ACS Chemistry for Life®

249th American Chemical Society National Meeting & Exposition

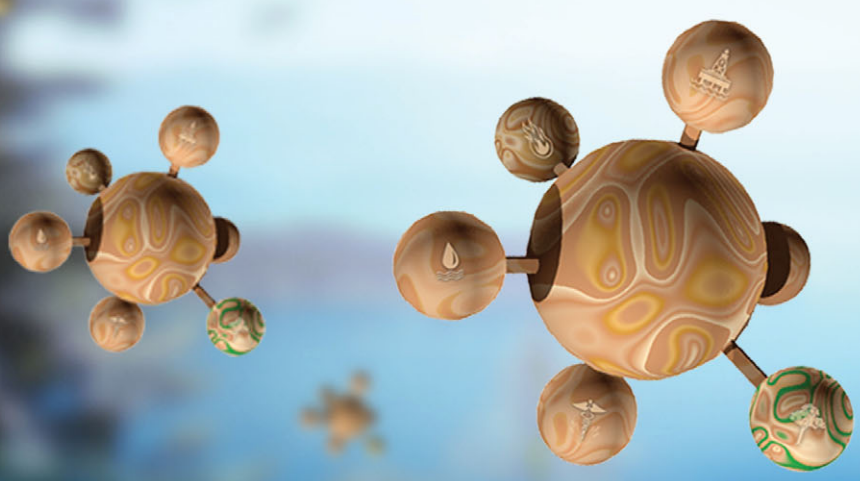
www.acs.org/denver2015

#acsdenver

CHEMISTRY OF NATURAL RESOURCES

Denver, CO • March 22–26, 2015

WWW.ACS.ORG/DENVER2015



Put this book in your pocket!

Download the free ACS Denver 2015 mobile app at www.acs.org/meetingapp

Available at amazon apps | ANDROID APP ON Google play | Download on the App Store

*Online version is also available for internet enabled devices.

IMPORTANT NOTICE

ACS NO RECORDING POLICY

The use of any device to capture images (e.g., cameras and camera phones) or sound (e.g., tape and digital recorders) or stream, upload or rebroadcast speakers or presentations is strictly prohibited at all official ACS meetings and events without express written consent from the ACS.

Questions? Contact NationalMeetings@acs.org

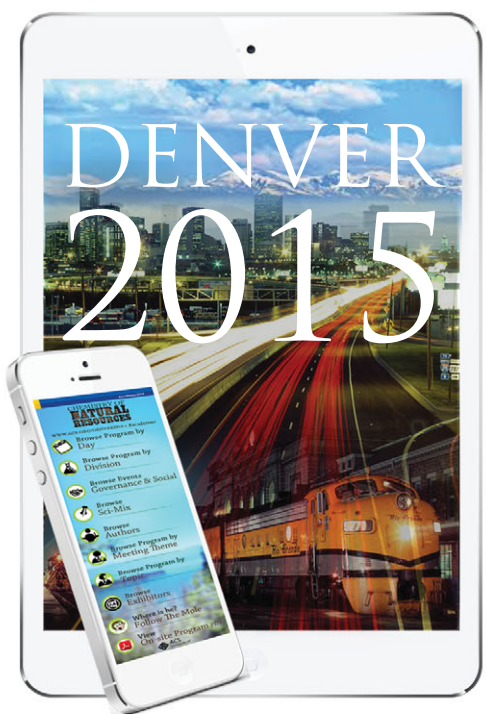
EMBRACING SUSTAINABILITY PRACTICES

The American Chemical Society continues to be a sustainability leader within the meeting and events community with most recently being the recipient of the 2014 Trade Show Executive's Gold 100 Award as the show with the Most Commendable Green Initiatives.

To continue to increase our support of sustainability efforts through engagement, education and reporting, we would like to remind you of the significant investments that we have made. One huge step in 2014 was the introduction of the mobile application for the National Meetings. The app received overwhelmingly positive feedback having over 6,500 downloads per meeting. The National Meetings app was also recognized in PCMA's *Convene* as Best in Show.

Additional efforts of our sustainability practices are briefly noted below. These changes not only support a greener meeting but also improve your meeting experience.

- Condensed Onsite Program book with enhancing the mobile application features
- Decreased print-run of the Onsite Program book due to digital and mobile applications
- Reformatted National Meeting website based on viewer analytics
- Increased Meeting Mail terminals at the Convention Center
- Free WiFi inside public areas at the Convention Center and many contracted hotels
- Established partnership with American Forests to offset carbon missions
- Audited contracted hotels on their sustainability efforts
- Partnered with Convention Center to source local foods for designated events
- Increased usage of digital signage
- Partnered with vendors that engaged in sustainability practices
- Increased attendee engagement through the Greener Meetings Challenge



Thank you for your support in making ACS a leader in sustainability. Further information can be found at: www.acs.org/greenermeetings. There you will find the ACS 2014 Sustainability Report including information on how to join the Greener Meetings Challenge.

ACS
Chemistry for Life®

249th American Chemical Society National Meeting & Exposition

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ACS OPERATIONS OFFICES

- **Colorado Convention Center – Room 210/212** 303-228-8400
- **Hyatt Regency Denver at Colorado Convention Center – Quartz A** 303-489-4976
- **Grand Hyatt Denver – Blanca Peak** 303-603-4305
- **Marriott City Center Denver - Homestead** 303-291-3657
- **Sheraton Denver Downtown Hotel – Aspen & Plaza Reg.** 303-352-2446 303-352-2447
- **Embassy Suites Denver—Downtown Convention Center – Quartz Boardroom** 720-587-0988
- **The Curtis—a DoubleTree by Hilton – Paper Room** 720-889-4753

INFORMATION CONTACTS

- **Attendee Registration – Colorado Convention Center, Lobby A/F** 303-228-8411
- **Career Fair Information Center, Colorado Convention Center, Hall B1** 303-228-8417
- **Exhibitor Registration, Colorado Convention Center, A/F Upper Lobby** 303-228-8414
- **Finance Office, Colorado Convention Center, Room 101** 303-228-8412
- **Host Local Section Booth, Colorado Convention Center, Lobby A/F** 303-228-8419
- **Housing Assistance, Colorado Convention Center, Lobby A/F** 303-228-8413
- **Member Services, Colorado Convention Center, Lobby A/F** 303-228-8418
- **Press Center, Colorado Convention Center, Room 104** 303-228-8406
- **Shuttle Desk, Colorado Convention Center, Outside Lobby F** 303-228-8420
- **Society Program Office, Hyatt Regency Denver at Colorado Convention Center** 303-486-4978
- **Governance Office, Hyatt Regency Denver at Colorado Convention Center** 303-486-4915

ACS OFFICERS

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American Chemical Society
1155 16th Street, NW, Washington, DC 20036
Tel: 800-227-5558 (US only) or 202-872-4600
Fax: 202-872-4615 E-mail: help@acs.org Website: www.acs.org

The American Chemical Society is a self-governed individual membership organization of more than 158,000 members at all degree levels and in all fields of chemistry. The Society provides a broad range of opportunities for peer interaction and career development, regardless of professional or scientifc interests. The programs and activities conducted by ACS today are the products of a tradition of excellence in meeting member needs that dates from the Society's founding in 1876.

This On-site Meeting Program is published by the American Chemical Society as a service to its attendees. Information contained herein is subject to change without notice. While every effort is made to ensure accuracy, ACS makes no warranties, expressed or implied, related to the information. For the official technical program for the 249th National Meeting & Exposition, refer to www.acs.org/denver2015. All San Francisco photos in this program are courtesy of the San Francisco Convention and Visitors Bureau and Shutterstock.

ACS Chemistry for Life®

American Chemical Society

Volunteer/National Meeting Attendee Conduct Policy

One of the key strengths of the ACS has been the enduring and varied contributions made by its thousands of dedicated volunteers.

Another unassailable strength of the ACS is its outstanding national meetings program. ACS national meetings are among the most respected scientific meetings in the world. ACS national meetings offer scientific professionals a legitimate platform to present, publish, discuss, and exhibit the most exciting research discoveries and technologies in chemistry and its related disciplines. Furthermore, ACS national meetings facilitate networking opportunities, career development and placement, and provide organizations with opportunities to exhibit products and services to targeted audiences.

The Society's Congressional Charter explicitly lists among its objectives "the improvement of the qualifications and usefulness of chemists through high standards of professional ethics, education and attainments...." The ACS expects its volunteers and national meeting attendees to display the highest qualities of personal and professional integrity in all aspects of their ACS-related activities. Indeed, every chemical professional has obligations to the public, to volunteer and staff colleagues, and to science.

Accordingly, and to foster a positive environment built upon a foundation of trust, respect, open communications, and ethical behavior, the ACS Board of Directors has issued this Conduct Policy. It applies to ACS Volunteers, i.e., it applies to individuals conducting the business and affairs of the ACS without compensation for that conduct. It also applies to attendees at ACS national meetings. Volunteers and national meeting attendees should at all times abide by this Conduct Policy. Specifically:

1. Volunteers should understand and support ACS's vision and mission.

2. Volunteers and national meeting attendees should contribute to a collegial, inclusive, positive, and respectful environment for their fellow volunteers and attendees, as well as for other stakeholders, including national meeting vendors and ACS staff.

3. Volunteers and national meeting attendees must avoid taking any inappropriate actions based on race, gen- der, age, religion, ethnicity, nationality, sexual orientation, gender expression, gender identity, marital status, political affiliation, presence of disabilities, or educational background. They should show consistent respect to colleagues, regardless of the level of their formal education and whether they are from industry, government or academia, or other scientific and engineering disciplines.

4. Volunteers and national meeting attendees should interact with others in a cooperative and respectful manner. Volunteers and national meeting attendees should refrain from using insulting, harassing, or otherwise offensive language in their ACS interactions. Disruptive, harassing, or inappropriate behavior toward other volunteers, stakeholders, or staff is unacceptable. Personal boundaries set by others must be observed. Harassment of any kind, including but not limited to unwelcome sexual advances, requests for sexual favors, and other verbal or physical harassment will not be tolerated.

5. Volunteers must obey all applicable laws and regulations of the relevant government authorities while acting on behalf of the ACS. Likewise, national meeting attendees must obey all applicable laws and regulations of the relevant government authorities while attending ACS national meetings. Volunteers and national meeting attendees alike should also ensure that they comply with all applicable safety guidelines relating to public chemistry demonstrations.

6. Volunteers and national meeting attendees should only use ACS's trademarks, insignia, name, logos, and other intellectual property in compliance with ACS regulations and directives as may be issued from time to time.

7. Violations of this Conduct Policy should be reported promptly to the ACS Secretary and General Counsel or to the Chair of the ACS Board of Directors. In cases of alleged persistent and/or serious violations of this Conduct Policy, the Board shall review the evidence and shall take such actions as may be appropriate, including but not limited to requiring volunteers to leave their volunteer position(s); precluding volunteers from serving in Society volunteer roles in the future; requiring national meeting attendees to leave the meeting; and, precluding meeting attendees from attending future ACS national meetings. ACS, through its Board of Directors, reserves the right to pursue additional measures as it may determine are appropriate.

Adopted by the Board of Directors 12/6/13

CHEMISTRY OF NATURAL RESOURCES

Denver, CO • March 22–26, 2015

WWW.ACS.ORG/DENVER2015

Where to Find Meeting Information

Official Meeting Website
www.acs.org/denver2015

Annoucements & Changes
www.acs.org/meetingupdates

Digital Meeting Program
www.acs.org/denver2015

follow us@acsnatlmtg
tweet using #acsdenver

www.facebook.com/
americanchemicalsociety

http://communities.acs.org/
community/science/meetings

Download the free mobile app
at www.acs.org/meetingapp

Text your question to
754.227.2012 *(Standard text rates apply)*

ACS
Chemistry for Life®

Welcome to Denver and the 249th ACS National Meeting

It is my pleasure to join all of you in the Mile High City, one of the most gorgeous locales for our meetings.

Diane Grob Schmidt
ACS President

Twenty-nine technical divisions and eight committees are hosting original programming based on the meeting theme of Chemistry of Natural Resources. More than 10,000 papers will be presented, and nearly 4,000 poster presentations will take place at the meeting. As well, there are a number of special events planned throughout the meeting. The ACS Board of Directors Open Session will be an opportunity to hear from Deborah Blum, bestselling author of The Poisoner's Handbook, discuss her thoughts on communicating chemistry. Please join your colleagues from noon to 1:00 p.m. in the Four Seasons Ballroom 4 of the Colorado Convention Center.

There are three Presidential Symposia I encourage you to attend as well as several others I am recommending. The first is on the morning of Sunday, March 22, titled Chemistry Without Borders: The Transnational Practice of Chemistry and Allied Sciences and Engineering (8:00 a.m.–12:00 p.m., Colorado Convention Center, Ballroom 3A,). The other two presidential symposia focus on nanotechnology, with the first beginning later that afternoon on Sunday, March 22, and continuing all day on Monday. Nanotechnology: Delivering on the Promise will highlight the fascinating research, development, and commercialization of nanochemistry and nanotechnology and will include 16 senior-level speakers from industry, academe, and government. The third presidential symposium (Tuesday, 8:30–11:30 a.m.), DOE Nanoscience Research Centers: National Resources for the Nanoscience Community, will feature the five heads of chemistry at U.S. national laboratories. This is the first symposium of its type to highlight these speakers collectively.

On Monday afternoon, Theodore Betley, Professor of Chemistry and Chemical Biology at Harvard University will deliver The Kavli Foundation Emerging Leader in Chemistry Lecture on 'Radical Frontiers in Catalysis.' He is followed by Laura Kiessling, at the University of Wisconsin - Madison with The Fred Kavli Innovations in Chemistry Lecture (Colorado Convention Center, Bellco Theater) who will speak on 'Us Versus Them: Distinguishing Humans from Microbes with Carbohydrates.'

The entire meeting program is filled with outstanding scientific, educational, and professional content. Please consult the listings in this program or go to www.acs.org/denver2015 for all the specific details pertaining to these events. There is plenty to select from and I am sure you will find something to satisfy your needs and expectations.

The exposition will feature more than 250 companies that will showcase services, instruments, books, lab equipment, and much more in more than 400 booths.

I express thanks to the members of the Colorado Local Section; the Committee on Meetings and Expositions; thematic program chair Robert S. Weber of the Pacific Northwest National Laboratory; the divisional program chairs and symposium chairs responsible for organizing this meeting's technical sessions; and the ACS staff for making it all happen. And thanks to you for contributing to the success of this meeting. Of course, thanks to all of you for attending.

Diane Grob Schmidt
ACS President

Welcome Message from Bob Weber, Denver Thematic Program Chair

The Spring 2015 ACS National Meeting, (Denver, March 22-26), will showcase the *Chemistry of Natural Resources*: their extraction, refining and conservation; a theme that resonates well with the history, biology and geology of the Mile-High City.

Bob Weber
Denver Thematic
Program Chair

The plenary session, on Sunday afternoon, March 22, will inaugurate the theme with three invited lectures: Prof. Carolyn Koh (Colorado School of Mines) will discuss "The Fundamentals of Gas Hydrates and Their Role in Energy Transport;" Dr. Paul Bryan (formerly manager of the Biomass program at DOE) will present "The Four Horsemen of the Advanced Biofuels Apocalypse—Sustainability, Technology, Profitability, and Politics," an overview of challenges and future opportunities for renewable fuels; and Dr. Peter Kareiva (Chief Scientist of The Nature Conservancy) will discuss "Water in the Anthropocene: Too Much, Too Little, Too Dirty." The afternoon of Monday, March 23 will see the Kavli Foundation Emerging Leader in Chemistry Lecture by Prof. Theodore Betley (Harvard University) "Radical Frontiers in Catalysis" and the Fred Kavli Innovations in Chemistry Lecture by Prof. Laura Kiessling (University of Wisconsin-Madison) "Us Versus Them: Distinguishing Humans from Microbes with Carbohydrate."

The technical program constructed by the ACS divisions includes both topical sessions and nearly 50 symposia honoring the winners of ACS awards. Symposia that resonate well with the overall theme of the meeting can be found in the sessions sponsored by AGFD, AGRO, ANYL, CATL, CEI, CELL, CINF, COLL, COMP, COMSCI, ENFL, ENVR, GEOC, HIST, I&EC, INOR, PHYS, SCHB, SOCED, and YCC.

Denver and its surroundings evoke many images: the American frontier, mining, forest products, coinage, civic zest, "Rocky Mountain Spring Water" and recently, the production of unconventional fossil fuels. To recollect and celebrate the region's traditions and resources, the local ACS chapter has put together a great social and enrichment program around local attractions. The Presidential Outreach Event, "Exploring Our World Through Chemistry," will take place at the Denver Zoo on Saturday, March 21. Denver authorities have also reminded me to note that spring skiing in Colorado is some of the best anywhere, easily reached by shuttles to the ski resorts (about 1.5 hours away from the meeting venue downtown): www.coloradomountainexpress.com/downtown-denver

The program for the meeting and other information is available online at the website of the meeting www.acs.org/denver2015.

I am very grateful to the members of the local section, the program chairs of the divisions listed above, and the ACS staff for their essential help in making the theme of this meeting cogent and coordinated. I look forward to meeting you in Denver.

Robert S Weber

Bob Weber
Thematic Program Chair

STATE OF COLORADO

EXECUTIVE CHAMBERS

136 State Capitol
Denver, CO 80203 - 1792
Phone (303) 866-2471

John Hickenlooper
Governor

March 22, 2015

Greetings:

On behalf of the State of Colorado, it is my distinct pleasure to welcome you to Denver for the 249th American Chemical Society National Meeting and Exposition.

You could not have chosen a better location to celebrate the chemistry of natural resources, as they are central to Colorado's heritage and an important part of our future. I commend all participants as you recognize and explore the transformative power of chemistry over the coming days. I wish you a productive and successful conference and look forward to learning about your ongoing research and discoveries. Outside of these activities, I hope you have some time to explore and enjoy our wonderful state.

Once again welcome to this exciting and informative event. You have my best wishes, now and in the years to come.

Sincerely,

John W. Hickenlooper

Michael B. Hancock
Mayor

City and County of Denver
OFFICE OF THE MAYOR
CITY AND COUNTY BUILDING
DENVER, CO 80202-5390
TELEPHONE: (720) 865-9090 • FAX: (720) 865-8787
TTY/ TTD: (720) 865-9010

March 22, 2015

American Chemical Society's 249th National Meeting
Colorado Convention Center
707 West 14th Street
Denver, CO 80202

Greetings:

On behalf of the City and County of Denver, it is my pleasure to extend a heartfelt welcome to the "Mile High City." We are excited that you have chosen Denver to advance the work of you organization.

The American Chemical Society has a long and rich history of support in the field of chemical science, engineering, and related fields. You are the leading source of authoritative scientific information through the Journal of the American Chemical Society and Chemical & Engineering News, and have been catalyst for education, research and publication, as well as advocate for information protection. Denver is a great location to continue this very important work.

While you are here, we invite you to take advantage of the many amenities that our city has to offer. Denver is one of the nation's most walkable cities and boasts a variety of attractions, including the nation's second largest performing arts complex, three art museums, three sports stadiums, a U.S. Mint, more than 300 restaurants and one of the largest city park systems in the country.

Also, please take advantage of the various transportation options we offer. We've made getting around the Mile High City easy with our 500 rental bikes available at 30 downtown stations, a free hybrid shuttle along the 16th Street pedestrian mall, and FasTracks, the nation's largest light rail initiative with 120 miles of track.

Again, welcome to Denver, have an informative and enjoyable time and please plan to return soon.

Respectfully,

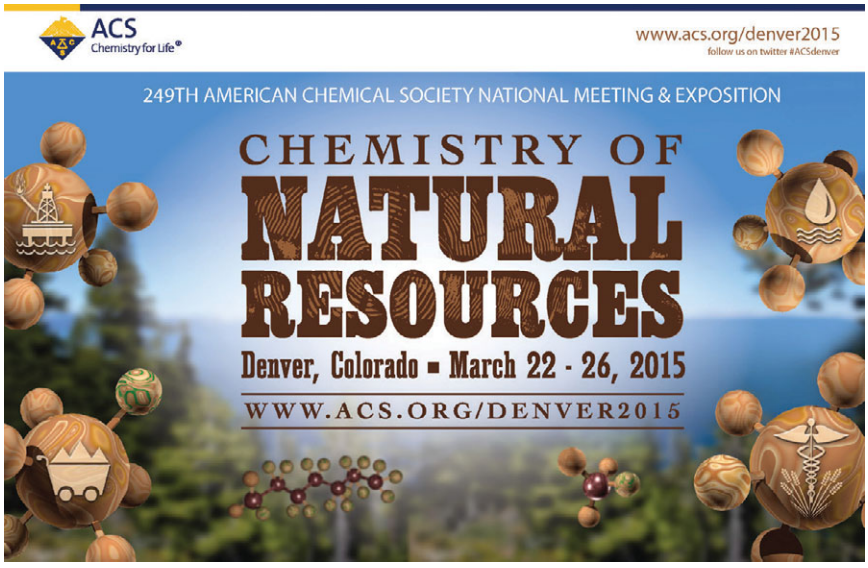
Michael B. Hancock
Mayor

PRESIDENTIAL SYMPOSIA

Sponsored by the ACS President

Photo: Peter Cutts Photography

Diane Grob Schmidt, Ph.D.
ACS President



Sunday and Monday – March 22-23, 2015

Nanotechnology: Delivering on the Promise

(Cosponsored by the following ACS Divisions and Committees and other scientific societies AGFD, AGRO, ANYL, CARB, CHAS, COLL, ENFL, HIST, I&EC, PMSE, POLY, SCHB, MPPG, CA, CCS, CCPA, COMSCI, DAC, IAC, SOCED; American Institute of Chemical Engineers, Gordon Research Conferences, Materials Research Society & National Academy of Engineering)

Sunday, March 22, 2015

1:30-5:30 PM

Nanotechnology: Delivering on the Promise – R&D

Monday, March 23, 2015

8:30-11:45 AM

Nanotechnology: Delivering on the Promise – Opportunities and Challenges for Health, Safety, and the Environment

Monday, March 23, 2015

1:30-4:45 PM

Nanotechnology: Delivering on the Promise – Bridging the Gap to a Thriving U.S. Marketplace

Colorado Convention Center, Mile High Ballroom 3A (Lower Level)

AIChE The Global Home of Chemical Engineers

Gordon Research Conferences

MRS ENDORSED MEETINGS

NATIONAL ACADEMY OF ENGINEERING OF THE NATIONAL ACADEMIES

249th American Chemical Society National Meeting & Exposition

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- Quick Access to the full technical program,maps, and search features.
- Build your schedule. Browse by day, division, theme topics, exhibitors or authors.
- Use your ACS ID to sync your schedule.
- Take notes and share them via email. Connect your meeting experience with social media and more!

The ACS Mobile Meeting Application is your free full greener guide to manage your experience at the 249th ACS National Meeting in Denver.

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Learn more at
www.acs.org/meetingapp
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Visit the Denver Mobile App Desk for a free app t-shirt — ***while supplies last.***
Colorado Convention Center, Lobby A/F

ACS Chemistry for Life®

www.acs.org/denver2015

JOIN THE
ACS BOARD OF DIRECTORS OPEN MEETING

Guest Speaker: **Deborah Blum**

2015 Grady Stack Award Recipient

Helen Firstbrook Franklin Professor
School of Journalism and Mass Communication
University of Wisconsin-Madison

Sunday, March 22, 2015
Noon – 1:00 PM
Four Seasons Ballroom 4 (Lower Level)
Colorado Convention Center

The Poisoner's Guide to Communicating Chemistry

Join the ACS Board of Directors at its Regular Session as they host lunchtime speaker Deborah Blum. Deborah is an American journalist, a columnist for the *New York Times*, a professor of journalism at the University of Wisconsin-Madison, and a blogger for *Wired*. She is also the author of several books including ***The Poisoner's Handbook***. She is a much sought out speaker and has appeared at several very well-attended ACS symposia focused on communicating chemistry/science to the public.

Deborah will be receiving the 2015 Grady-Stack Award at the ACS National Meeting in Denver, March 2015, for her achievements in public outreach, engagement and communications.

Sandwiches available for first 200 attendees.

GENERAL MEETING INFORMATION

YOUR MEETING REGISTRATION entitles you to a wide range of programming, including 987 scientific sessions, invited symposia, poster sessions, special lectures and events, award presentations, workshops, and the exposition. Interact with chemical scientists from around the world by participating in social events, networking opportunities, exhibitor sessions, and educational activities, with many events offered at no additional charge. Certain workshops, short courses, and ticketed events require a separate entry fee, as indicated in this program.

REGISTRATION

ALL ATTENDEES, including speakers and poster presenters, must register for the meeting to participate in the technical sessions. Sponsored speakers should contact their symposium organizer or division program chair to clarify the terms of their invitation and to determine who will complete the speaker's registration. Attendees must display their badge at all times for admission to all official ACS sessions and events.

Early Registration. Attendees within the U.S. who registered prior to Feb. 13 received their badge credentials by mail before the meeting. International registrants must pick up their badge credentials at ACS Attendee Registration (this includes Canada and Mexico).

Standard & On-Site Registration. Attendees who registered after Feb. 13 must pick up their badge credentials on-site.

MEETING INFO ON THE WEB

Registration, housing, technical programming, special events, participating exhibitors, and other meeting details are available at www.acs.org/denver2015.

Registration Changes. Attendees can modify their existing registration or generate a receipt from the registration website by following the instructions in their confirmation message. Attendees can also update their registration on-site at ACS Attendee Registration. Bring your confirmation and/or badge credentials with you to the meeting for faster processing.

Registration Methods. All registrants received a confirmation via the original method of registration.

Internet. Register online at www.acs.org/meetings until March 26. A valid credit card is required to register online, and online registrations are real-time transactions.

Telephone. Call the ACS National Meeting Registration Center by March 26 at 800-251-8629 (U.S./Canada only) or 508-743-0192 (international), Monday to Friday, 9:00 AM to 5:00 PM EST.

Fax/Mail. Submit the registration form by fax: 508-743-9605 or mail: ACS Registration, c/o CDS, 107 Waterhouse Rd., Bourne, MA 02532. Mailed registrations will be accepted until March 26.

On-site. Register during the meeting at ACS Attendee Registration at standard registration rates. ACS Attendee Registration will be open at the Colorado Convention Center, Lobby A/F, on Saturday, 3:00 to 6:00 PM; Sunday, 7:30 AM to 7:30 PM; Monday, 7:30 AM to 9:30 PM; Tuesday, 7:30 AM to 5:00 PM; Wednesday, 7:30 AM to 4:00 PM; and Thursday, 7:30 AM to 1:00 PM.

REGISTRATION PAYMENTS. Registration fees can be paid by check, money order, credit card (American Express, Discover, MasterCard, or VISA), or bank wire transfer. Make checks payable in U.S. dollars to the American Chemical Society, and include a completed registration form with each payment. Registration fees should not be combined with any other payment (such as membership dues). Purchase orders and training requests are not accepted. For wire transfer payments, contact the ACS Finance Department at 202-872-6106 or e-mail bankwires@acs.org. **Registration forms received without payment will not be processed.**

BADGES

All attendees are required to wear their badges for all technical sessions, poster sessions, and other official meeting events. Our badge holders are recyclable and biodegradable. Please discard appropriately.

REGISTRATION CATEGORY	FEE: EARLY BY JAN. 30	FEE: STANDARD AFTER FEB. 13
MEMBERS		
ACS member or society affiliate	$390	$470
Postdoctoral member	390	470
Emeritus or retired member	200	240
50-year member	No fee	No fee
Unemployed member (Dues waiver required)	No fee	No fee
Precollege teacher	110	110
Graduate student	200	200
Undergraduate	110	110
One-day registrant	200	240
NONMEMBERS		
Chemical scientist	$680	$820
Postdoctoral scientist	680	820
Visitor: Nonchemical scientist or chemical technician	390	470
Precollege teacher	110	110
Graduate student	390	390
Undergraduate	200	200
One-day registrant	390	470
Guest of registrant[a]	50	50
EXPOSITION-ONLY VISITORS		
Adult, exposition only	$60	$60
Student, exposition only	30	30

a Registration is restricted to a spouse or family member of registered attendee having no affiliation with the field of chemical science and who is not eligible to become an ACS member. Only one guest registration is allowed per registering attendee, and the guest registration must be completed and paid by the registering attendee at time of original registration.

ACS BADGE REPRINT POLICY

1st badge reprint: no charge, upon proper identification and confirmation of registration payment, a duplicate badge is issued.
2nd badge reprint: attendee completes a duplicate badge request, shows identification (which we copy), a charge of $25 is paid (cash/credit card), a duplicate badge is issued.
3rd badge reprint: attendee completes a duplicate badge request, shows identification (which we copy), a charge of $50 is paid (cash/credit card), a duplicate badge is issued.
For any badge beyond the 3rd: attendee completes a duplicate badge request, shows identification (which we copy), a charge of $100 is paid (cash/credit card), a duplicate badge is issued.

REGISTRATION ASSISTANCE. The ACS National Meeting Registration Center will be available from 9:00 AM to 5:00 PM EST by telephone, fax, mail, or e-mail. Service representatives can be reached at 800-251-8629 (U.S./Canada only) or 508-743-0192 (international); fax: 508-743-9605; e-mail: acs@xpressreg.net; or mail: ACS Registration, c/o CDS, 107 Waterhouse Rd., Bourne, MA 02532.

Registration Cancellations/Refunds. All cancellations and refund requests must be submitted in writing to guarantee the registrant a full refund less a $50 administrative fee. Refund requests made after March 6 will not be honored. Your registration badge credentials and a copy of your registration confirmation must be attached to your request. All refunds will be issued via the original payment method, and refunds will be processed within 30 days after the meeting. Send your request to ACS Registration Cancellation, c/o CDS, 107 Waterhouse Rd., Bourne, MA 02532 or fax 508-743-9605 (save your fax confirmation sheet).

Social Event Ticket Cancellations/Refunds. Social event cancellations received by March 6 entitle the registrant to a full refund. Refund requests made after March 6 will not be honored. Event tickets and a copy of your registration confirmation must be attached to your request.

Abstract Cancellations/Refunds. Abstract USB flash drives (thumb drives) and their shipping costs are nonrefundable.

MEMBER REGISTRATION. You must enter a valid ACS membership number during registration to register as a member and receive your ACS member discount on registration fees. Your registration options will automatically appear in accordance with your current membership status in the ACS membership database. Your ACS membership number can be found on your ACS membership card or your ***Chemical & Engineering News*** address label. Address questions about your membership status to ACS Member Services at 800-333-9511 (U.S./Canada only), 614-447-3776 (international), or e-mail: service@acs.org.

NONMEMBER REGISTRATION. Save money on registration fees by joining ACS. You can join ACS now through the online ACS membership application at www.acs.org/join or by contacting ACS Member Services and then registering for the meeting at your member rate. To receive your meeting discount, you must join the society before you register for the meeting. New memberships or questions about membership status should be handled through ACS Member Services at 800-333-9511 (U.S./Canada only), 614-447-3776 (international), or e-mail: service@acs.org.

PRESS/MEDIA REGISTRATION. Press registration is complimentary for credentialed members of the news media (restricted to reporters and editors working full-time for print or broadcast news) who are approved by the ACS Office of Communications. Press badges may be picked up with valid media credentials from the Press Room at the Colorado Convention Center. For more information, visit www.acs.org/pressroom.

EXPO-ONLY ADMISSION. All meeting attendees with a valid badge receive complimentary admittance into the exposition as part of their registration. Individuals who want to visit the exposition without registering for the meeting's technical sessions can register for an expo-only adult badge for $60 or $30 for students with school identification. Register online or in person at ACS Attendee Registration.

EXHIBITOR REGISTRATION. Exhibitor registration is handled exclusively through ACS National Expositions at www.acs.org/expositions.

CAREER FAIR EMPLOYER REGISTRATION. ACS Career Fair Employer registration is handled exclusively through ACS Careers at www.acs.org/careers.

ACCOMMODATIONS

ORCHID EVENT SOLUTIONS is the official housing bureau for the ACS national meeting in Denver. ACS does not endorse booking hotel reservations through any other sources. All attendees who made their reservations through Orchid Event Solutions will receive complimentary internet access in their sleeping rooms and automatically entered in the ACS Housing Drawing.

On-site Housing. During the meeting an on-site housing desk will be located at the Colorado Convention Center in the registration area. Staff will be available to assist with last-minute housing changes or needs.

Reservation Confirmation. All registrants who booked their reservations through Orchid Event Solutions received a confirmation. Each confirmation contains a unique number that is proof of your reservation.

Keep Your Meeting Affordable. Attendee support of the official hotels allows ACS to utilize meeting space at a discount and keep registration fees to a minimum.

ACS GREENER MEETINGS

THE AMERICAN CHEMICAL SOCIETY Department of Meetings & Expositions Services and the Committee on Meetings & Expositions are committed to greener meetings. For each national meeting, we collaborate with the destination city, convention center, and our hotel and vendor partners to reduce our environmental footprint and raise the bar with regard to industry sustainability practices.

Interested in learning more about how we're leading the way? Go to www.acs.org/greenermeetings to read about our greener meeting initiatives and access our annual Event Sustainability Report.

For our efforts, ACS has been recognized by the Capital Chapter of the Professional Convention Management Association as a sustainable event leader and received the Trade Show Executive's Gold 100 Award for the Show with the Most Commendable Green Initiatives. Here are a few reasons why:

■ ACS offsets all shuttle transport emissions and staff-related emissions (1,193 tons of carbon dioxide were offset in 2014, equivalent to not driving 2,840,476 miles in an average passenger vehicle).

Take the greener meeting Challenge

Take the Greener Meetings Challenge at **www.acs.org/greenermeetings**. Tell your story or simply show your support for the ACS Greener Meetings Program. All participants will receive a special thank you (*While supplies last*.). Three participants having the best stories will be awarded prizes on **April 27, 2015.**

To be a catalyst for positive change! Here's what you can do:

1

Take advantage of linen reuse and other initiatives at your hotel, and always turn the lights off when away from your room. If you are staying at the Westin or Sheraton, enroll in their Make A Green Choice program.

2

Responsibly dispose of recyclable materials (paper, plastic, glass, aluminum) at the convention center and hotels.

3

Download the national meeting mobile app or digital program. Limited quantities of the printed Onsite Program are available.

4

Avoid the use of taxis by walking when safe and possible. Stop by the Greener Meetings Booth for your pedometer (***While supplies last).*** Burn calories, and enjoy the city.

5

Ride the ACS carbon-neutral shuttle service when walking isn't an option between your hotel and the center. Shuttle service will be provided between many ACS contracted properties.

6

Avoid the use of disposable, plastic water bottles. Stop by the ACS Colorado Host Local Section Booth to pick up a free, reusable water bottle (***While supplies last).*** Avoid the cost and waste associated with disposable bottles.

Colorado Convention Center, Lobby A/F

Greener Meetings Booth

Sun., 3 – 6 PM
Mon., 8 – 1PM
Tues., 8 – 1 PM

Colorado Host Local Section Booth

Sat., 3 to 6 PM
Sun., 7:30 AM to 7:30 PM
Mon., 7:30 AM to 9 PM
Tues., 7:30 AM to 5 PM
Wed., 7:30 AM to 4 PM
Thurs., 7:30 AM to 1 PM

■ ACS partnered with conservation group American Forests to offset ACS staff-related emissions (related to travel, accommodations, and show management freight) through tree-planting efforts in Lower Rio Grande Valley National Wildlife Refuge and the Dinkey Collaborative Reforestation project.

■ ACS performed on-site walk-throughs for 98% of our hotel room block properties in 2014, surveying hotels on more than 40 sustainability practices.

■ ACS designates Sci-Mix as a "zero waste" event. We achieved nearly 100% diversion for meetings in both Dallas and San Francisco. Help us keep up the great work!

Be A Catalyst For Change In Denver. Facilities are only as effective as the people who operate and occupy them. That means you! Go to www.acs.org/greenermeetings and take the Greener Meeting Challenge to show your support and share your personal national meeting sustainability story. Challenge participants are eligible to win fantastic prizes. Challenge activities include the following:

■ Take advantage of linen reuse initiatives at your hotel, decline delivery of unread newspapers, and turn off the lights when away from your hotel room.

■ Responsibly dispose of recyclable materials (paper, plastic, glass, aluminum) in the convention center and hotels.

■ Use the meeting mobile app and digital program instead of the printed on-site program.

■ Enjoy the city, burn calories, and travel carbon dioxide-neutral by walking to and from your hotel.

■ When walking isn't an option, use the ACS carbon-offset shuttle service.

■ Bring a reusable water bottle to avoid the cost and waste associated with disposable, petroleum-based plastic water bottles.

Suggestions? end them to ACS National Meetings & Expositions at NationalMeetings@acs.org.

TRAVEL & TRANSPORTATION

DENVER is easily accessible by air or train, and the city offers several options to get around, including the ACS shuttle, taxis, and buses.

AIRPORT. Numerous ground transportation options are available at Denver International Airport. The Ground Transportation Information Counter is located in the central area on Level 5 of Jeppesen Terminal. Counter hours are 6:00 AM to 11:30 PM daily. For more information, call 303-342-4059.

SUPERSHUTTLE. ACS has established a 10% discount for attendees of our meeting. Take advantage of this savings by going to www.supershuttle.com or www.execucar.com and entering the discount code 94D3G in the "Group/Discount Code" box on the first page of the website.

TAXIS are readily available and provide service to the Denver metro area and surrounding counties. From Denver International Airport to downtown Denver there is a flat rate of $55.15 (one-way fare, airport access fee already included). Taxis pick up and drop off from Jeppesen Terminal, Level 5, Island 1, outside doors 507 through 511 (Terminal East) and doors 506 through 510 (Terminal West).

PUBLIC TRANSPORTATION. Public bus service is scheduled and provided within the local metro area by the Regional Transportation District (RTD). Please contact RTD directly, or visit their booth in the Jeppesen Terminal, for information on specific routes, schedules, and fares. Riders must have exact change. RTD buses pick up and drop off from Jeppesen Terminal Level 5, outside doors 504, 506, and 510 (west side).

TRANSPORTATION DISCOUNTS. ACS has negotiated special travel discounts with the partners listed below. To get the best rates and avoid service fees, it is recommended to make reservations online (except Amtrak).

AIRLINES:

Delta
delta.com; 800-328-1111 (please note that ticketing charges will apply for bookings by phone)
Discount Codes: NMK2Y, NMJTX (international)

United
united.com; 800-426-1122
Offer Code: ZT6E969361

Southwest
swabiz.com
Corporate ID: 99329790
Online Reservations Only

TRAIN:

Amtrak
amtrak.com; 800-872-7245
Convention Fare Discount: #X03V-918

RENTAL CARS:

Advantage Rent A Car
advantage.com; 800-777-5500
Discount Code: CD02C826E8

Avis
avis.com; 800-331-1600
Avis Worldwide Discount (AWD): B923099

Hertz
hertz.com; 800-654-2240
Discount Code: CV# 02UZ0014

TRAVELING TO MEETING VENUES

The Colorado Convention Center is located at 700—14th St., Denver, CO 80202.

ACS Shuttle. Complimentary shuttle service will be provided between the Colorado Convention Center and official ACS hotels, with the exception of hotels within walking distance. Buses will run from 7:00 AM to 11:00 PM from Sunday to Wednesday and 7:00 AM to 6:00 PM on Thursday. Buses will run approximately every 15 to 30 minutes. Visit the meeting website for a route map and to download the shuttle schedule.

If you require wheelchair access or for any other inquiries, please e-mail nationalmeetings@acs.org to schedule.

Parking. Daily parking is limited and expensive in downtown Denver. You should contact your hotel to inquire about daily parking policies and fees.

GETTING AROUND THE CITY

Walking. The Colorado Convention Center and ACS hotels are conveniently located in downtown Denver. Do your part to reduce our environmental impact by walking to ACS properties.

Denver's Regional Transportation District (RTD). Denver's Regional Transportation District (RTD) offers

eco-friendly transportation by bus or light-rail services within and around the city of Denver. RTD also offers a shuttle services "skyRide" to and from Denver International Airport. For routes, fares, and other pertinent information, call 303-299-6000 or visit the website at www.rtd-denver.com.

ACS MEMBER SERVICES

ACS MEMBER SERVICES. ACS staff can assist you on-site with joining ACS, renewing memberships, completing adjustments to member records, and answering general membership questions. ACS members receive discounted rates when registering for the meeting.

ACS Member Services is located in Lobby A/F near registration in the Colorado Convention Center and is open Saturday, March 21, 3:00 to 6:00 PM; Sunday, March 22, 7:30 AM to 7:30 PM; Monday, March 23, 7:30 AM to 9:00 PM; Tuesday, March 24, 7:30 AM to 5:00 PM; Wednesday, March 25, 7:30 AM to 4:00 PM; and Thursday, March 26, 7:30 AM to 1:00 PM.

ONLINE SOCIAL NETWORKING TOOLS. Start discussions and connect with other attendees on the ACS Network and the ACS Facebook page. Follow ACS national meetings on Twitter.

ATTENDEE NATIONAL MEETING E-NEWSLETTER. Receive official updates on ACS national meetings, including locations, registration and accommodation dates, information and discounts, resources, and event details. You can sign up and manage your subscriptions with your free ACS ID. Subscribe at www.emailpref.acs.org.

BUSINESS CENTER. The UPS Store, located in Concourse A, offers in-store and online printing, notary services, document finishing, packing and shipping, and a variety of other services tailored to help you make the best of the convention.

MEMBER INSURANCE PROGRAM. Exposition Booth 624. The ACS Member Insurance Program offers coverage and policies for every stage of life, from college student to young professional, from raising a family to enjoying retired life and everything in between. Stop by the Member Insurance Station to learn how you can sign up for Life & Health Insurance, Auto & Homeowners Plus, Disability Income, Long-Term Care, Medicare Supplement, Medical Discount Cards, Pet Insurance, and Professional Liability.

Also learn more about two new policies available to ACS members: International Life Insurance and Commercial Business Insurance. We look forward to showing you how you can receive great value for your insurance dollars. For additional information, visit www.acs.org/insurance.

Access meeting information and the On-site Program at **www.acs.org/denver2015**

ON-SITE MEETING ARRANGEMENTS

ADA-COMPLIANT MEETING. The Colorado Convention Center provides service ramps to entrances and elevated areas, braille instructions and directions throughout the building, and pay phones on each level of the facility with (TDD) hearing-impaired functions. More information is available at denverconvention.com.

ACS is dedicated to ensuring that no individual with a disability is excluded, denied services, segregated, or otherwise treated differently because of the absence of auxiliary aids and services identified in the Americans with Disabilities Act. If you require special accommodations to participate in the meeting, communicate your needs to ACS Meeting Services by e-mail: nationalmeetings@acs.org; fax: 202-872-6128; or phone: 202-872-6111 by Feb. 5 to allow enough time to fulfill your request. Keep in mind that ACS may not be able to accommodate last-minute requests.

If you have an emergency or need immediate assistance during the meeting, contact any ACS Operations Office.

ASSISTANCE. Our information clerks will be positioned throughout the convention center and can help you navigate the On-site Program, find a particular session or room, and answer questions. Lost-and-found items at the convention center should be directed to the ACS Operations Office located in Rooms 210/212. Messages left at the ACS Operations Office will be conveyed to attendees via the Meeting Mail system, but ACS cannot accept responsibility for the delivery of any messages, mail, or packages.

ATTENDEE BADGES. Attendees and guests must be registered and display their badges at all times to be admitted to all official ACS sessions and events.

ATTENDEE MESSAGING/MEETING MAIL. After registering for the meeting, you will be assigned a temporary electronic mailbox to exchange personal messages with other registered attendees via Meeting Mail. Meeting Mail will be available before, during, and after the meeting at www.acs.org/denver2015. Use the Meeting Mail terminals located in the Colorado Convention Center. Telephone messages left at the ACS Information Booth will be conveyed to attendees via the electronic message center, but ACS cannot accept responsibility for the delivery of any messages. No one will be paged in meeting rooms.

AUDIOTAPING, PHOTOGRAPHY & VIDEOTAPING. The use of any device to capture images (e.g., cameras and camera phones) or sound (e.g., tape and digital rebroadcast) of speakers or presentations is strictly prohibited at all ACS meetings and events without express written consent from ACS.

CHILD CARE. Camp ACS will be available to all meeting attendees free of charge from 7:00 AM to 6:00 PM on Sunday, March 22, through Thursday, March 26. At Camp ACS, children two (and potty-trained) to 16 years of age can participate in age-appropriate activities, including arts and crafts and active games, while you enjoy the meeting. For your child's safety, the location of Camp ACS will not be communicated until your registration is confirmed. On-site registration will be accepted at the ACS Operations Office, Colorado Convention Center, room 210/212 and on the space available basis.

LUGGAGE & COAT CHECK. A luggage and coat check station will be available during registration hours from Sunday through Thursday at the Colorado Convention Center, Lobby A/F. Items left beyond published hours of operation will be turned over to building security at the end of each day.

ELECTRONIC DEVICES. As a courtesy to other meeting attendees, electronic devices must be operated in silent/vibrate mode in technical or educational sessions. Cell phone conversations are not permitted in meeting rooms.

EMERGENCIES DURING ACS MEETING EVENTS. ACS will place detailed instructions inside each meeting room to be used if an emergency occurs during an ACS meeting event. These instructions will revolve around following the established emergency guidelines of the facility where the emergency occurs. Report emergencies to the nearest security guard or to any ACS Operations Office during the meeting. Should a catastrophic event occur, attendees should follow safety and security instructions issued by the facility where they are located at the time of the event.

HOST LOCAL SECTION. ACS gratefully acknowledges the cooperation and assistance of the ACS Colorado local section and its members in handling local arrangements. Volunteers have planned many interesting activities; the Host Local Section booth will be located in the Colorado Convention Center, Lobby F.

INTERNATIONAL REGISTRANTS. Many international visitors are required to hold a visa to be admitted to the U.S. All visa applicants are advised to apply for their visa in their home country as soon as possible. Detailed information for international attendees can be found at www.acs.org/denver2015.

INTERNET & COMPUTER SERVICES. Use our electronic communication services before, during, and after the meeting. Once you get to the meeting, you can access your e-mail and the Internet as well as your personal Meeting Mail mailbox from Meeting Mail terminals, which will be located throughout the Colorado Convention Center.

LITERATURE & PRODUCT DISTRIBUTION. Promotions, posters, and literature distribution by attendees, exhibitors, or other groups during the meeting must be done within their own contracted meeting space or exhibit booth and not in public meeting space, with the exception of designated marketing opportunities. No one except the ACS Operations Office is authorized to place any promotional items in public meeting space at a given location. Items left in violation of this policy will be removed and discarded. Literature distribution at specific division tables is under the control of that division, and permission must be secured from the division before placing any items on their table.

MEETING OFFICES. The following ACS offices will be located in the Colorado Convention Center:

Attendee Registration: Lobby A/F

Career Fair: Hall B1

Exhibitor Registration: Upper Lobby A/F

Exposition: Halls A/F

Finance Office: Room 101

Host Local Section Center: Lobby F

Member Services: Lobby A/F

Press Center: Room 104

Shuttle Desk: Outside F Lobby

The following offices are located at the identified properties:

Operations Offices: Colorado Convention Center, Hyatt Regency Denver at Colorado Convention Center, Grand Hyatt Denver, Marriott City Center Denver, Sheraton Denver Downtown Hotel, Embassy Suites Denver—Downtown Convention Center, The Curtis—a DoubleTree by Hilton

Governance Office: Hyatt Regency Denver at Colorado Convention Center

Society Programs: Hyatt Regency Denver at Colorado Convention Center

MOTHERS ROOM. For your convenience and privacy, ACS will provide a room for nursing mothers at the Colorado Convention Center. Please see the Operations Office in Room 210/212 for access to the room.

SMOKING. ACS policy prohibits smoking in all rooms during ACS functions at the convention center and official hotels. Additionally, the convention center and many of the official hotels are designated as smoke-free environments at all times.

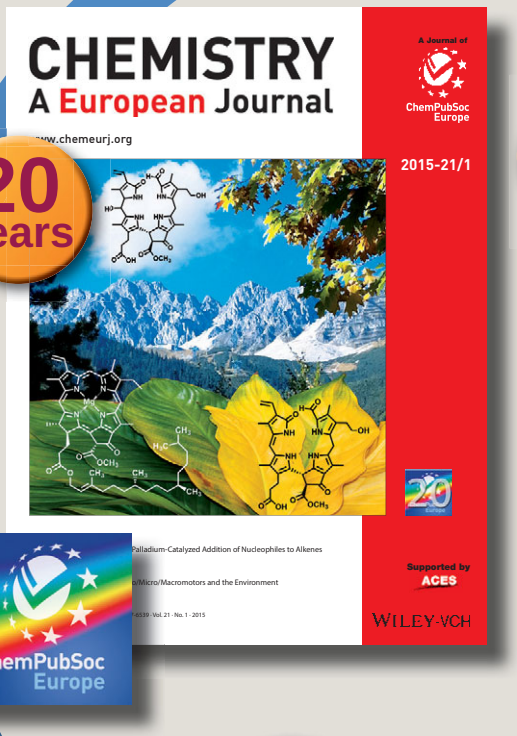
THANK YOU

The society thanks the many volunteers of the Colorado local section who are contributing to the 249th ACS National Meeting & Exposition by participating as division officers or program chairs, symposium organizers, session or award presiders, oral and poster presenters, short course or workshop instructors, career consultants, and society governance members.

TIPS FOR A SAFE STAY IN DENVER

- Attendees should be aware of their surroundings at all times.
- Don't wear your meeting badge outside the convention center or hotels.
- Don't wear fancy jewelry or carry expensive technology in plain sight.
- Carry your briefcase, tote bag, purse, or laptop carrier close to your body.
- Don't leave valuables in your hotel room. Get a hotel safe deposit box.
- Walk in open and in well-lit areas at night.
- Travel in groups. Don't be a loner, particularly in the evening.
- Use common sense. If someone or someplace looks suspicious, report it and/or avoid it.
- If an emergency occurs during a meeting event, refer to detailed instructions placed by ACS staff inside each meeting room to follow in case of emergencies. Report emergencies to the nearest security guard or to any ACS Operations Office during the meeting.
- If an emergency occurs outside an ACS event, contact police or emergency assistance by dialing 911 or seeking assistance from the facility where the emergency occurs.
- Should a catastrophic event occur while the meeting is underway, follow safety and security instructions issued by the facility where you are located at the time of the event.

Let's celebrate
leading society journals...



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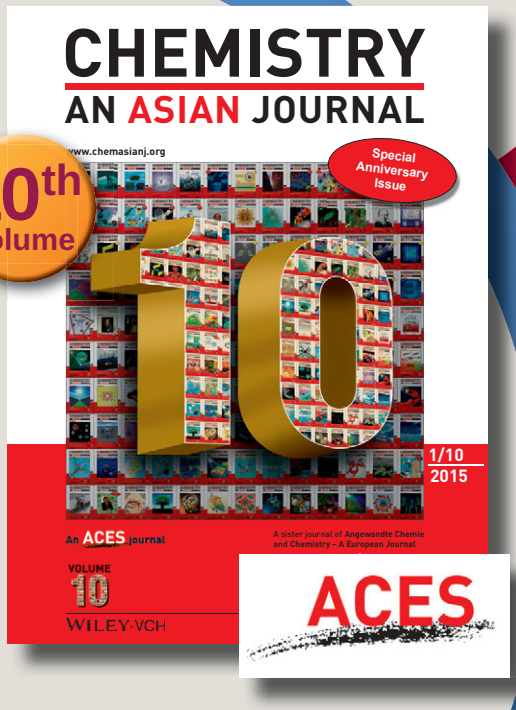

10th volume

ACES

ChemPubSoc Europe

5 years

ChemistryViews

... with a piece of cake

3:00 pm
Monday & Tuesday
March 23rd & 24th
Colorado Convention Center
Wiley Booth # 700

WILEY-VCH

WILEY

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THE AMERICAN CHEMICAL SOCIETY INVITE YOU TO

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PACIFICHEM 2015 raci NZIC KCS CCS Canadian Society for Chemistry ACS Chemistry for Life

GOVERNANCE & BUSINESS MEETINGS

MANY MEMBERS PARTICIPATE in meetings concerning the business of the Society, technical divisions, and governance committees in conjunction with the meeting. On the following pages, you will find a listing of the open meetings scheduled for Denver. ACS encourages it's members to get active in governance at all levels in order to contribute their vision to the direction of the Society. You can share ideas and insights into the Society and the chemical profession, network with peers, and catch up with friends through these volunteer connections. With nearly thirty national governance committees and leadership opportunities in technical divisions and local sections to choose from, there are many opportunities for members to become actively involved in ACS at the national level. If you are an ACS member interested in volunteering for a governance committee, contact the Office of the Secretary by email at secretary@acs.org or by phone 202-872-4461. Someone will put you in contact with the ACS Committee on Committees to discuss your desire to volunteer for a committee assignment. If you wish to volunteer with a specific technical division or local section, contact the officers listed at www.acs.org to explore your specific interests.

ACS COUNCIL

The ACS Council meeting will begin at 8:00 AM, Wednesday, March 25, at the Hyatt Regency Denver at the Colorado. The meeting will be preceded by a continental breakfast for councilors beginning at 7:00 AM. Councilors are asked to check in beginning at 7:00 AM and proceed to the breakfast area, keeping in mind that the meeting starts promptly at 8:00 AM. Space will be available for ACS members and nonmembers to observe the council in action. We hope that many will take advantage of this opportunity to learn firsthand of the society's operation. Alternate councilors and division and local section officers are particularly urged to attend.

Colorado Convention Center PHOTO.UA / SHUTTERSTOCK.COM

ACS Chemistry for Life®

www.acs.org

ACS Committee on Science
Emerging Frontiers in Science Symposium

Advanced Materials for Solar Energy
Transitioning Between Academic Research into Practical Use

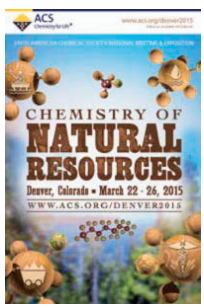
Monday, March 23
8:30 AM – 12:30 PM (Colorado Convention Center, Room 301)

Hear leading experts from:

Academia (Harry B. Gray-Caltech, James McCone-Cornell),
Government (John Turnel, NREL, Cheryl Martin, DOE ARPA-E) &
Industry (Anik R. Duggal, GE Global Research)

This distinguished panel will discuss key challenges and opportunities in advanced materials for solar energy and their commercial applications.

An ACS Presidential Event and Feature of the ACS Thematic Program (MPPG)
Cosponsored by the Division of Inorganic Chemistry



GOVERNANCE MEETINGS

For the complete list of committee meetings and agendas, please consult www.acs.org/denver2015.

BOARD & COUNCIL MEETINGS

ACS BOARD OF DIRECTORS. Board of Directors meeting, open to members who wish to participate, will be held in the Colorado Convention Center, Four Seasons Ballroom 4, from noon to 1:00 PM on Sunday, March 22. The guest speaker will be Deborah Blum, 2015 Grady Stack Award Recipient, and author of "The Poisoner's Handbook."

ACS COUNCIL. The ACS Council meeting will begin at 8:00 AM, Wednesday, March 25, at the Hyatt Regency Denver at Colorado Convention Center. The meeting will be preceded by a continental breakfast for councilors beginning at 7:00 AM. Councilors are asked to check in beginning at 7:00 AM and proceed to the breakfast area, keeping in mind that the meeting starts promptly at 8:00 AM. Space will be available for ACS members and nonmembers to observe the council in action. We hope that many will take advantage of this opportunity to learn firsthand of the society's operation. Alternate councilors and division and local section officers are particularly urged to attend.

COUNCIL POLICY COMMITTEE

The Council Policy Committee will open the floor during its meeting at 11:00 AM on Tuesday, March 24, to councilors who would like to raise issues of concern that affect them and/or their local sections or divisions. For further information, contact Alan M. Ehrlich, vice chair of CPC, at cpc@acs.org. For more committee meeting details and agendas, please consult the meeting website at www.acs.org/denver2015 or the on-site program distributed during the meeting.

COUNCILOR CAUCUS MEETINGS

District II Councilor Caucus
Sunday, March 22, 6:00 – 7:00 PM
Hyatt Regency Denver at Colorado Convention Center
Mineral Hall C

Middle Atlantic Councilor Caucus
Sunday, March 22, 6:00 – 7:00 PM
Hyatt Regency Denver at Colorado Convention Center
Mineral Hall D

District IV Councilor Caucus
Sunday, March 22, 6:00 – 7:00 PM
Hyatt Regency Denver at Colorado Convention Center
Mineral Hall E

District V Councilor Caucus
Sunday, March 22, 6:00 – 7:00 PM
Hyatt Regency Denver at Colorado Convention Center
Mineral Hall F

District VI Councilor Caucus
Sunday, March 22, 6:00 – 7:00 PM
Hyatt Regency Denver at Colorado Convention Center
Mineral Hall G

Division Officers/Councilors Caucus
Tuesday, March 24, 4:00 – 6:00 PM
Colorado Convention Center
Room 502

District I Councilor Caucus
Tuesday, March 24, 5:30 – 7:00 PM
Hyatt Regency Denver at Colorado Convention Center
Mineral Hall C

COMMITTEE AGENDA

THE COMMITTEE ON COMMITTEES has clarified three types of committee meetings:

OPEN. May be attended by any ACS member. At these sessions, members are encouraged to voice concerns, issue compliments, offer suggestions, express interest in, or raise questions about matters over which the committee has purview. The assumption is that participation is welcomed and will be orderly and courteous. Only committee members can vote.

EXECUTIVE. Attendance and participation are limited to officially appointed/elected committee members, associates, advisers, consultants, staff liaisons, and the appointed Committee on Committees liaison. Liaisons from other groups and ex officio and elected councilors may attend; participation by these groups would be at the invitation of the chair. Only committee members can vote.

CLOSED. The committee chair must declare any EXECUTIVE session CLOSED when confidential or sensitive personnel, financial, or legal matters of the society are discussed. At that point, only officially appointed/elected committee members, associates, consultants, staff liaisons, and the appointed Committee on Committees liaison shall remain in the session. Others may stay in the session at the discretion of the chair. Once these discussions have been completed, the committee should return to EXECUTIVE mode.

During the open and executive committee meetings, ACS members are given a chance to express their views on issues under consideration before these issues are acted on by the board or the council, or to bring up other subjects that deserve attention. Members are urged to examine the agenda and make known any opinions or ideas they may have. If you cannot attend the particular sessions involved, write to the officers listed or ask someone attending the session to speak on your behalf. For further information, contact the officers listed.

BUDGET & FINANCE

Kristen M. Omberg, chair; b_ffeedback@acs.org

Open Meeting
Saturday, March 21, 8:00 AM to noon
Hyatt Regency Denver at Colorado Convention Center, Centennial A

1. *Report of the Chair*
2. *Report of the Treasurer & CFO:*
   a. *Budgetary Performance Report for the Year Ended December 31, 2014*
3. *Reports from the B&F Subcommittees:*
   a. *Financial Impact of Constitution & Bylaw Changes*
   b. *Communications*
   c. *Program Funding Requests*
   d. *Program Review*

CHEMICAL SAFETY

Elizabeth M. Howson, chair; safety@acs.org

Open Executive Session
Monday, March 23, 8:30 to 11:30 AM
Hyatt Regency Denver at Colorado Convention Center, Centennial F

1. *Welcome*
2. *Minutes of August 11 Meeting*
3. *Reports of the Chair/Staff Liaison*
4. *Report of Subcommittees and Task Forces*
5. *Old and new business*

CHEMISTRY & PUBLIC AFFAIRS

Susan B. Butts, chair; sbbuttsdc@gmail.com

Open Meeting
Saturday, March 21, 8:00 AM to 4:00 PM
Hyatt Regency Denver at Colorado Convention Center, Capitol 1/2

1. *Welcome*
2. *Minutes of August 11 Meeting*
3. *Reports of the Chair/Staff Liaison*
4. *Report of Subcommittees and Task Forces*
5. *Old and new business*

CHEMISTS WITH DISABILITIES

John J. Johnston, chair; USDA-FSIS, Fort Collins, CO 80526-8116

Combined Open and Executive Meeting
Sunday, March 22, 8:30 AM to 4:30 PM
Hyatt Regency Denver at Colorado Convention Center, Capitol 3

1. *Welcome*
2. *Chair Report*
   a. *Update of CWD Activities/Events, and Collaborative Opportunities*
   b. *Diversity & Inclusion Advisory Group Report*
   c. *Strategic Planning Retreat*
   d. *Minutes from San Francisco, 2014*
3. *Staff Report*
4. *Future Event and Programming Planning*
5. *Subcommittee Progress Reports*
   a. *CWD Poster Project*
6. *Reports of Liaisons to/from other committees*
7. *Ongoing Business*
8. *New Business*

COMMITTEES

Wayne E. Jones Jr., chair; Department of Chemistry, Binghamton University (SUNY), Vestal Pkwy. East, Binghamton, NY 13902-6000

Open Session
Monday, March 23, 1:30 to 2:00 PM
Hyatt Regency Denver at Colorado Convention Center, Capitol 2

1. *Welcome*
2. *Minutes of August 11-13, 2014*
3. *Reports of chair/staff liaison*
4. *Report of Subcommittees and Task Forces on:*
   a. *Diversity*
   b. *Leadership Development*
5. *Topics from floor*

COMMUNITY ACTIVITIES

George L. Heard, chair; University of North Carolina, Asheville; glheard@gmail.com

Open Executive Session
Sunday, March 22, 7:45 AM to noon
The Curtis Hotel, Four Square B

CCA/LSAC Joint Open Meeting
Tuesday, March 24, 2:00 to 3:30 PM
The Curtis Hotel, Four Square Ballroom

1. *Reports of chair, subcommittee chairs, staff liaison*
2. *Training materials for outreach*
3. *Reports of committee liaisons*

CONSTITUTION & BYLAWS

James C. Carver, chair, The Carver Law Firm, Baton Rouge, LA; bylaws@acs.org

Open Meetings
Sunday, March 22, 1:15 to 1:45 PM
Hyatt Regency Denver at Colorado Convention Center, Mineral F

Executive Session (Closed)
Sunday, March 22, 9:00 AM to noon

1. *Open forum to discuss bylaws, petitions, and other issues that may arise*

Executive Session
Sunday, March 22, 1:45 to 4:30 PM
Hyatt Regency Denver at Colorado Convention Center, Mineral F

1. *Status of unit bylaws*
2. *Bylaw review process*
3. *Reports from liaisons from other committees*
4. *Petition on Member Expulsion*
5. *Petition on Preferential Voting*
6. *Open discussion*

CORPORATION ASSOCIATES

Dawn Mason, chair; P.O. Box 431, Kingsport, TN 37662

Open Meeting
Monday, March 23, 8:00 AM to noon
Hyatt Regency Denver at Colorado Convention Center, Capitol 3

1. *Welcome*
2. *Approval of Minutes*
3. *Reports of Chair/Staff Liaison*
4. *Report of Subcommittees*
5. *Open Discussion and New Business*

COUNCIL POLICY

Alan M. Ehrlich, vice chair; cpc@acs.org

Open Meeting
Tuesday, March 24, 9:30 AM to noon
Hyatt Regency Denver at Colorado Convention Center, Capitol 1

1. *Committee and Officer Reports*
2. *Report of CPC vice chair*
3. *Reports of Subcommittees and Task Forces on:*
   a. *Petitions, Constitution and Bylaws*
   b. *Long Range Planning*
   c. *Task Forces: to review Councilor Travel Reimbursement Program; on Councilor and Member Duties and Conduct; on Divisor Communications*
5. *Schedule of business sessions, fall 2015*
6. *Review of Council agenda*
7. *Open forum*
8. *Old and new businessss*

DIVISIONAL ACTIVITIES

Michael J. Morello, chair; mike.morello@pepsico.com

Open Session
Sunday, March 22, 8:00 AM to noon
Hyatt Regency Denver at Colorado Convention Center, Mineral E

1. *Welcome*
2. *Review Denver Agenda*
3. *Minutes from 248th ACS National Meeting in San Francisco, CA*
4. *DAC Chair Report*
5. *Subcommittee Reports*

ECONOMIC & PROFESSIONAL AFFAIRS

Rick Ewing, chair; william.ewing@bms.com

Executive Session
Saturday, March 21, 8:00 AM to 5:30 PM
Colorado Convention Center

Open Executive Session
Sunday, March 22, 8:00 AM to noon
Colorado Convention Center, Room 601

1. *Opening Remarks/Introductions*
2. *Priorities and Strategic Plan*
3. *Subcommittee Meetings*
4. *Staff Reports*
5. *Wrap-Up and Process Check*
6. *Subcommittee Reports*
   a. *Public Policy*
   b. *Events, Volunteers and Employment Services*
   c. *Marketing and Research*
   d. *Standards and Ethics*
7. *Reports from Liaisons to and from CEPA*
8. *Old Business / New Business*

EDUCATION

Diane Krone, chair; kroned@alumni.stevens.edu

Open Meeting
Monday, March 23, 3:00 to 4:00 PM
Hyatt Regency Denver at Colorado Convention Center, Mineral D

Executive Session
Friday, March 20, 1:00 to 5:30 PM
Hyatt Regency Denver at Colorado Convention Center, Centennial E

1. *K-12 science topics, including ChemCom,* ChemMatters*, the American Association of Chemistry Teachers, High School Chemistry Clubs, Chemistry Olympiad, Science Coaches, and teacher professional development*
2. *College/university topics, including two-year college chemistry, undergraduate programs, graduate and postdoctoral education,* Chemistry in Context*, and professional development*

Items 1-2 open to all Councilors with prior approval of the Chair

ENVIRONMENTAL IMPROVEMENT

Laura Pence, chair; lpence@hartford.edu

Open Executive Session
Saturday, March 21, 4:00 to 6:00 PM
Hyatt Regency Denver at Colorado Convention Center, Centennial E

1. *Chair's report and review of interim actions*
2. *Subcommittee on Member Involvement*
3. *Subcommittee on Programming and Education*
4. *Subcommittee on Public Policy*
5. *Staff reports from OPA and GCI*
6. *Reports of Other Working Groups and Liaisons*
7. *Committee Business*
8. *Open Discussion*

ETHICS

Keith Vitense, chair; Cameron University, Physical Science Department, 2800 West Gore Blvd., Lawton, OK 73505-6320

Open Executive Session
Sunday, March 22, 9:00 AM to 4:30 PM
Hyatt Regency Denver at Colorado Convention Center, Capitol 5

1. *Welcome & Introductions*
2. *Approval of Minutes from San Francisco Meeting*
3. *Review of Committee on Ethics Charge*
4. *Chair/Staff Liaison Reports*
5. *Liaison Reports*
6. *Subcommittee Progress Reports*
   a. *Communications and Awareness*
   b. *Education and Materials*
   c. *Programming and Screening*
7. *Committee Discussion*
8. *Subcommittee Working Sessions*
9. *Old Business /New Business/ Action Items*

INTERNATIONAL ACTIVITIES

H. N. Cheng, chair; c/o ACS Office of International Activities, 1155–16th St., N.W., Washington, DC 20036

Open Meeting
Saturday, March 21, 1:00 to 3:00 PM
Hyatt Regency Denver at Colorado Convention Center, Centennial F/G

1. *Welcome*
2. *Minutes of August 9, 2014*
3. *Reports of Chair/Staff Liaison*
4. *Report of Subcommittees:*
   a. *Subcommittee on Africa and the Americas*
   b. *Subcommittee on Europe and the Middle East*
   c. *Subcommittee on Asia / Pacific Rim*
5. *New Business*

LOCAL SECTION ACTIVITIES

Martin Rudd, chair; martin.rudd@uwc.edu

LSAC/CCA Joint Open Meeting
Tuesday, March 24, 2:00 to 3:30 PM
The Curtis Hotel, Four Square Ballroom

Open Executive Session
Sunday, March 22, 8:00 AM to noon
The Curtis Hotel, Four Square A

1. *Report from the LSAC and CCA Executive Sessions*
2. *Interactive session: questions, answers and best practices*

Open Executive Session

1. *Report of chair, subcommittee chairs, staff liaison*
2. *Review of petitions for council consideration*
3. *Reports of committee liaisons*

MEETINGS & EXPOSITIONS

Will E. Lynch, chair; Department of Chemistry & Physics, Armstrong Atlantic State University, 11935 Abercorn St., Savannah, GA 31419-1997

Open Executive Session
Sunday, March 22, 7:00 AM to noon
Colorado Convention Center, Room 207

1. *Welcome*
2. *Minutes from San Francisco National Meeting*
3. *Chair's report*
4. *Subcommittee reports*
5. *Finance/Staff Liaison Report*
6. *Registration Fee Vote*
7. *New Business*

MEMBERSHIP AFFAIRS

James M. Landis Jr., chair; jim.landis@gt.org

Open Session
Sunday, March 22, 2:00 to 3:00 PM
Hyatt Regency Denver at Colorado Convention Center, Capitol 1/2

1. *Welcome*
2. *Minutes of August 11-12, 2014*
3. *Reports of Chair/Staff Liaison*
4. *Reports of Subcommittees*
   a. *Categories & Dues*
   b. *Retention, Benefits & Services*
   c. *Recruitment & Admissions*
5. *Petition on Member Expulsion (For Consideration)*
6. *Topics from floor*

MINORITY AFFAIRS

Madeleine Jacobs, chair; c/o ACS Office of Diversity Programs, 1155—16th St., N.W., Washington, DC 20036

Executive Session
Sunday, March 22, 8:00 AM to 12:30 PM
Hyatt Regency Denver at Colorado Convention Center, Centennial D

1. *Opening Remarks*
2. *Staff Report*
3. *Subcommittee Meetings*

Open Session
Sunday, March 22, 12:30 to 2:00 PM
Hyatt Regency Denver at Colorado Convention Center, Centennial D

1. *Subcommittee Reports*
2. *Old Business*
4. *New Business*
5. *Open Discussion*
6. *Adjournment*

NOMENCLATURE, TERMINOLOGY & SYMBOLS

Albert C. Censullo, chair; 1595 Cordova Dr., San Luis Obispo, CA 93405

Open Session
Monday, March 23, 2:00 to 5:00 PM
Hyatt Regency Denver at Colorado Convention Center, Centennial H

1. Review minutes from San Francisco meeting
2. Chair/Staff Liaison reports
3. Reports from subcommittees
a.Communication/Outreach
   b. Education
   c. Committee Liaison
   d. Long Range Planning
4. *IUPAC Reports*
5. *Update to Kilogram, Amount of Substance and Mole Issues*
6. *Task Force on new SI definitions*

NOMINATIONS & ELECTIONS

D. Richard Cobb, chair; nomelect@acs.org

Open Executive Session
Monday, March 23, 11:00 AM to noon
Hyatt Regency Denver at Colorado Convention Center, Mineral C

1. *Report of the Executive Session*
2. *Topics from the floor*

PATENTS & RELATED MATTERS

Sadiq Shah, chair; sadiq@utpa.edu

Open Meeting
Saturday, March 21, 9:00 AM to 5:00 PM
Hyatt Regency Denver at Colorado Convention Center, Capitol 4

1. *Legislation & Regulation Subcommittee.*
2. *Education and Outreach Subcommittee.*
3. *Awards Subcommittee.*
4. *Executive Session*

PROFESSIONAL TRAINING

Thomas J. Wenzel, chair; cpt@acs.org

Open Meeting
Sunday, March 22, noon to 1:00 PM
Marriott Denver City Center, Gold Coin

1. *Implementation of New Guidelines for ACS Approval*
2. *Expectations for Polymer Chemistry*
3. *Supplements to the New Guidelines*
4. *Planning for Graduate Work in the Chemical Sciences*
5. *Survey of PhD Recipients*
6. *Directory of Undergraduate Research*
7. *Topics from floor*

PROJECT SEED

Anna G. Cavinato, chair, Eastern Oregon University, Department of Chemistry, One University Blvd., LaGrande, OR 97850-2807

Open Session
Sunday, March 22, 9:30 to 10:30 AM
Hyatt Regency Denver at Colorado Convention Center, Agate B

1. *Report from executive session*
2. *Topics from the floor*

Executive Session
Saturday, March 21, 10:30 AM to 5:00 PM
Hyatt Regency Denver at Colorado Convention Center, Mineral C

1. *Subcommittee meetings 10:30 AM – noon*
2. *Minutes of August 9, 2014*
2. *Reports of Chair/Staff Liaison*
3. *Report of Subcommittees*
4. *Old and new business*

PUBLICATIONS

Stephanie Brock, chair; Wayne State University, Chemistry, 5101 Cass Ave., Detroit, MI 48202-3929

Open Meeting
Friday, March 20, 4:30 to 5:00 PM
Hyatt Regency Denver at Colorado Convention Center, Mineral F/G

1. *Updates from ACS Publications Division*
2. *Open Discussion*

Executive Session
Friday, March 20, 1:00 to 5:00 PM
(Closed Executive Session until 4:30 PM)
Hyatt Regency Denver at Colorado Convention Center, Mineral F/G
(Closed Executive Session until 4:30 PM)

1. *Report of C&EN Editorial Board*
2. *Reports of the Publications Division and of the Governing Board for Publishing*
3. *Reports from Other Committees*
4. *Discussion of Journal Monitoring Reports and Editor Appointments*
5. *Open Session:*

a. Updates from ACS Publications Division
   b. Open Discussion

SCIENCE

Katherine Glasgow, chair; Nomacorc, 400 Vintage Park Dr., Zebulon, NC 27597-3803;

Open Meeting

Saturday, March 21, 8:00 AM to 4:30 PM

Hyatt Regency Denver at Colorado Convention Center, Centennial B

1. *Welcome*
2. *Approval of Minutes*
3. *Reports of Chair/Staff Liaison*
4. *Report of Subcommittees:*
   a. *Science and Technology,*
   b. *Awards,*
   c. *Public Policy and Communication*
5. *Subcommittee Breakouts*
6. *Subcommittee Reports from Breakouts*

SENIOR CHEMISTS

George Heinze, chair; 30 Bunker Hill Run, East Brunswick, NJ 08816-3317

Open Meeting

Monday, March 23, 8:00 AM to noon

Hyatt Regency Denver at Colorado Convention Center, Mineral B

1. *Welcome & Introductions*
2. *Discussion and approval of San Francisco Meeting Minutes*
3. *Reports of Chair & Staff Liaison*
4. *Subcommittee Reports*
   a. *Newsletter*
   b. *National Meeting Programming*
      1. *Denver*
      2. *Boston*
   c. *Senior Activities in Local Sections*
      1. *Mini Grant Awards*
   d. *Consulting & Mentoring*
      1. *Undergraduate Speed Networking Event*
   e. *Planning and Priorities*
5. *Old Business*
   a. *Senior Chemists Breakfast*
6. *New Business*
   a. *ChemLuminary Awards*
7. *Adjournment*

TECHNICIAN AFFAIRS

Susan S. Marine, chair; CTA@acs.org

Closed Executive Session

Sunday, March 22, 8:30 AM to 2:00 PM

Hyatt Regency Denver at Colorado Convention Center, Centennial A

1. *Welcome*
2. *Minutes of Fall Meeting*
3. *Reports of Chair/Staff Liaison*
4. *Subcommittee breakout*
5. *Subcommittee reports*
6. *New business*
7. *Final comments/Feedback*

Open Session

Sunday, March 22, 2:00 to 2:30 PM

Hyatt Regency Denver at Colorado Convention Center, Centennial A

1. *Welcome*
2. *Chair's Report*
3. *Subcommittee Reports*
4. *Topics from Floor*
5. *Adjourn*

WOMEN CHEMISTS

Amber F. Charlebois, chair; afcharleb@gmail.com

Closed Executive Session

Saturday, March 21, 8:00 AM to 5:00 PM

Hyatt Regency Denver at Colorado Convention Center, Centennial D

1. *Welcome*
2. *Review of Fall Action Items & Minutes*
3. *Reports of Chair/Staff Liaison*
4. *Subcommittee Meetings*
5. *Report of Subcommittees and Task Forces:*
   a. *Awards & Recognition*
   b. *Communications & Technology*
   c. *Professional Development*
   d. *Programs & Events*
6. *New Business*

YOUNGER CHEMISTS

Douglas B. Hausner, chair; doug.hausner@gmail.com

Open and Executive Session

Sunday, March 22, 8:00 AM to noon

Hyatt Regency Denver at Colorado Convention Center, Centennial C

1. *Welcome*
2. *Staff Report*
3. *Subcommittee Reports*
   a. *Communications*
   b. *Governance Interface and Outreach*
   c. *Membership Engagement*
4. *Liaison Reports*
5. *Petitions (CLOSED)*
6. *New Business*
7. *Visitors*

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ACS ATTENDEE WELCOME RECEPTION

Meet exhibitors and employers while networking and enjoying the reception!
Colorado Convention Center
Exhibit Halls A/F, Sunday
March 22, 6 - 8:30 PM

DAILY RAFFLE, BOOTH 339

Visit the Daily Prize Raffle area on Sunday through Tuesday for a chance to win a prize.

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Get scanned by 20 exhibitors on Sunday through Tuesday and be entered into a raffle for a terrific prize.

ENJOY POSTERS ON EXPO FLOOR

Join us on Tuesday, inside the Colorado Convention Center Exhibit Halls A/F, for poster sessions on the show floor.

Monday, March 23

Spectroscopy Simplified – How to Run a Research FT-IR System with the Touch of a Button
Sponsor: Thermo Scientific, 9:30 AM - 12:00 PM
Colorado Convention Center
Exhibit Halls A/F, Exhibitor Workshop Room 1

Innovative Technologies to Engage Your Student's Learning Experience
Sponsor: McGraw Hill Higher Education, 9:30 AM - 12:00 PM
Colorado Convention Center, Room 103

SciFinder Training Session
Sponsor: CAS, 12:30 PM - 3:00 PM
Colorado Convention Center
Exhibit Halls A/F, Exhibitor Workshop Room 1

Thermo Fisher Chromatography and Mass Spectrometry
Sponsor: Thermo Scientific, 12:30 PM - 3:00 PM
Colorado Convention Center, Exhibit Halls A/F
Exhibitor Workshop Room 2

Innovative Technologies to Engage Your Student's Learning Experience
Sponsor: McGraw Hill Higher Education, 12:30 PM - 3:00 PM
Colorado Convention Center, Room 103

Online Homework with Targeted Instructional Feedback Leads to Improved Student Learning Outcomes
Sponsor: Sapling Learning, 3:30 PM - 6:00 PM
Colorado Convention Center, Room 103

Tuesday, March 24

SciFinder Training Session
Sponsor: CAS, 9:30 AM - 12:00 PM
Colorado Convention Center
Exhibit Halls A/F, Exhibitor Workshop Room 1

Tuesday, March 24, Cont'd

A Survey of Accelerated Materials Research Using Raman Microscopy and Imaging
Sponsor: Thermo Scientific, 9:30 AM - 12:00 PM
Colorado Convention Center, Room 103
Exhibit Halls A/F, Exhibitor Workshop Room 2

Compact Mass Spectrometry: A Swiss Army Knife Approach to Chemistry Challenges
Sponsor: Advion, 9:30 AM - 12:00 PM
Colorado Convention Center, Room 103

Intelligent Real-Time Reaction Monitoring In The Fume Hood Using Benchtop NMR
Sponsor: Thermo Scientific, 12:30 PM - 3:00 PM
Colorado Convention Center
Exhibit Halls A/F, Exhibitor Workshop Room 1

Analysis of Polymers by Vibrational Spectroscopy and Microscopy
Sponsor: Bruker, 12:30 PM - 3:00 PM
Colorado Convention Center
Exhibit Halls A/F, Exhibitor Workshop Room 2

Advances in Atomic and Molecular Spectroscopy
Sponsor: Agilent Technologies, 12:30 PM - 3:00 PM
Colorado Convention Center, Room 103

Chromatography and Mass Spectrometry Tips, Tricks, and Advanced Techniques
Sponsor: Agilent Technologies, 3:30 PM - 6:00 PM
Colorado Convention Center, Room 103

Wednesday, March 25

Designing Inhibitors with MOE Structure-Based Drug Design Tools
Sponsor: Chemical Computing Group, 3:30 PM - 6:00 PM
Colorado Convention Center, Room 103

DIVISION MEETINGS & SOCIAL EVENTS

Division of Agricultural & Food Chemistry— AGFD

Membership Committee— Special Meeting	Sunday, March 22	12:00 PM - 1:00 PM	Room 113, Colorado Convention Center
Executive Committee Meeting	Sunday, Ma rch 22	5:00 PM - 8:00 PM	Mineral B Room, Hyatt Regency Denver
Future Programs Planning Meeting	Monday, March 23	12:00 PM - 1:00 PM	Room 701, Colorado Convention Center
AGFD Chair's Reception	Tuesday, March 24	6:00 PM - 8:00 PM	Crystal Ballroom B, Embassy Suites Denver Downtown

Division of Analytic Chemistry— ANYL

Sci-Mix	Monday, March 23	8:00 PM - 10:00 PM	Hall C, Colorado Convention Center
Analytical Posters	Tuesday, March 24	7:00 PM - 9:00 PM	Hall C, Colorado Convention Center

Division of Biological Chemistry— BIOL

Current Topics in Biological Chemistry	Sunday, March 22	8:15 PM - 9:45 PM	Hall B2, Colorado Convention Center

Division of Biochemical Technology— BIOT

Company Seminar Luncheon	Sunday, March 22	12:30 PM - 2:00 PM	Capitol Peak B, Grand Hyatt Denver
Company Seminar Luncheon	Monday, March 23	12:30 PM - 2:00 PM	Capitol Peak B, Grand Hyatt Denver
Company Seminar Luncheon	Tuesday, March 24	12:30 PM - 2:00 PM	Capitol Peak B, Grand Hyatt Denver
Future Programming (Closed Meeting)	Tuesday, March 24	12:30 PM - 2:00 PM	Grays Peak, Grand Hyatt Denver
Program Chair Meeting (Closed Meeting)	Wednesday, March 25	11:30AM - 2:30 PM	Maroon Peak, Grand Hyatt Denver
Company Seminar Luncheon	Wednesday, March 25	12:30 PM - 2:00 PM	Capitol Peak B, Grand Hyatt Denver
Networking Session	Wednesday, March 25	6:00 PM - 8:00 PM	Capitol Peak B, Grand Hyatt Denver

Division of Business Development & Management— BMGT

BMGT Reception	Monday, March 23	5:30 PM - 7:30 PM	Crystal Ballroom B&C, Embassy Suites Denver Downtown

Division of Carbohydrate Chemistry— CARB

2015 Carbohydrate Division Award Banquet (Ticketed Event)	Monday, March 23	7:00 PM - 10:00 PM	Appaloosa Grill

Division of Catalysis and Surface Science— CATL

Division Board/Leadership Meeting	Monday, March 23	6:00 PM - 8:00 PM	Room 108, Colorado Convention Center
Program Committee Meeting	Tuesday, March 24	6:00 PM - 8:00 PM	Room 605, Colorado Convention Center

Division of Cellulose and Renewable Materials— CELL

Anselme Payen Award Banquet (Ticketed Event)	Tuesday, March 24	6:30 PM - 10:00 PM	Coohills Restaurant
Business Meeting	Wednesday, March 25	5:00 PM - 6:00 PM	Room 404, Colorado Convention Center

Note: Due to space limitations, hotel abbreviations are used in these tables.

Division of Chemistry and Law— CHAL

CHAL Reception	Monday, March 23	5:00 PM - 8:00 PM	Crystal Peak A, Grand Hyatt Denver

Division of Chemical Health & Safety— CHAS

Laboratory Safety Workshop	Friday, March 20	7:30 AM - 5:30 PM	CCB 1, Embassy Suites Denver
Laboratory Waste Management Workshop	Friday, March 20	7:30 AM - 5:30 PM	CCB 2, Embassy Suites Denver
Chemical Reactivity Hazards: Laboratory-Scale Recognition & Control Workshop	Saturday, March 21	7:30 AM - 5:30 PM	CCB1, Embassy Suites Denver
Job Hazard Analysis Workshop	Saturday, March 21	7:30 AM - 5:30 PM	CCB 2, Embassy Suites Denver
How to be a More Effective Chemical Hygiene Officer Workshop	Saturday, March 21	7:30 AM - 5:30 PM	Silverton Ballroom 1, Embassy Suites Denver
NRCC Certification Exams	Sunday, March 22	8:00 AM - 12:00 PM	Rexford Room, Embassy Suites Denver
Executive Committee Meeting	Sunday, March 22	8:00 AM - 12:00 PM	Silverton Ballroom 3, Embassy Suites Denver

Division of Chemical Education— CHED

Chemical Education Research Committee	Sunday, March 22	7:00 AM - 9:00 AM	Plaza Court 6, Sheraton Denver Downtown
High School/College Interface Luncheon (Ticketed Event)	Sunday, March 22	12:00 PM - 1:00 PM	Silver Room, Sheraton Denver Downtown
Workshop 1	Sunday, March 22	8:00 AM - 12:00 PM	Plaza Court 3, Sheraton Denver Downtown
Workshop 2	Sunday, March 22	1:00 PM - 5:00 PM	Plaza Court 4, Sheraton Denver Downtown
Workshop 3	Monday, March 23	8:00 AM - 12:00 PM	Plaza Court 3, Sheraton Denver Downtown
Workshop 4	Monday, March 23	1:00 PM - 5:00 PM	Plaza Court 4, Sheraton Denver Downtown

Division of Chemical Information— CINF

Education Committee Meeting (Closed Meeting)	Saturday, March 21	1:00 PM - 3:00 PM	Room 604, Colorado Convention Center
Program Commttee Meeting (Clossed Meeting)	Saturday, March 21	1:00 PM - 3:00 PM	Room 606, Colorado Convention Center
Awards Committee Meeting (Closed Meeting)	Saturday, March 21	1:00 PM - 3:00 PM	Room 608, Colorado Convention Center
Executive Meeting (Closed Meeting)	Saturday, March 21	3:00 PM - 6:00 PM	Room 604, Colorado Convention Center
Open Business Meeting	Sunday, March 22	6:00 PM - 6:30 PM	Silverton Ballroom 3, Embassy Suites Denver
Welcoming Reception	Sunday, March 22	6:30 PM - 8:30 PM	Silverton Ballroom 3, Embassy Suites Denver
Luncheon (Ticketed Event)	Tuesday, March 24	12:00 PM - 1:30 PM	Silverton Ballroom 3, Embassy Suites Denver

Division of Colloid & Surface Chemistry— COLL

Open Business Meeting/Social Hour with Poster Session	Sunday, March 22	5:30 PM - 8:00 PM	Hall E, Colorado Convention Center
Luncheon	Tuesday, March 24	12:00 PM - 1:45 PM	Penrose Ballroom 1, Denver Marriott City Center

Division of Computers in Chemistry— COMP

Programming & Executive Board Meeting	Saturday, March 21	8:00 AM - 6:30 PM	Room 108, Colorado Convention Center
Poster and Awards Session	Tuesday, March 24	6:00 PM - 8:30 PM	Hall B2, Colorado Convention Center

Division of Energy & Fuel— ENFL

Division Dinner (Ticketed Event)	Tuesday, March 24	7:30 PM - 9:00 PM	Maggiano's Little Italy

Division of Environmental Chemistry— ENVR

Program Planning Committee Meeting	Sunday, March 22	2:00 PM - 3:00 PM	Room 207, Colorado Convention Center
Long Range Planning Committee Meeting	Sunday, March 22	3:00 PM - 5:00 PM	Room 605, Colorado Convention Center
Executive Committee Meeting	Sunday, March 22	7:00 PM - 10:00 PM	Room 603, Colorado Convention Center
Reception (Ticketed Event)	Tuesday, March 24	6:00 PM - 7:30 PM	Wynkoop Brewing Company

Division of Geochemistry— GEOC

Business Committee Meeting	Tuesday, March 24	5:30 PM - 7:30 PM	Room 603, Colorado Convention Center

Division of Industrial & Engineering Chemistry— I&EC

Subcommittee Meeting (Closed Meeting)	Sunday, March 22	12:00 PM - 2:00 PM	Crystal Ballroom C, Embassy Suites Denver
General Posters Session	Tuesday, March 24	5:00 PM - 6:30 PM	Hall C, Colorado Convention Center

Division of Inorganic Chemistry— INOR

Dow Energy Water Nexus Reception	Tuesday, March 24	4:00 PM - 5:00 PM	Room 207, Colorado Convention Center

Division of Medicinal Chemistry— MEDI

Business Meeting	Sunday, March 22	5:30 PM - 6:30 PM	Room 605, Colorado Convention Center

Division of Nuclear Chemistry & Technology— NUCL

Social Hour	Monday, March 23	7:00 PM - 9:00 PM	Silverton Ballroom 2, Embassy Suites Denver

Division of Organic Chemistry— ORGN

Executive Committee Meeting (Closed Meeting)	Sunday, March 22	1:00 PM - 5:00 PM	Room 603, Colorado Convention Center

Division of Physical Science— PHYS

Poster Session	Wednesday, March 25	6:00 PM - 8:00 PM	Hall C, Colorado Convention Center

Division of Polymer Chemistry— POLY

POLY/PMSE Awards Reception	Wednesday, March 25	5:30 PM - 8:30 PM	Plaza Ballroom A/B, Sheraton Denver Downtown

Division of Professional Relations— PROF

Professional Relations Executive Committee Meeting	Tuesday, March 24	3:00 PM - 5:00 PM	Capitol 3, Hyatt Regency Denver

Division of Small Chemical Business— SCHB

SCHB & PROF Luncheon	Sunday, March 22	11:30 AM = 1:30 PM	Silverton Ballroom 2, Embassy Suites Denver
SCHB & HACH Award Luncheon	Monday, March 23	11:30 AM - 1:30 PM	Silverton Ballroom 2, Embassy Suites Denver
SCHB/HACH Award Reception	Monday, March 23	5:30 PM - 7:30 PM	Cactus Club

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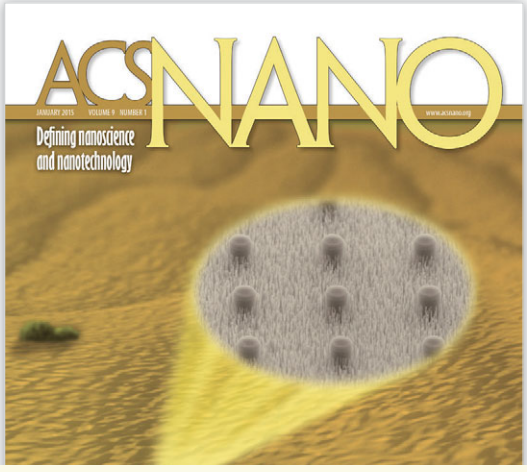
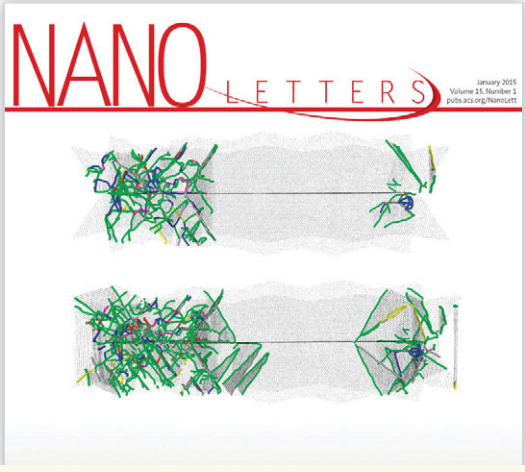
Symposium at the 2015 ACS Spring National Meeting





TUESDAY, MARCH 24 | 9:00 AM – 11:40 AM

Denver, CO | Colorado Convention Center | Mile High Ballroom 3A

Paul Weiss
Editor-in-Chief, *ACS Nano*

Paul Alivisatos
Co-Editor, *Nano Letters*

Join the Editors of *ACS Nano* and *Nano Letters* for the next joint session at the 2015 ACS Spring National Meeting Denver, CO. The session was specially designed for the National Meeting theme with world-renowned speakers presenting. All speakers are editors of *ACS Nano* or *Nano Letters*.

GUEST SPEAKERS	PRESENTATIONS
Naomi Halas, Rice University	*Your anion is my plasmonic nanostructure: Discovering molecular plasmonics*
Shuit-Tong Lee, Soochow University	*Silicon nanostructures for new energy applications*
Andrey Rogach, City University of Hong Kong	*Design of colloidal heterostructures for photocatalytic hydrogen generation*
Uri Banin, The Hebrew University of Jerusalem	*Dimensionality matters: Dimensio-nality effects on optoelectronic behavior of semiconductor nanocrystals*
Paula T. Hammond, Massachusetts *Institute of Technology*	*Nanomaterials design for programmed multi- and staged release*

SOCIAL & EDUCATIONAL EVENTS

PRESIDENTIAL EVENTS

DIANE GROB SCHMIDT, the 2015 ACS president, welcomes attendees to the 249th ACS National Meeting.

Schmidt's first presidential symposia, titled "Chemistry without Borders: The Transnational Practice of Chemistry & Allied Sciences & Engineering," will take place the morning of Sunday, March 22. This symposium will touch on the ever-increasing practice of researchers, students, and professionals working overseas and efforts to attract and build a workforce to benefit the worldwide success of chemistry.

The next presidential symposium begins later that afternoon on Sunday, March 22, and continues all day on Monday. "Nanotechnology: Delivering on the Promise" will highlight the fascinating research, development, and commercialization of nanochemistry and nanotechnology and will include 16 senior-level speakers from industry, academe, and government.

The third presidential symposium, "DOE Nanoscience Research Centers: National Resources for the Nanoscience Community," will feature the five heads of chemistry at U.S. national laboratories. This is the first symposium of its type to highlight these speakers collectively.

Always a highlight at the ACS national meetings are the Kavli lectures, which will take place on Monday, March 23, at the Colorado Convention Center. The first is The Kavli Foundation Emerging Leader in Chemistry Lecture given by Theodore Betley, a professor of chemistry and chemical biology at Harvard University, from 4:00 to 5:00 PM. Following shortly afterward, from 5:30 to 6:30 PM, is The Fred Kavli Innovations in Chemistry Lecture, given by Laura L. Kiessling, Steenbock Professor of Chemistry and Laurens Anderson Professor of Biochemistry at the University of Wisconsin, Madison, which will focus on how the features of carbohydrates on cell surfaces differ between mammals and microbes.

Details of presidential events and other recommended symposia can be found at www.acs.org/denver2015 and in the on-site program.

2015 NATIONAL AWARDS

THE ACS NATIONAL awards recognize individual or team accomplishments in diverse fields of the chemical sciences. Award recipients traditionally receive their national award in person during the ACS awards dinner and general meeting and deliver an award address on the scientific work that is being recognized to an appropriate division.

This year's event will be held on the evening of Tuesday, March 24, at the Sheraton Denver Downtown Hotel, Ballroom. Dinner begins at 7:30 PM, and the general meeting begins at 8:30 PM. Jacqueline K. Barton will deliver the Priestley Medal Address at the general meeting. See Ticketed Events on page 71 for ticket information.

Several awards, such as the Arthur C. Cope Scholar Awards and the Arthur C. Cope Award, will be presented at the Arthur C. Cope Symposium in conjunction with the 250th ACS National Meeting in Boston in August.

ACS Award for Achievement in Research for the Teaching & Learning of Chemistry, sponsored by Pearson Education, **Vickie M. Williamson,** Texas A&M University. Address to be presented before the Division of Chemical Education. March 23; Sheraton Denver Downtown Hotel; Gold Room; 3:35 PM.

ACS Award for Affordable Green Chemistry, sponsored by Dow Chemical and endowed by Rohm and Haas, **John Frye** and **Alan H. Zacher,** Pacific Northwest National Laboratory, and **Todd Werpy,** Archer Daniels Midland. Address to be presented before the Division of Cellulose & Renewable Materials. March 25; Colorado Convention Center; Room 403; 4:45 PM & 5:10 PM

ACS Award for Computers in Chemical & Pharmaceutical Research, sponsored by the ACS Division of Computers in Chemistry, **David A. Case,** Rutgers University. Address to be presented before the Division of Computers in Chemistry. March 24; Colorado Convention Center; Mile High Ballroom 1D; 3:45 PM.

ACS Award for Creative Advances in Environmental Science & Technology, sponsored by the ACS Division of Environmental Chemistry, *Environmental Science & Technology*, and *Environmental Science & Technology Letters*, Paul B. Shepson, Purdue University. Address to be presented before the Division of Environmental Chemistry at the fall ACS national meeting in Boston.

ACS Award for Creative Invention, sponsored by ACS Corporation Associates, **Jotham W. Coe,** Pfizer. Address to be presented before the Division of Organic Chemistry. March 24; Colorado Convention Center; Four Seasons Ballroom 1; 11:10 AM.

ACS Award for Creative Research & Applications of Iodine Chemistry, sponsored by SQM S.A., **Karl O. Christe,** University of Southern California. Address to be presented before the Division of Inorganic Chemistry. March 23; Colorado Convention Center; Bellco Theatre; 10:00 AM.

ACS Award for Creative Work in Fluorine Chemistry, sponsored by the Juhua Group Technology Center (China), **Véronique Gouverneur,** University of Oxford. Address to be presented before the biennial Winter Fluorine Conference in January 2015 and the Division of Fluorine Chemistry. March 22; Embassy Suites Denver– Downtown Covention Center; Silverton Ballroom; 4:20 PM.

ACS Award for Creative Work in Synthetic Organic Chemistry, sponsored by Aldrich Chemical Co., **F. Dean Toste,** University of California, Berkeley. Address to be presented before the Division of Organic Chemistry. March 24; Colorado Convention Center; Four Seasons Ballroom 2&3; 11:05 AM.

ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry, sponsored by Strem Chemicals, **Kim R. Dunbar,** Texas A&M University. Address to be presented before the Division

of Inorganic Chemistry. March 23; Colorado Convention Center; Bellco Theatre; 10:45 AM.

ACS Award for Encouraging Disadvantaged Students into Careers in the Chemical Sciences, sponsored by the Camille & Henry Dreyfus Foundation, **Catherine H. Middlecamp,** University of Wisconsin, Madison. Address to be presented before the Division of Chemical Education. March 23; Sheraton Denver Downtown Hotel; Columbine Room; 1:50 PM.

ACS Award for Encouraging Women into Careers in the Chemical Sciences, sponsored by the Camille & Henry Dreyfus Foundation, **E. Ann Nalley,** Cameron University. Address to be presented before the Division of Professional Relations and the ACS Women Chemists Committee. March 24; Hyatt Regency Denver– Colorado Convention Center; Capitol Ballroom 6; 11:15 AM.

ACS Award for Research at an Undergraduate Institution, sponsored by Research Corporation for Science Advancement, **George C. Shields,** Bucknell University. Address to be presented before the Division of Computers in Chemistry. March 24; Colorado Convention Center; Mile High Ballroom 1E; 4:30 PM.

ACS Award for Team Innovation, sponsored by ACS Corporation Associates, **Ryan Gaston, James R. Keenihan, Abhijit A. Namjoshi, Stephen Pisklak,** and **Jason A. Reese,** Dow Chemical. Address to be presented before the Division of Energy & Fuels. March 24; Colorado Convention Center; Mile High Ballroom 4A; 8:05 AM.

ACS Award in Analytical Chemistry, sponsored by Battelle Memorial Institute, **John R. Yates III,** Scripps Research Institute, La Jolla, Calif. Address to be presented before the Division of Analytical Chemistry at the fall ACS national meeting in Boston.

ACS Award in Applied Polymer Science, sponsored by Eastman Chemical, **Geoffrey W. Coates,** Cornell University. Address to be presented before the Division of Polymeric Materials: Science & Engineering. March 22; Sheraton Denver Downtown Hotel; Governor's Square 16; 4:45 PM.

ACS Award in Chromatography, sponsored by Sigma-Aldrich/ Supelco, **Milton T. W. Hearn,** Monash University, in Australia. Address to be presented before the Division of Analytical Chemistry. March 23; Embassy Suites Denver– Downtown Covention Center; Aspen Room A; 8:05 AM.

ACS Award in Colloid & Surface Chemistry, sponsored by Colgate-Palmolive Co., **Paul S. Weiss,** University of California, Los Angeles. Address to be presented before the Division of Colloid & Surface Chemistry. March 24; Marriott City Center Denver; Colorado F; 3:40 PM.

ACS Award in Industrial Chemistry, sponsored by the ACS Division of Business Development & Management and the ACS Division of Industrial & Engineering Chemistry, **Thomas J. Colacot,** Johnson Matthey. Address to be presented before the Division of Business Development & Management and the Division of Industrial & Engineering Chemistry. March 23; Embassy Suites Denver– Downtown Convention Center; Crystal Ballroom B/C; 4:40 PM.

ACS Award in Inorganic Chemistry, sponsored by Aldrich Chemical Co., **John T. Groves,** Princeton University. Address to be presented before the Division of Inorganic Chemistry. March 23; Colorado Convention Center; Bellco Theatre; 9:30 AM.

ACS Award in Organometallic Chemistry, sponsored by the Dow Chemical Co. Foundation, **William J. Evans,** University of California, Irvine. Address to be presented before the Division of Inorganic Chemistry. March 23; Colorado Convention Center; Bellco Theatre; 9:00 AM.

ACS Award in Polymer Chemistry, sponsored by ExxonMobil Chemical, **Nikos Hadjichristidis,** King Abdullah University of Science & Technology, Thuwal, Saudi Arabia. Address to be presented before the Division of Polymeric Materials: Science & Engineering. March 25; Sheraton Denver Downtown Hotel; Governor's Square 15; 5:00 PM.

ACS Award in Pure Chemistry, sponsored by Alpha Chi Sigma Fraternity and Alpha Chi Sigma Educational Foundation, **Adam E. Cohen,** Harvard University, Howard Hughes Medical Institute. Address to be presented before the Division of Physical Chemistry. March 24; Colorado Convention Center; Room 607; 10:05 AM.

ACS Award in Separations Science & Technology, sponsored by Waters Corp., **Richard D. Noble,** University of Colorado, Boulder. Address to be presented before the Division of Industrial & Engineering Chemistry. March 22; Embassy Suites Denver– Downtown Covention Center; Crystal Ballroom A; 2:00 PM.

ACS Award in the Chemistry of Materials, sponsored by E. I. du Pont de Nemours & Co., **Mark E. Thompson,** University of Southern California. Address to be presented before the Division of Inorganic Chemistry. March 23; Colorado Convention Center; Bellco Theatre; 11:45 AM.

ACS Award in Theoretical Chemistry, sponsored by ACS, **Mark S. Gordon,** Iowa State University. Address to be presented before the Division of Physical Chemistry. March 24; Colorado Convention Center; Room 607; 9:35 AM.

Award for Volunteer Service to the American Chemical Society, sponsored by ACS, **Cynthia K. Larive,** University of California, Riverside. Address to be presented before the ACS ChemLuminary Awards at the ACS fall national meeting in Boston.

Roger Adams Award in Organic Chemistry, sponsored by Organic Reactions Inc. and Organic Syntheses Inc., **Larry E. Overman,** University of California, Irvine. Address to be presented before the biennial National Organic Chemistry Symposium of the ACS national meeting in July at the University of Maryland.

Alfred Bader Award in Bioinorganic or Bioorganic Chemistry, sponsored by the Alfred R. Bader Fund, **Michael A. Marletta,** Scripps Research Institute, La Jolla, Calif. Address to be presented before the Division of Biological Chemistry. March 22; Hyatt Regency Denver– Colorado Convention Center; Capitol Ballroom 4; 7:00 PM.

Earle B. Barnes Award for Leadership in Chemical Research Management, sponsored by the Dow Chemical Co. Founda-

tion, **Christopher P. Austin,** National Institutes of Health. Address to be presented before the Division of Medicinal Chemistry. March 25; Colorado Convention Center; Mile High Ballroom 1A/1B; 4:15 PM.

Ronald Breslow Award for Achievement in Biomimetic Chemistry, sponsored by the Ronald Breslow Award Endowment, **Eric T. Kool,** Stanford University. Address to be presented before the Division of Organic Chemistry. March 22; Colorado Convention Center; Four Seasons Ballroom 2&3; 3:25 PM.

Herbert C. Brown Award for Creative Research in Synthetic Methods, sponsored by the Purdue Borane Research Fund and the Herbert C. Brown Award Endowment, **Gary A. Molander,** University of Pennsylvania. Address to be presented before the Division of Organic Chemistry. March 23; Colorado Convention Center; Four Seasons Ballroom 2&3; 4:10 PM.

James Bryant Conant Award in High School Chemistry Teaching, sponsored by Thermo Fisher Scientific, **Jenelle L. Ball,** Chico High School, California. Address to be presented before the Division of Chemical Education. March 22; Sheraton Denver Downtown Hotel; Silver Room; 1:00 PM.

Arthur C. Cope Award, sponsored by the Arthur C. Cope Fund, **Paul A. Wender,** Stanford University. Address to be presented before the Division of Organic Chemistry at the ACS fall national meeting in Boston.

Arthur C. Cope Scholar Awards, sponsored by the Arthur C. Cope Fund, **Michelle Chang,** University of California, Berkeley; **Debbie C. Crans,** Colorado State University, Fort Collins; **Antonio M. Echavarren,** Institute of Chemical Research of Catalonia, in Spain; **Ben L. Feringa,** University of Groningen, in the Netherlands; **Miguel A. Garcia-Garibay,** UC Los Angeles; **Neil K. Garg,** UC Los Angeles; **Chuan He,** University of Chicago; **Kenichiro Itami,** Nagoya University, in Japan; **Kenneth M. Nicholas,** University of Oklahoma; **Richmond Sarpong,** UC Berkeley. Address to be presented before the Division of Organic Chemistry at the ACS fall national meeting in Boston.

Elias J. Corey Award for Outstanding Original Contribution in Organic Synthesis by a Young Investigator, sponsored by the Pfizer Endowment Fund, **Jin-Quan Yu,** Scripps Research Institute, La Jolla, Calif. Address to be presented before the Division of Organic Chemistry. March 23; Colorado Convention Center; Four Seasons Ballroom 2&3; 11:00 AM.

F. Albert Cotton Award in Synthetic Inorganic Chemistry, sponsored by the F. Albert Cotton Endowment Fund, **Jaqueline L. Kiplinger,** Los Alamos National Laboratory. Address to be presented before the Division of Inorganic Chemistry. March 23; Colorado Convention Center; Bellco Theatre; 8:30 AM.

Peter Debye Award in Physical Chemistry, sponsored by E. I. du Pont de Nemours & Co., **Xiaoliang Sunney Xie,** Harvard University. Address to be presented before the Division of Physical Chemistry. March 24; Colorado Convention Center; Room 607; 8:05 AM.

Frank H. Field & Joe L. Franklin Award for Outstanding Achievement in Mass Spectrometry, sponsored by Waters Corp., **Hilkka I. Kenttämaa,** Purdue University. Address to be presented before the Division of Analytical Chemistry. March 25; Embassy Suites Denver–Downtown Convention Center; Aspen Room A; 3:40 PM.

Francis P. Garvan-John M. Olin Medal, sponsored by the Francis P. Garvan-John M. Olin Medal Endowment, **Angela K. Wilson,** University of North Texas. Address to be presented before the Division of Physical Chemistry. March 24; Colorado Convention Center; Room 607; 9:05 AM.

James T. Grady-James H. Stack Award for Interpreting Chemistry for the Public, sponsored by ACS, **Deborah L. Blum,** University of Wisconsin, Madison. Address to be presented before the ACS Office of Public Affairs. March 22; Colorado Convention Center; Four Seasons Ballroom 4; 12:20 PM.

Harry Gray Award for Creative Work in Inorganic Chemistry by a Young Investigator, sponsored by the Gray Award Endowment, **Emily A. Weiss,** Northwestern University. Address to be presented before the Division of Inorganic Chemistry. March 23; Colorado Convention Center; Bellco Theatre; 11:15 AM.

Ernest Guenther Award in the Chemistry of Natural Products, sponsored by Givaudan, **Thomas R. Hoye,** University of Minnesota. Address to be presented before the Division of Organic Chemistry. March 24; Colorado Convention Center; Four Seasons Ballroom 2&3; 3:45 PM.

Kathryn C. Hach Award for Entrepreneurial Success, sponsored by the Kathryn C. Hach Award Fund, **Terry L. Brewer,** Brewer Science Inc. Address to be presented before the Division of Small Chemical Businesses. March 23; Embassy Suites Denver– Colorado Convention Center; Cripple Creek Ballroom 2; 10:50 AM.

E. B. Hershberg Award for Important Discoveries in Medicinally Active Substances, sponsored by Merck Research Laboratories, **Ruth R. Wexler,** Bristol-Myers Squibb. Address to be presented before the Division of Medicinal Chemistry. March 24; Colorado Convention Center; Mile High Ballroom 2A/2B; 11:20 AM.

Joel Henry Hildebrand Award in the Theoretical & Experimental Chemistry of Liquids, sponsored by ExxonMobil Research & Engineering, **Mark Maroncelli**, Pennsylvania State University. Address to be presented before the Division of Physical Chemistry. March 24; Colorado Convention Center; Room 607; 8:35 AM.

E. V. Murphree Award in Industrial & Engineering Chemistry, sponsored by ExxonMobil Research & Engineering, **Joseph R. Zoeller,** Eastman Chemical. Address to be presented before the Division of Industrial & Engineering Chemistry. March 24; Embassy Suites Denver– Downtown Convention Center; Crystal Ballroom A; 4:00 PM.

Nakanishi Prize, sponsored by the Nakanishi Prize Endowment, **Fred W. McLafferty,** Cornell University. Address

to be presented before the Division of Analytical Chemistry. March 26; Embassy Suites Denver– Downtown Convention Center; Aspen Room A; 11:20 AM.

Nobel Laureate Signature Award for Graduate Education in Chemistry, sponsored by Avantor Performance Materials, **Denis Malyshev** (student), Synthorx, and **Floyd E. Romesberg** (preceptor), Scripps Research Institute, La Jolla, Calif. Address to be presented before the Division of Biological Chemistry. March 22; Hyatt Regency Denver– Colorado Convention Center; Capitol Ballroom 4; 8:30 AM & March 23; Hyatt Regency Denver– Colorado Convention Center; Capitol Ballroom 4; 10:45 AM.

James Flack Norris Award in Physical Organic Chemistry, sponsored by the ACS Northeastern Section, **Charles L. Perrin,** University of California, San Diego. Address to be presented before the Division of Organic Chemistry. March 24; Colorado Convention Center; Four Seasons Ballroom 1; 3:50 PM.

George A. Olah Award in Hydrocarbon or Petroleum Chemistry, sponsored by the George A. Olah Award Endowment, **Jingguang G. Chen,** Columbia University. Address to be presented before the Division of Catalysis Science & Technology. March 24; Colorado Convention Center; Room 108; 11:15 AM.

Charles Lathrop Parsons Award, sponsored by ACS, **Paul H. L. Walter,** Skidmore College. Address to be presented before the ACS Board of Directors. March 22; Hyatt Regency Denver– Colorado Convention Center; Centennial H; 1:30 PM.

George C. Pimentel Award in Chemical Education, sponsored by Cengage Learning and the ACS Division of Chemical Education, **I. Dwaine Eubanks,** Clemson University. Address to be presented before the Division of Chemical Education. March 24; Sheraton Denver Downtown Hotel; Columbine Room; 4:40 PM.

Priestley Medal, sponsored by ACS, **Jacqueline K. Barton,** California Institute of Technology. Address to be presented before the general meeting of the American Chemical Society, Tuesday, March 24, at the Sheraton Denver Downtown Hotel, BCEF Ballroom.

Glenn T. Seaborg Award for Nuclear Chemistry, sponsored by the ACS Division of Nuclear Chemistry & Technology, **Heino Nitsche** (deceased), University of California, Berkeley. Address to be presented before the Division of Nuclear Chemistry & Technology. March 22; 8:30 AM & March 23; Embassy Suites Denver– Downtown Convention Center; Crestone Ballroom A; 8:10 AM.

Gabor A. Somorjai Award for Creative Research in Catalysis, sponsored by the Gabor A. & Judith K. Somorjai Endowment Fund, **Maurice Brookhart,** University of North Carolina, Chapel Hill. Address to be presented before the Division of Catalysis Science & Technology. March 23; Colorado Convention Center; Room 207; 4:50 PM.

George & Christine Sosnovsky Award for Cancer Research, sponsored by the George & Christine Sosnovsky Endowment Fund, **Christopher P. Leamon,** Endocyte, Inc.; **Philip Low**, Purdue University; **Joseph A. Reddy** and **Iontcho Vlahov**, Endocyte, Inc. Address to be presented before the Division of Medicinal Chemistry. March 25; Colorado Convention Center; Mile High Ballroom 1A/1B; 2:45 PM & 3:30 PM.

E. Bright Wilson Award in Spectroscopy, sponsored by the ACS Division of Physical Chemistry, **R. J. Dwayne Miller,** Max Planck Institute for the Structure & Dynamics of Matter, Hamburg, Germany, and University of Toronto. Address to be presented before the Division of Physical Chemistry. March 24; Colorado Convention Center; Room 607; 11:25 AM.

Ahmed Zewail Award in Ultrafast Science & Technology, sponsored by the Ahmed Zewail Endowment Fund established by Newport Corp., **Shaul Mukamel,** University of California, Irvine. Address to be presented before the Division of Physical Chemistry. March 24; Colorado Convention Center; Room 607; 10:55 AM.

National Fresenius Award, sponsored by Phi Lambda Upsilon, the National Chemistry Honor Society, **Abigail G. Doyle,** Princeton University. Address to be presented before the Division of Organic Chemistry. March 25; Colorado Convention Center; Four Seasons Ballroom 2&3; 11:10 AM.

SOCIAL & TICKETED EVENTS

A VARIETY of social and special events will be held by event organizers during the meeting. Event participation is open to all interested registrants. View an updated listing of social and special events, including event locations, at www.acs.org/meetings.

The following social events require purchase of a ticket (event number in red), which can be purchased through Attendee Registration. Tickets will remain on sale until the evening prior to the event, if available. All tickets are sold on a first-come, first-served basis. Cancellations or refund requests must be made by March 8. No tickets will be refunded after that date.

FRIDAY, MARCH 20

CHAS Workshop: Laboratory Waste Management
7:30 AM to 5:30 PM
Embassy Suites Denver - Downtown Convention Center
Cripple Creek Ballroom 2

CHAS Workshop: Laboratory Safety
7:30 AM to 5:30 PM
Embassy Suites Denver - Downtown Convention Center
Cripple Creek Ballroom 1

SATURDAY, MARCH 21

CHAS Workshop: How to be a More Effective Chemical Hygiene Officer
7:30 AM to 5:30 PM
Embassy Suites Denver - Downtown Convention Center
Silverton Ballroom 1

CHAS Workshop: Reactivity Hazards: Laboratory Scale Recognition & Control
7:30 AM to 5:30 PM
Embassy Suites Denver - Downtown Convention Center
Cripple Creek Ballroom 1

CHAS Workshop: Job Hazard Analysis
7:30 AM to 5:30 PM
Embassy Suites Denver - Downtown Convention Center
Cripple Creek Ballroom 2

COACh Workshop: COACHing Strong Women in the Art of Strategic Persuasion – Jr. Faculty
8:30 AM to 5:00 PM
Grand Hyatt Denver
Mt. Harvard

COACh Workshop: COACHing Strong Women in the Art of Strategic Persuasion – Sr. Faculty
8:30 AM to 5:00 PM
Grand Hyatt Denver
Mt. Princeton

Presidential Outreach Event – Exploring Our World Through Chemistry
Kids and families can learn more about the fascinating world of chemistry through hands-on, age-appropriate activities at the Denver Zoo.
10:00 AM to 2:00 PM
Denver Zoo
2300 Steele Street
Denver

COACh Reception
5:00 PM to 7:00 PM
Grand Hyatt Denver
Maroon Peak

SUNDAY, MARCH 22

CHAS Executive Committee Meeting
8:00 AM to 12:00 PM
Embassy Suites Denver - Downtown Convention Center
Silverton Ballroom 3

CHED Workshop 1
8:00 AM – 12:00 PM
Sheraton Denver Downtown
Plaza Court 3

NRCC Certification Exams
8:00 AM to 12:00 PM
Embassy Suites Denver - Downtown Convention Center
Rexford Room

ACS Career Fair Workshops: Career Pathways II
8:30 AM to 5:00 PM
Colorado Convention Center, Room 604

ACS Career Fair Workshops: Career Workshop
8:30 AM to 5:00 PM
Colorado Convention Center, Room 701

Undergraduate Hospitality Center
8:00 AM to 5:00 PM
Sheraton Denver Downtown, Majestic Ballroom

Undergraduate Workshop: Making the Most of Your First National Meeting
9:00 AM to 9:45 AM
Sheraton Denver Downtown, Majestic Ballroom

Society Communication Workshop: Improv Training
Room 1/SE03/SE03A/$10
9:00 AM to 12:00 PM
The Curtis – a DoubleTree by Hilton, Dodgeball Room

Undergraduate Workshop: Graduate School Reality Check: Getting In
10:00 AM to 11:15 AM
Sheraton Denver Downtown, Plaza Ballroom AB

Harvey Mudd College Alumni & Friends Brunch
10:00 AM to 1:00 PM
Hotel Monaco – Panzano
1717 Champa Street
Denver

Chem Demo Exchange
11:00 AM to 12:30 PM
Colorado Convention Center, Hall B2

Undergraduate Workshop: Graduate School Reality Check: You're in-Now What?
11:15 AM to 12:30 PM
Sheraton Denver Downtown, Plaza Ballroom AB

SCHB/PROF Luncheon
11:30 AM to 1:30 PM
Embassy Suites Denver - Downtown Convention Center
Silverton Ballroom 2

ACS Board Open Session & Luncheon
(Open to staff and attendees)
12:00 PM to 1:00 PM
Colorado Convention Center, Four Seasons Ballroom 4

ACS Career Fair Workshops: Career Pathways I
12:00 PM to 5:30 PM
Colorado Convention Center, Room 602

ACS Career Fair Workshops: Career Pathways III
12:00 PM to 5:30 PM
Colorado Convention Center, Room 606

CHED High School/College Interface Luncheon/SE05/$0
(Included at no charge with high school teacher registration.)
12:00 PM to 1:00 PM
Sheraton Denver Downtown, Silver

Undergraduate Workshop: How to be a Successful ACS Student Chapter
1:00 PM to 2:30 PM
Sheraton Denver Downtown, Plaza Ballroom DE

Undergraduate Workshop: Networking Social with Graduate School and Research Opportunity Representatives
1:00 PM to 5:00 PM
Sheraton Denver Downtown, Grand Ballroom

CHED Workshop 2
1:00 PM to 5:00 PM
Sheraton Denver Downtown, Plaza Court 4

Charles Lathrop Parsons Award, sponsored by ACS
Paul H. L. Walter, Skidmore College
Address to be presented before the ACS Board of Directors
1:30 PM to 2:30 PM
Hyatt Regency Denver, Centennial H

Society Communication Workshop: Improv Training
Room 1/SE04/SE04A/$10
1:30 PM to 4:30 PM
The Curtis – a DoubleTree by Hilton, Keep Away Room

UPAB/CPC Strategy Cafe
(Co-sponsored by CPC)
2:45 PM to 4:00 PM
Hyatt Regency Denver at Colorado Convention Center
Centennial B

Undergraduate Workshop: Can You Have a Life and Career
(Co-sponsored by WCC)
2:45 PM to 4:00 PM
Sheraton Denver Downtown, Plaza Ballroom DE

Chemistry of Natural Resources Plenary
3:00 to 5:20 PM
Bellco Theater, Colorado Convention Center

Characterizing Structure and Chemistry of Functional Nanomaterials
Sponsor: FEI Company
3:30 PM to 6:00 PM
Colorado Convention Center, Room 103

Undergraduate Workshop: Improving Scientific Communication Skills
4:00 PM to 5:30 PM
Sheraton Denver Downtown, Plaza Ballroom AB

Undergraduate Workshop: Careers in Teaching Chemistry
4:00 PM to 5:30 PM
Sheraton Denver Downtown, Plaza Ballroom DE

Nominees Town Hall Meeting
4:30 to 5:30 PM
Hyatt Regency Denver at Colorado Convention Center
Centennial F/G

Grady-Stack Award Reception Honoring Deborah Blum
4:30 PM to 6:00 PM
Hyatt Regency Denver at Colorado Convention Center
Centennial A

ACS Diversity Reception
5:00 PM to 7:00 PM
Hyatt Regency Denver at Colorado Convention Center
Centennial C

PNNL 50th Anniversary Reception
5:00 PM to 6:30 PM
Colorado Convention Center, Room 203

University of Wisconsin – Madison Alumni & Friends
5:00 PM to 7:00 PM
Marriott City Center Denver
Penrose Ballroom 1

Chemistry at Illinois Alumni & Friends Reception
5:00 PM to 8:00 PM
Marriott City Center Denver
Penrose Ballroom 2

CHED Social Reception
5:30 PM to 7:00 PM
Colorado Convention Center, Room 207

International Welcome Reception/ SE06/$No Fee
5:30 PM to 7:30 PM
Hyatt Regency Denver at Colorado Convention Center
Centennial D

Research Corporation Reception in Honor of the Awardee for Research at an Undergraduate Institution
5:30 PM to 7:30 PM
Marriott City Center Denver, Colorado Ballroom E

COLL Social Hour/ Poster Session/Open Business Meeting
5:30 PM to 8:00 PM
Colorado Convention Center, Hall E

CINF Open Business Meeting
6:00 PM to 6:30 PM
Embassy Suites Denver - Downtown Convention Center
Silverton Ballroom 3

Mid Atlantic Councilor Caucus
6:00 PM to 7:00 PM
Hyatt Regency Denver at Colorado Convention Center
Mineral D

District IV Councilor Caucus
6:00 PM to 7:00 PM
Hyatt Regency Denver at Colorado Convention Center
Mineral E

District V Councilor Caucus
6:00 PM to 7:00 PM
Hyatt Regency Denver at Colorado Convention Center
Mineral F

District II Councilor Caucus
6:00 PM to 7:00 PM
Hyatt Regency Denver at Colorado Convention Center
Mineral C

District VI Councilor Caucus
6:00 PM to 7:00 PM
Hyatt Regency Denver at Colorado Convention Center
Mineral G

CELL & INOR Poster Session
6:00 to 8:00 PM
Colorado Convention Center, Hall C

Expo Attendee Welcome Reception
6:00 PM to 8:30 PM
Colorado Convention Center, Halls A/F

CINF Division Welcoming Reception
6:30 PM to 8:30 PM
Embassy Suites Denver - Downtown Convention Center
Silverton Ballroom 3

CHED Posters Session
7:00 PM to 9:00 PM
Colorado Convention Center, Hall C

BIOL Poster Session
8:15 PM to 9:45 PM
Colorado Convention Center, Hall B2

MEDI & COLL Poster Session
7:00 to 9:00 PM
Colorado Convention Center, Hall E

ACS Student Chapter Awards Ceremony
7:00 PM to 8:30 PM
Colorado Convention Center, Bellco Theater

ORGN Poster Session
8:00 to 10:00 PM
Colorado Convention Center, Hall C

Undergraduate Social
8:30 PM to 11:00 PM
Colorado Convention Center, Four Seasons Ballroom

MONDAY, MARCH 23

WCC Women in the Chemical Enterprise Breakfast/SE01/$40 (regular)/ SE02/$20 (student)
7:30 AM to 9:00 AM
(A limited number of student tickets are available. Students may purchase regular tickets if student tickets are sold out.)
Hyatt Regency Denver at Colorado Convention Center
Centennial E

CHED Workshop 3
8:00 AM to 12:00 PM
Sheraton Denver Downtown, Plaza Court 3

Undergraduate Hospitality Center
8:00 AM to 5:00 PM
Sheraton Denver Downtown, Majestic Ballroom

ACS Career Fair Workshop: Career Pathways I
8:30 AM to 5:30 PM
Colorado Convention Center, Room 602

ACS Career Fair Workshop: Career Pathways II
8:30 AM to 5:30 PM
Colorado Convention Center, Room 604

ACS Career Fair Workshop: Career Pathways III
8:30 AM to 5:30 PM

Colorado Convention Center, Room 606

ACS Exposition
9:00 AM to 5:00 PM
Colorado Convention Center, Halls A/F

University of Wisconsin – Milwaukee Workshop: Scale Interventions for Lecture & Laboratory
9:00 AM to 12:00 PM
Sheraton Denver Downtown, Plaza Court 2

Spectroscopy Simplified – How to Run a Research FT-IR
Sponsor: Thermo Scientific
9:30 AM to 12:00 PM
Colorado Convention Center, Exhibit Halls A/F, Exhibitor Workshop Room 1

Innovative Technologies to Engage Your Student's Learning Experience
Sponsor: McGraw Hill Higher Education,
9:30 AM to 12:00 PM
Colorado Convention Center, Room 103

Driving Separations Success.
Sponsor: Waters Corporation
9:30 AM to 12:00 PM
Colorado Convention Center, Exhibit Halls A/F, Exhibitor Workshop Room 2

Undergraduate Workshop: Networking 101
9:45 to 11:00 AM
Colorado Convention Center, Rooms 601/603

Undergraduate Workshop: Chemists Celebrate Earth Day (Co-sponsored by Committee on Community Activities)
9:45 to 11:45 AM
Sheraton Denver Downtown, Grand Ballroom II

Women Chemists of Color Social
10:00 AM to 11:30 AM
Hyatt Regency Denver at Colorado Convention Center, Mineral D

Undergraduate Poster Session
12:00 PM to 2:00 PM
Colorado Convention Center, Hall C

Committee on Minority Affairs Luncheon/SE07/$50
11:30 AM to 1:30 PM
Hyatt Regency Hotel at Colorado Convention Center
Centennial E

SCHB/HACH Luncheon
11:30 AM to 1:30 PM
Embassy Suites Denver - Downtown Convention Center
Silverton Ballroom 2

CHAL Luncheon/SE08/$40
12:00 PM to 1:30 PM
Embassy Suites Denver - Downtown Convention Center
Silverton Ballroom 3

SciFinder Training Session System with the Touch of a Button
Sponsor: CAS
12:30 PM – 3:00 PM
Colorado Convention Center, Exhibit Hall A/F, Exhibitor Workshop Room 1

Protecting Our Natural Resources with GC-MS and LC-MS from Thermo Fisher Scientific
Sponsor: Thermo Scientific
12:30 PM to 3:00 PM
Colorado Convention Center, Exhibit Halls A/F, Exhibitor Workshop Room 2

Innovative Technologies to Engage Your Student's Learning Experience
Sponsor: McGraw Hill Higher Education,
12:30 PM - 3:00 PM, Colorado Convention Center, Room 103

CHED Workshop 4
1:00 PM to 5:00 PM
Sheraton Denver Downtown, Plaza Court 4

College of Wooster Alumni,Students, Faculty & Friends of Helen Murray Free
2:30 to 4:30 PM
Colorado Convention Center, Room 701

CHED Younger Chemistry Education Scholars Social
3:00 PM to 5:00 PM
Sheraton Denver Downtown, Windows

WCC 'Just Cocktails'
3:30 PM to 4:30 PM
Hyatt Regency Denver at Colorado Convention Center
Capitol 5

Online Homework with Targeted Instructional Feedback Leads to Improved Student Learning Outcomes
Sponsor: Sapling Learning
3:30 PM to 6:00 PM,
Colorado Convention Center, Room 103

Undergraduate Speed Networking with Chemistry Professionals
3:45 PM to 5:15 PM
Hyatt Regency Denver at Colorado Convention Center
Centennial D/E

The Kavli Foundation Emerging Leader in Chemistry Lecture
4:00 PM to 5:05 PM
Colorado Convention Center, Bellco Theater

CHAL Reception
5:00 PM to 8:00 PM
Grand Hyatt Denver, Capital Peak A

The Fred Kavli Innovations in Chemistry Lecture
5:30 PM to 6:30 PM
Colorado Convention Center, Bellco Theater

Colorado State University Chemistry Alumni & Friends Reception
7:00 PM to 8:00 PM
CSU Denver Event Center
475 17th Street, Suite 200
Denver

Purdue Department of Chemistry Alumni Event/SE10/$10
7:00 PM to 8:30 PM
The Curtis – a DoubleTree by Hilton, Keep Away Room

ACS Graduate & Postdoctoral Scholars Reception
7:00 PM to 8:30 PM
Colorado Convention Center, Four Seasons Ballroom 4

2015 CARB Award Banquet/SE09/$60
7:00 PM to 10:00 PM
Appaloosa Grill – 535 16th Street, Denver

NUCL Social Hour
7:00 PM to 9:00 PM
Embassy Suites Denver - Downtown Convention Center
Silverton Ballroom 2

Sci-Mix Interdivisional Poster Session & Mixer
(Drink Ticket with registration)
8:00 PM to 10:00 PM
Colorado Convention Center, Hall C

TUESDAY, MARCH 24

Senior Chemists Breakfast/SE11/$20
7:30 AM to 9:30 AM
Hyatt Regency Denver at Colorado Convention Center
Centennial A/B

University of Minnesota Alumni & Friends Breakfast/SE20/$5
7:30 AM to 9:30 AM
Colorado Convention Center, Room 207

ACS Career Fair Workshop: Career Pathways I
8:30 AM to 5:30 PM
Colorado Convention Center, Room 602

ACS Career Fair Workshop: Career Pathways II
8:30 AM to 5:30 PM
Colorado Convention Center, Room 604

ACS Career Fair Workshop: Career Pathways III
8:30 AM to 5:30 PM
Colorado Convention Center, Room 606

ACS Exposition
9:00 AM to 5:00 PM
Colorado Convention Center, Halls A/F

SciFinder Training Session
Sponsor: CAS
9:30 AM to 12:00 PM
Colorado Convention Center, Exhibit Halls A/F, Exhibitor Workshop Room 1

A Survey of Accelerated Materials Research Using Raman Microscopy and Imaging
Sponsor: Thermo Scientific
9:30 AM to 12:00 PM
Colorado Convention Center, Exhibit Halls A/F, Exhibitor Workshop Room 2

Compact Mass Spectrometry: A Swiss Army Knife Approach to Chemistry Challenges
Sponsor: Advion
9:30 AM to 12:00 PM
Colorado Convention Center, Room 103

Alpha Chi Sigma Fraternity Luncheon
11:00 AM to 1:30 PM
Bubba Gump Shrimp Co.
1437 California St., Denver

Eli Lilly Poster Session
11:00 AM to 12:00 PM

Access meeting information and the On-site Program at **www.acs.org/denver2015**

Hyatt Regency Denver at Colorado Convention Center, Centennial A-C

CINF Division Luncheon/ SE12/$15 (students)/ SE12A $20 (regular)
12:00 PM to 1:30 PM
Embassy Suites Denver - Downtown Convention Center
Silverton Ballroom 3

WCC Eli Lilly Travel Award Poster Session & Luncheon/SE14/$50 (regular)/SE15/$25 (student)
12:00 PM to 1:30 PM
Hyatt Regency Denver at Colorado Convention Center
Centennial A – C

COLL Luncheon/SE13/$40
12:00 PM to 1:45 PM
Marriott City Center Denver, Penrose Ballroom 1

Committee on Environmental (CEI) Film Series — Thin Ice: The Inside Story of Climate Science
12:00 PM to 2:00 PM
Sheraton Denver Downtown, Grand Ballroom I

PerkinElmer Workshop: Nano FFF & SP-ICP-MS
12:00 PM to 6:00 PM
Colorado School of Mines
1500 Illinois Street, Golden, CO

Intelligent Real-Time Reaction Monitoring In The Fume Hood Using Benchtop NMR
Sponsor: Thermo Scientific
12:30 PM to 3:00 PM
Colorado Convention Center
Exhibit Halls A/F, Exhibitor Workshop Room 1

Analysis of Polymers by Vibrational Spectroscopy and Microscopy
Sponsor: Bruker
12:30 PM to 3:00 PM
Colorado Convention Center, Exhibit Halls A/F, Exhibitor Workshop Room 2

Advances in Atomic and Molecular Spectroscopy
Sponsor: Agilent Technologies
12:30 PM to 3:00 PM
Colorado Convention Center, Room 103

ENFL Poster Session
2:00 to 4:00 PM
Colorado Convention Center, Halls A/F

Chromatography and Mass Spectrometry Tips, Tricks, and Advanced Techniques
Sponsor: Agilent Technologies
3:30 PM to 6:00 PM
Colorado Convention Center, Room 103

AGFD Poster Session
3:30 to 5:30 PM
Colorado Convention Center, Hall C

Dow Energy Water Nexus Reception
4:00 PM to 5:00 PM
Colorado Convention Center, Room 207

Division Councilors & Division Officers Caucus
4:00 PM to 6:00 PM
Colorado Convention Center, Room 502

I&EC Poster Session
5:00 to 6:30 PM
Colorado Convention Center, Hall C

VUV Analytics ACS Reception
5:00 PM to 7:30 PM
Colorado Convention Center, Mile High Ballroom 4D

District I Councilor Caucus
5:30 PM to 7:00 PM
Hyatt Regency Denver at Colorado Convention Center
Mineral C

ENVR Reception/SE16/$10
6:00 PM to 7:30 PM
Wynkoop Brewing Company
1634 18th Street, Denver

PMSE/POLY Joint Poster Session
6:00 to 8:00 PM
Colorado Convention Center, Hall E

CATL & INOR Poster Session
6:00 to 8:00 PM
Colorado Convention Center, Hall C

COMP Poster and Award Session
6:00 to 8:30 PM
Colorado Convention Center, Hall B2

BIOT Poster Session
6:00 to 9:00 PM
Grand Hyatt Denver, Imperial Ballroom

AGFD Chair's Reception
6:00 PM to 8:00 PM
Embassy Suites Denver - Downtown Convention Center
Crystal Ballroom B

ACS National Awards Reception, Banquet Ceremony &General Meeting of the Society/SE17/$130
6:30 PM to 10:00 PM
Sheraton Denver Downtown Hotel, Plaza Ballroom BCEF

CELL Anselme Payen Award Banquet/SE18/$65
6:30 PM to 10:00 PM
Coohills Restaurant
1400 Wewatta St., Denver

CARB & ANYL Poster Session
7:00 to 9:00 PM
Colorado Convention Center, Hall C

ENFL Division Dinner/SE19/$65
7:30 PM to 9:00 PM
Maggiano's Little Italy
500 16th St., Ste 150, Denver

ORGN Poster Session
8:00 to 10:00 PM
Colorado Convention Center, Hall C

WEDNESDAY, MARCH 25

ACS Career Fair Workshop: Career Pathways I
8:30 AM to 5:30 PM
Colorado Convention Center, Room 602

ACS Career Fair Workshop: Career Pathways II
8:30 AM to 5:30 PM
Colorado Convention Center, Room 604

ACS Career Fair Workshop: Career Pathways III
8:30 AM to 5:30 PM
Colorado Convention Center, Room 606

New Developments in Isothermal Titration Calorimetry from MicroCal
Sponsor: Malvern Instruments
9:30 AM to 12:00 PM
Colorado Convention Center, Room 103

PerkinElmer Workshop: Nano FFF & SP-ICP-MS
12:00 PM to 6:00 PM
Colorado School of Mines
1500 Illinois Street, Golden, CO

Designing Inhibitors with MOE Structure-Based Drug Design Tools
Sponsor: Chemical Computing Group
3:30 PM to 6:00 PM
Colorado Convention Center, Room 103

POLY/PMSE Awards Reception
5:30 PM to 8:30 PM
Sheraton Denver Downtown Hotel, Plaza Ballroom A/B

PHYS & ENVR Poster Session
6:00 PM to 8:00 PM
Colorado Convention Center, Hall C

Joint MEDI & ORGN Poster Session
7:00 PM to 10:00 PM
Colorado Convention Center, Four Seasons Ballroom

STUDENT & TEACHER ACTIVITIES

EDUCATION-FOCUSED programs and specialty activities are being held for undergraduate students, graduate students, high school teachers, and chemical professionals. Explore these opportunities in depth at www.acs.org/denver2015.

UNDERGRADUATE PROGRAM. A vibrant program designed especially for undergraduate students has been planned by the Society Committee on Education's Undergraduate Programs Advisory Board. This educational and career-oriented program includes technical symposia and workshops on essential skills for employment in chemistry and success in graduate school. Eminent scientist Henry Kohlbrand from Dow Chemical will discuss sustainability from a research and industrial point of view.

SUNDAY, MARCH 22

Undergraduate Hospitality Center, 8:00 AM to 5:00 PM

Undergraduate Research Papers (Oral), (sponsored by CHED), 8:30 AM to 5:00 PM

Making the Most of Your First ACS Meeting, 9:00 to 9:45 AM

Graduate School Reality Check, Step I: Getting In, 10:00 to 11:15 AM

Graduate School Reality Check, Step II: You're In—Now What? 11:15 AM to 12:30 PM

Chem Demo Exchange, 11:00 AM to 12:30 PM

Networking Social with Graduate School Recruiters, 1:00 to 5:00 PM

Networking Social with Graduate School and Research Opportunity Representatives, 1:00 to 2:30 PM

Can You Have a Life and Career? (cosponsored by WCC), 2:45 to 4:00 PM

Workshop: Careers in Teaching Chemistry, 4:00 to 5:30 PM

Workshop: Improving Scientific Communication Skills, 4:00 to 5:30 PM

Student Chapter Awards Ceremony, 7:00 to 8:30 PM

Undergraduate Social, 8:30 to 11:00 PM

MONDAY, MARCH 23

Undergraduate Hospitality Center, 8:00 AM to 5:00 PM

Undergraduate Research Papers (Oral), (sponsored by CHED), 8:30 AM to 5:00 PM

Technical Symposium: NREL Biomass to Fuel & Products (cosponsored by CELL and ENFL), 9:00 to 10:30 AM

Workshop: Networking 101, 9:45 to 11:00 AM

Workshop: Chemists Celebrate Earth Day, (cosponsored by CCA) 9:45 to 11:45 AM

Technical Symposium: Forensic Toxicology of Marijuana (cosponsored by BMGT and TOXI), 10:45 to 11:45 AM

Undergraduate Research Poster Session (sponsored by CHED), noon to 2:00 PM

Eminent Scientist Lecture: "Sustainability in the 21st Century: Optimizing Complex Interdependent Systems," with Henry Kohlbrand, Dow Chemical (cosponsored by CELL and ENFL), 2:30 to 3:30 PM

Speed Networking with Chemistry Professionals, 3:45 to 5:15 PM

Sci-Mix/Successful Student Chapter Posters, 8:00 to 10:00 PM

TUESDAY, MARCH 24

Chemistry and the Environment Film Series, noon to 2:00 PM.

All events are sponsored or cosponsored by the Society Committee on Education's Undergraduate Programs Advisory Board. Chair: Matthew Mio, University of Detroit, Mercy. Program Chair: Daniel Swartling, Tennessee Technological University, Cookeville. For more information, go to www.acs.org/undergrad or contact the ACS Undergraduate Programs Office at 800-227-5558 ext. 4480.

GRADUATE & POSTDOCTORAL SCHOLARS OFFICE. With support from the Graduate Education Advisory Board, this office provides and promotes programs and resources for graduate students and postdoctoral scholars. All events will take place at the Colorado Convention Center.

MONDAY, MARCH 23

Graduate & Postdoctoral Scholars Reception, 7:00 to 8:30 PM.

For more information about this reception and other ACS programs offered to graduate students and postdocs, visit www.acs.org/grad or contact the ACS Graduate & Postdoctoral Scholars Office at GradEd@acs.org.

HIGH SCHOOL TEACHERS PROGRAM. The Division of Chemical Education and the ACS Education Division are sponsoring the High School Teachers Program. It will include presentations and demonstrations on current pedagogies, resources, and activities that align with the meeting theme, "Chemistry of Natural Resources." The High School/College Interface Luncheon will bring together educators from all grade levels with the goal of facilitating an exchange of ideas and networking among teachers.

High school teachers can register for the program directly through Attendee Registration; the special registration fee includes course materials, lunch, access to the full ACS meeting (Sunday through Thursday), and entry to the exposition (Sunday to Tuesday). Attendees can track professional development (based on clock hours) for sessions attended at the ACS national meeting. Upon completion and submission of ACS forms, participants will be mailed a certificate documenting their participation in the conference.

SUNDAY, MARCH 22

High School Teachers Program, 8:30 AM to 4:30 PM; Sheraton Denver Downtown Hotel.

For more information, contact the Office of High School Chemistry at education@acs.org or call 800-227-5558 ext. 2105.

WORKSHOPS

THE FOLLOWING workshops require a separate registration process and/or entry fee to participate in the event, as indicated in this listing. Participation is open to all interested registrants.

Division of Chemical Health & Safety (CHAS)-sponsored workshop fees (unless otherwise indicated). CHAS member: $300; non-CHAS member: $350. Registration is required for all CHAS workshops. Register online at dchas.org.

Laboratory Waste Management. Friday, March 20, 7:30 AM to 5:30 PM, Embassy Suites Denver, Cripple Creek Ballroom 2. ***Sponsored by CHAS.*** Presenter: Russ Phifer. This comprehensive course will identify various regulatory requirements that apply to laboratories that generate hazardous waste, as well as provide insight on the options for on-site management and off-site disposal. The focus will include discussion of recycling/reclamation techniques, economical handling of waste, and liability issues.

Laboratory Safety. Friday, March 20, 7:30 AM to 5:30 PM, Embassy Suites Denver, Cripple Creek Ballroom 1. ***Sponsored by CHAS.*** Presenters: James Kaufman and/or Jack Breazeale. This presentation on laboratory safety by the Laboratory Safety Institute has been attended by thousands of safety professionals. With experience in both industrial and academic laboratories, the presenters take a real-world approach to safety issues in the lab. Interactive demonstrations will teach you about issues such as creative wiring in the lab and how to work with administrators to keep a safe working environment. This workshop provides an excellent forum to speak openly about safety in the workplace.

How To Be a More Effective Chemical Hygiene Officer. Saturday, March 21, 7:30 AM to 5:30 PM, Embassy Suites Denver, Silverton Ballroom 1. ***Sponsored by CHAS.*** Presenter: Russ Phifer. Take a close look at the Chemical Hygiene Officer (CHO) position, and prepare at the same time for the CHO Certification exam, which will be held on Sunday, March 22, through the National Registry of Certified Chemists. This workshop will focus on what you do and how you can do it better. The course covers all of the content areas of the certification exam and includes a sample test in the same format as the real one. Request an application packet for the CHO Certification examination at www.acs.org/dchas.

Chemical Reactivity Hazards: Laboratory-Scale Recognition & Control. Saturday, March 21, 7:30 AM to 5:30 PM, Embassy Suites Denver, Cripple Creek Ballroom 1. ***Sponsored by CHAS.*** Presenter: Neal Langerman. This workshop addresses the risks associated with chemicals such as *t*-butyllithium and processes such as thermal distillations. The objective is to provide participants with the knowledge and skills to screen processes for potential hazards, to recognize when reactive hazards are present, and to implement appropriate controls to reduce the risk of an incident associated with the hazards. Workshop attendees will review case studies of actual incidents and do screening examples to understand the screening and recognition process. Group discussions of control methods will allow participants to share their experiences and to evaluate methods for controlling reactivity risks. Preregistration for this event is required.

Job Hazard Analysis Workshop. Saturday, March 21, 7:30 AM to 5:30 PM, Embassy Suites Denver, Cripple Creek Ballroom 2. ***Sponsored by CHAS.***

249th American Chemical Society National Meeting & Exposition

www.acs.org/denver2015
#acsdenver

CHEMISTRY OF NATURAL RESOURCES

Denver, CO • March 22–26, 2015

Organized by Robert S. Weber, Senior Scientist and Operating Officer, Institute for Integrated Catalysis, Pacific Northwest National Laboratory; Associate Editor, Energy & Fuels.

Chemistry of Natural Resources Plenary Session

Colorado Convention Center, Bellco Theater

Sunday, March 22, 2015, 3:00 – 5:00 PM

Dr. Carolyn A. Koh

Department of Chemical & Biological Engineering
Colorado School of Mines

Fundamentals of Gas Hydrates and Their Role in Energy Transportation and Storage

Understanding of the economic and environmental components of gas hydrates.

Dr. Peter Kareiva

Chief Scientist for The Nature Conservancy

Water in the Anthropocene: Too Much, Too Little, Too Dirty

Understanding water as it relates to science, policy and financial incentives.

Dr. Paul F. Bryan

Department of Chemical & Biomolecular Engineering
University of California, Berkeley

The Four Horsemen of the Advanced Biofuels Apocalypse – Sustainability, Technology, Profitability, and Politics

Understanding Advanced Biofuels (ABF), government funding, their technology, and development.

Kavli Foundation Lecture Series

The Kavli Foundation Lecture Series promotes groundbreaking discovery and public understanding of the world's mounting challenges and how chemistry can provide solutions.

The American Chemical Society gratefully acknowledges The Kavli Foundation's generous support for The Fred Kavli Innovations in Chemistry Lecture and The Kavli Foundation Emerging Leader in Chemistry Lecture.

The Kavli Foundation Emerging Leader in Chemistry Lecture

Colorado Convention Center, Bellco Theatre

Monday, March 23, 2015
4:00 – 5:00 PM

Dr. Theodore Betley

Professor of Chemistry and Chemical Biology
Harvard University

Radical Frontiers in Catalysis

Understanding of factors contributing to the promotion of productive small molecule activation processes.

The Fred Kavli Innovations in Chemistry Lecture

Colorado Convention Center, Bellco Theatre

Monday, March 23, 2015
5:30 – 6:30 PM

Dr. Laura L. Kiessling

Steenbock Professor of Chemistry
Laurens Anderson Professor of Biochemistry
University of Wisconsin-Madison

Us Versus Them: Distinguishing Humans from Microbes with Carbohydrates

How the features of carbohydrates on the cell surfaces differ between mammals and microbes.

ACS Chemistry for Life®

Theme-Related Technical Symposia & Programming

Full Program information is available online at www.acs.org/denver2015

Division of Agricultural and Food Chemistry (AGFD)

- Water Our Most Critical Resource

Division of Biochemical Technology (BIOT)

- Biofuels & Sustainable Energy: Engineering Microbes to Utilize Next Generation Feedstocks
- Biofuels & Sustainable Energy: Development of Sustainable & Low-cost Feedstocks for Biofuels & Bioproducts
- Biofuels & Sustainable Energy: Biomass Pretreatment & Hydrolysis
- Biofuels & Sustainable Energy: Biological Fuel & Energy Production Using Photons & Electrons
- Downstream Processing: Downstream Processing for the Biobased Industries

Division of Catalysis Science & Technology (CATL)

- Catalytic Materials and Technologies for Upgrading of COx and Natural Gas
- Electrocatalysis and Photocatalysis
- Theoretical and Experimental Synergies at the Frontiers of Renewable Energy Catalysis
- Novel Catalytic Materials for Renewable Fuels/Chemicals

Division of Cellulose & Renewable Materials (CELL)

- Advances in Lignocellulosic Materials and Chemistry: A Tribute to W.G. Glasser
- Cellulose Dissolution: New Solvents and Mechanisms
- Cellulose in Solid State and Solution: Structure, Chemistry and Reaction Mechanisms: Anselme Payen Award Symposium in Honor of Thomas Rosenau
- Conservation Science of Cellulosic Materials: Recent Developments
- Frontiers in Glycoscience
- Functional Lignocellulosics and Nanotechnology
- CELL General Posters
- Lignin Biosynthesis, Characterization and Modifications
- Renewable Resources for Materials and Energy: Recent Research and Developments in Ibero-America
- Application of Computational Chemistry to Biomass Chemistry and Utilization
- Research on Renewable Materials: US and EU Perspectives
- Smart and Responsive Composites from Renewable Building Blocks

Division of Chemical Education (CHED)

- Citizens First: Communicating Climate Science to the Public

Division of Chemical Information (CINF)

- Information Sources on Natural Resources

Division of Computers in Chemistry (COMP)

- Computational Pyrolysis & Upgrading of Bio-Oils

Division of Energy & Fuels (ENFL)

- 12th International Symposium on Heavy Oil Upgrading, Production & Characterization
- Catalysis for Un-conventional Energy Sources
- Enhanced Extraction & Utilization of Unconventional Energy Sources: Hydrofracking, EOR and Novel Approaches
- Nanomaterials for Solar Energy Conversion & Storage

Division of Environmental Chemistry (ENVR)

- Advances in Analytical Chemistry for Discovering Emerging Contaminants in the Natural Environment
- Assessing Toxicity of Environmental Contaminants
- Bioavailability and Biogeochemical Interactions Affecting Remediation of Hazardous Substances in the Environment
- Biogenically Enhanced Recovery and Bioremediation in Fossil Fuel Reservoirs
- Chemical Processes at Environmental Interfaces
- Chemistry in the Marine Boundary Layer
- Environmental Chemistry and Health Impacts of Fine and Ultrafine Particulate Matter
- Environmental Chemistry: Pedagogical Models and Practices

Division of Environmental Chemistry (ENVR)

- Environmental Reactivity of Organic Micropollutants and their Transformation Products in Receiving Waters
- Microalgae: A Renewable Energy Source and a Sustainable Solution for the Environment
- Modern Analytical Approaches for the Characterization of Natural Organic Matter in the Environment
- Hydraulic Fracturing Impacts on Water, Soil and Air Quality
- Solutions to Metals Contamination of Water
- Surface Physicochemical Processes in Engineered and Natural Systems
- Trace Materials in Air, Soil, and Water
- Water Recycling in Domestic Use, Energy Extraction, and Agricultural Use
- Water Sustainability in Oil and Gas Exploration: Treatment Issues

Division of Geochemistry (GEOC)

- Coupled Cycling of Biogeochemical Critical Elements and Contaminants
- Geochemistry and Reactive Transport in Nano-Pore Geomaterials
- How Do Geologic Processes Drive the Structure and Function of Aquatic and Riparian Ecosystems?
- Iron Oxides: Formation, Structure, Reactivity and Applications
- Molecular-Scale Processes Controlling Reactivity at Mineral-Water Interfaces
- Understanding the Geochemical Interactions of Organic Compounds in the Subsurface

Division of the History of Chemistry (HIST)

- Chemical Technology in Antiquity

Division of Industrial & Engineering Chemistry (I&EC)

- Uranium in Seawater

Division of Inorganic Chemistry (INOR)

- Earth-Abundant Materials for Sustainable Hydrogen Production and Storage
- Environmental and Energy-Related Inorganic Chemistry
- Chemistry of the Energy Water Nexus: Focus on Fracking

Multidisciplinary Program Planning Group (MPPG)

- Chemistry of Natural Resources Plenary
- The Kavli Foundation Lecture Series
- Nanoscience and Nanotechnology of Natural Resources

Division of Organic Chemistry (ORGN)

- Chemistry of Natural Resources

Division of Small Chemical Businesses (SCHB)

- Water is the Next Oil: Small Businesses Percolating to the Top

Society Committee on Education (SOCED)

- Sustainability in the 21st Century: Optimizing Complex Interdependent Systems
- Biomass to Fuel and Products
- Forensic Toxicology of Marijuana

Presenter: Sammuela Sigmann. Job Hazard Analysis (JHA) is one method to consider hazards associated with lab research and guide the control of those hazards. JHA can assist a researcher in uncovering potential hazards in synthesis, instrumental studies, physical manipulations, and more. Identified hazards can then be mitigated or eliminated. In this workshop, participants will learn the basic principles, required elements, and format of the common JHA. Examples of completed tools, such as nitric acid disgestion of metal samples, cryogenic work, and HPLC with THF/DCM/Water, will be utilized to examine the technique. Each participant will create a ready-to-use JHA based on some task applicable to their lab, so attendees should come with a specific idea of a chemical or process they would like to investigate.

COACh-the-COACHes. Saturday, March 21, 8:30 AM to 5:00 PM, Grand Hyatt Denver, Mt. Wilson. ***Sponsored by COACh.*** This workshop is designed for women faculty who are interested in being trained to offer COACh workshops to graduate students and postdoctoral associates at their academic institution and/or regional professional meetings and who have attended COACh workshops in the past. This session will be a refresher of the negotiation and communication skills taught in faculty COACh workshops and also cover interview techniques, CV and website building, and effective scientific presentation. Participants will need to attend the full day of activities from 8:00 AM to 4:00 PM. The traditional COACh reception will follow the day's activities. Participants must have attended a COACh workshop previously. Apply at: coach.uoregon.edu. For more information, contact Priscilla Lewis: coach@uoregon.edu; phone: 541-346-0116. Fee: Free.

COACHing Strong Women in the Art of Strategic Persuasion—Senior Faculty. Saturday, March 21, 8:30 AM to 4:30 PM, Grand Hyatt Denver, Mt. Princeton.

COACHing Strong Women in the Art of Strategic Persuasion—Junior Faculty. Saturday, March 21, 8:30 AM to 5:00 PM, Grand Hyatt Denver, Mt. Havard. ***Sponsored by COACh.*** These workshops will help professional women be more effective when leading or participating in discussions, meetings, or group negotiations. Learn about strategic rather than reactive behaviors and effective speaking voices while tuning out stress and tension, which will allow you to be heard. The workshops combine presentation, leadership training, and faculty development in an interactive format that encourages highly personal learning. Topics include communication styles effective for women; projecting confidence and credibility through voice, image, and body language; dealing with difficult conversations; and using powerful rather than weak words. Preregistration is required; visit coach.uoregon.edu. For more information, contact Priscilla Lewis at coach@uoregon.edu or (541) 346-0116. Fee: Free.

Improv Training. Sunday, March 22. 9:00 AM to noon and 1:30 to 4:00 PM, The Curtis Hotel, Training Rooms 1 thru 4. ***Sponsored by Society Communications.*** $10 per session. Catalyze your communication skills at this improv sesson with trainers from the acclaimed Alan Alda Center for Communicating Science. You'll learn how to connect with the audience and create effective delivery that will captivate and inform. Whether you're new to communicating or want to pick up some new tips, this workshop is for you.

"Scale Interventions for Lecture & Laboratory" Monday, March 23, 9:00 AM to noon, Sheraton Denver Downtown, Plaza Court 2. ***Sponsored by the University of Wisconsin, Milwaukee.*** According to AAAS and NRC, an important component of a student's science literacy is scale and concepts relating to scale. We have created both lecture and laboratory instructional materials, which can easily be incorporated into any general chemistry course, on the subject of scale and the skills related to understanding quantity within chemistry concepts. At this workshop, we will present the continuing results of our experiments on scale, share how we measure the scale knowledge of our students, introduce and describe several of the activities we have incorporated into our curriculum, and provide resources for educators who wish to incorporate our activities into their own courses.

Nano FFF & SP-ICP-MS. Tuesday, March 24, noon to 6:00 PM, and Wednesday, March 25, noon to 6:00 PM, Colorado School of Mines. ***Sponsored by PerkinElmer and Colorado School of Mine***s. This hands-on workshop will allow researchers to learn from the experts on single particle-ICP-MS and field flow fractionation (FFF) technologies in a working laboratory setup. Learn more and register at acsnanoworkshop.eventbrite.com.

ACS CAREER NAVIGATOR

ACS CAREER NAVIGATOR is your home for career services, leadership development, in-person and online professional education, and market intelligence resources. We offer comprehensive and easily identified tools that allow you to achieve your career goals by landing a new job, finding a new career path, or comparing your salary and viewing current trends in the field to make better-informed decisions.

Opportunities abound at the ACS national meeting in Denver to take advantage of the many resources and tools the ACS Career Navigator offers to help you succeed in the global scientific enterprise. Are you ready to get started? Refresh skills and branch into new areas of emerging science and

advanced applications with a short course or with an ACS Leadership Development Systems course that gives you skills that can be immediately applied in school or on the job. If you are an ACS member, stop by the ACS Career Fair in the convention center and speak to a personal career consultant. In short, whatever your career goals, the ACS Career Navigator is here to help you achieve and exceed them. We'll see you in Denver.

ACS PROFESSIONAL EDUCATIONAL SHORT COURSES

REFRESH YOUR SKILLS or branch into new areas with an ACS short course. Held in conjunction with ACS national meeting in Denver, courses taught by our expert instructors give you the opportunity to stay on top of new technology, growing trends in the industry, and the skills you need to advance your career. ACS member, advanced registration, and group discount rates are available. A course fee and registration separate from the national meeting are required. For more information on ACS Short Courses in Denver or to register, visit www.proed.acs.org/denver. If you have questions, call 202-872-4508, fax 202-872-6336, or e-mail proed@acs.org.

NRCC CERTIFICATION EXAMS

WHAT: Certification exams of the National Registry of Certified Chemists
WHEN: Sunday, March 22, 8:00 AM to noon
WHERE: Embassy Suites Denver Downtown, Rexford Room
HOW: Advance registration and completion (with approval) of application must be done before March 2. Applications may be downloaded from www.nrcc6.org.

ANALYTICAL

1-D & 2-D NMR Spectroscopy: Structure Determination of Small-Molecule Organic Compounds, March 20–21

Practical & Applied Gas Chromatography, March 20–21

COMPUTERS/STATISTICS/ ENGINEERING

Experimental Design for Productivity & Quality in Research & Development, March 20–22

ORGANIC/PHYSICAL CHEMISTRY

1-D & 2-D NMR Spectroscopy: Structure Determination of Small-Molecule Organic Compounds, March 20–21

Dispersions in Liquids: Suspensions, Emulsions & Foams, March 22–23

POLYMER CHEMISTRY

Polymer Science & Technology, March 20–21

Surfactants & Block Copolymers, March 22

PROFESSIONAL DEVELOPMENT

Effective Supervision of Scientists & the Technical Staff, March 20–21

Effective Technical Writing, March 20–21

Project Management for Technical Professionals, March 20–21

Write Your Own Patent Applications, half-day course, March 22

Intellectual Property Strategies for Technical Professions, half-day course, March 22

REGULATORY/ENVIRONMENTAL

Methods Development, Validation Procedures & Regulatory Compliance Issues, March 20–21

2015 LEADERSHIP DEVELOPMENT SYSTEM COURSE OFFERINGS

WHETHER YOU are a manager, experienced professional, or new to the workforce, we invite you to attend an ACS Leadership Development Systems course held at the ACS national meeting. The following four-hour facilitated courses require a fee of $150 each for ACS members and $300 each for nonmembers. Register for these courses when you register for the meeting. For more information and full course descriptions, visit www.acs.org/leadershipdevelopment.

Leading Without Authority. Sunday, March 22, 1:00 to 5:00 PM. We've all been in situations where we are leading projects or teams and need to direct everyone's effort but don't have complete control of the project's resources, including the people. Learn practical tools to help you gain cooperation without formal authority and motivate your colleagues or volunteers.

Engaging Colleagues in Dialogue. Monday, March 23, 8:00 AM to noon. Communication underlies everything we do and has a direct correlation to the success of a project. It is one of the most important skills we need to be successful in school, on the job, and in volunteer situations. This hands-on, interactive course helps develop your one-to-one communication skills. You will learn how to improve both sides of the communication exchange: first, working to understand how to better communicate your messages and second, working on listening and acknowledging others' messages. You will have an opportunity to assess your own communication skills through conversations with colleagues.

Coaching & Feedback. Monday, March 23, 1:00 to 5:00 PM. Most managers will tell you that coaching is important, and yet they avoid actually coaching anyone. Some who try find it harder than expected. The reason? Most managers lack the skills and confidence to be effective in the coaching role. But good coaching is central to your success as a leader and to the success of your team members, employees, and volunteers on ACS committees. Coaching will help you increase performance, expand your team's capabilities, and improve relationships and morale. This course provides leaders with a proven process, practical tools, and a hands-on opportunity to coach volunteers and employees more effectively.

Strategic Planning. Tuesday, March 24, 8:00 AM to noon. Of the various responsibilities of a leader, none is more critical than setting goals and direction. Whether you are leading at the level of a local section, division, or national committee, your members look to you to establish the strategic plan that will guide the group's activities. This course will help you improve your understanding of the planning process while giving you the opportunity to start developing a strategic plan that aligns with the ACS Board of Directors' strategic goals.

Fostering Innovation. Tuesday, March 24, 1:00 to 5:00 PM. Keeping pace in an environment of constant change requires continuous innovation. Whether you are in a nonprofit, business, or academic environment, the ability to contribute to the creation of new ideas, new processes, and new approaches is a key to personal and organizational success. But coming up with new ideas is challenging, and few of us have the tools and skills. This course teaches a proven, systematic process to generate ideas. You will gain understanding and tools to help you tap into your own innovation style and learn how to stimulate innovative thinking among team members and colleagues.

ACS CAREER FAIR ON-SITE AND ONLINE

JOB SEEKERS, are you looking to jumpstart your job search or enhance your professional development? **Employers,** are you looking to hire scientists and engineers? Then you need to attend the ACS Career Fair, open Sunday, March 22, 9:00 AM to 5:30 PM; Monday, March 23; 9:00 AM to 5:00 PM; Tuesday, March 24, 9:00 AM to 5:00 PM; and Wednesday, March 25, 8:30 AM to 12:30 PM (workshops only) in the Colorado Convention Center. The Virtual Career Fair will be held on March 23 and 24, 8:00 AM to 6:00 PM (central time). Whether on-site or online, the career fair is the place where the best talent and the best employers in chemistry meet.

LET ACS HELP YOU REACH YOUR CAREER GOALS. ACS will help you prepare for your next career move by providing resources that make it possible to map out your personal job search strategy, strengthen your résumé, and build your interview skills, all with the support of career consultants. During the career fair, participants can take full advantage of the following:

- Networking opportunities
- Résumé reviews
- One-on-one career consulting
- Interview practice and skills building
- More than 30 career-related workshops
- Keynote speakers presented live and via webcast
- Request live and virtual interviews

On-site job seekers must be ACS members, be registered for the national meeting, and complete career fair registration at www.acs.org/careers (pick up a career fair registration badge beginning Sunday, March 22).

GET ONLINE AND OPTIMIZE YOUR JOB SEARCH! The virtual portion of the ACS Career Fair eliminates geographical barriers, enabling job seekers and employers to connect with each other from their home, from their office, or from the dedicated computer stations at the meeting. Interviews and informal discussions will take place in virtual booths via text or video chat. Additionally, job seekers can schedule time with ACS career consultants for one-on-one consultations and attend live events via webcast. In today's tough economy, it makes good sense to enhance your job search by participating fully in both the on-site and online ACS career fairs. Register at www.acs.org/vcf.

Please note: We cannot guarantee that you will secure interviews at the ACS Career Fair or online at the Virtual Career Fair. Interviewing is strictly contingent on the availability of positions and the credentials and qualifications that employers are seeking.

EMPLOYERS—ACS HAS THE TALENT YOU ARE LOOKING FOR. Leading employers around the world trust and depend on ACS to provide them with the talent they need to innovate and excel. At our last event, approximately 1,000 global job seekers—from recent grads to seasoned professionals—met with on-site and virtual recruiters seeking to fill positions in all facets of chemistry, pharmaceuticals, and biotechnology.

The ACS Careers Jobs Database can help manage your employer account, post jobs, search for qualified candidates, and schedule career fair interviews. Moreover, participating in the ACS Career Fair enables you to accomplish the following:

- Connect with top talent via on-site and online interviews.
- Screen candidates and make appointments in advance.
- Find the personnel your company needs to thrive, from entry- to executive-level positions.
- Meet qualified candidates informally via on-site and online networking forums.
- Extend your presence for 30 days after the career fair via the ACS jobs database and your virtual booth.

ACS CAREER FAIR AND THE ACS EXPOSITION TEAM HAVE JOINED FORCES. Employers can purchase booth space inside the exposition hall, enabling your company to maximize its ability to showcase products and services and connect with job seekers. Employers can sign up for the ACS Career Fair Recruiters Row package by contacting Garretta Rollins at 800-227-5558 ext. 6209 (U.S./Canada only), 202-872-6209 (international), or e-mail g_rollins@acs.org.

Employers will receive an e-mail confirmation and must visit the ACS Career Fair Information Booth in the Convention Center to pick up their blue badge. For more information, please visit www.acs.org/careerfair. You can also contact Garretta Rollins at 800-227-5558 ext. 6209 (U.S./Canada only), 202-872-6209 (international), or e-mail g_rollins@acs.org.

ONE-ON-ONE CAREER CONSULTING. Individual 30-minute appointments with career consultants are available both on-site and online. These consults can help you strengthen your résumé, improve your interviewing skills, and design a job search or comprehensive professional growth

strategy. Please bring a copy of your résumé or CV to all appointments. All one-on-one on-site career consulting sessions will take place in the Résumé Review/Mock Interview area. Sign-up begins at 9:00 AM on Sunday, March 22, on a first-come, first-served basis.

CAREER AND PROFESSIONAL DEVELOPMENT WORKSHOPS. More than 30 career-related workshops will help you with everything from your résumé to optimizing job performance to how to ace an interview. Workshop times are subject to change. Please consult the online workshop schedule at www.acs.org/careerfair for location.

SUNDAY, MARCH 22

Acing the Interview, 8:30 AM to 12:30 PM; 1:30 to 5:30 PM

New Technology To Find Jobs & Manage Your Career, 10:00 to 11:30 AM

Soups to Nuts of Entrepreneurship, noon to 1:30 PM

Foreign National Scientist Obtaining a Job in the U.S., 1:30 to 3:00 PM

Finding your Path, 1:30 to 5:30 PM

Working in Industry, 1:30 to 5:30 PM

Writing Excellent Proposals, 3:30 to 5:00 PM

MONDAY, MARCH 23

Working for Yourself, 8:30 AM to 12:30 PM

Working in Government, 8:30 AM to 12:30 PM

Working in Higher Education, 8:30 AM to 12:30 PM

Acing the Interview, 1:30 to 5:30 PM

Finding Your Path, 1:30 to 5:30 PM

Working in Industry, 1:30 to 5:30 PM

TUESDAY, MARCH 24

Acing the Interview, 8:30 AM to 12:30 PM

Finding Your Path, 8:30 AM to 12:30 PM

Working in Industry, 8:30 AM to 12:30 PM

Working in Government, 1:30 to 5:30 PM

Working in Higher Education, 1:30 to 5:30 PM

Working for Yourself, 1:30 to 5:30 PM

WEDNESDAY, MARCH 25

Acing the Interview, 8:30 AM to 12:30 PM

Finding Your Path, 8:30 AM to 12:30 PM

Working in Industry, 8:30 AM to 12:30 PM

EXPOSITION

SEE WHAT'S NEW INSIDE THE EXPOSITION. Visit the ACS National Exposition at the Colorado Convention Center, Halls A/F, from Sunday, March 22, through Tuesday, March 24. The show hours will be Sunday, 6:00 to 8:30 PM, and Monday and Tuesday, 9:00 AM to 5:00 PM.

Companies will showcase services, instruments, books, computer hardware, scientific software, and an array of chromatographic, lab, and safety equipment. Technical personnel will be available to give demonstrations, answer questions, and discuss your specific needs and interests. You can also visit the ACS Career Fair Recruiters Row inside the exposition where employers will showcase their products and services. Also, join us at the ACS Booth in the middle of the exposition floor where ACS staff units will present the many benefits, services, products, and merchandise offered by ACS.

Online Exposition. The Online Exposition is a component within the Exhibitor Directory that enables attendees to view videos, press releases, brochures, and flyers of participating exhibitors. Access the Online Exposition at www.acs.org/denver2015 to learn more about exhibiting companies and to download product information that meets your needs.

Free Exhibitor Workshops. Free workshops will be hosted by exhibitors on the exposition floor and in private rooms inside the Colorado Convention Center. These workshops will introduce new products and services, build skills with specific tools and techniques, and highlight innovative applications that may improve your productivity. Exhibitor workshop registration is now available at www.acs.org/denver2015.

Presentations, Prizes & Special Events. Visit the Daily Prize Raffle area on Sunday through Tuesday for a chance to win a prize. Then automatically be entered in our special prize giveaway Sunday through Tuesday after being scanned by 20 exhibitors. Don't forget to join us on Sunday from 6:00 to 8:30 PM for the Attendee Welcome Reception. Also, visit the Networking Lounge inside the exposition for poster sessions and to connect with colleagues.

Internet & Technology. Use free Internet access and leave messages for one another at the Meeting Mail terminals located inside the Networking Lounge. Enjoy free Wi-Fi service at designated areas in the Colorado Convention Center.

Admission Requirements & Expo-Only Registration. Exposition admission is complimentary for all national meeting registrants; however, you are required to wear your badge. Individuals who want to visit the exhibits without registering for the technical component of the national meeting can obtain an expo-only badge for $60. Students with school identification can obtain an expo-only badge for $30. Registration can be handled online, by mail, or in person at ACS Attendee Registration, Colorado Convention Center, Lobby A/F.

EXHIBITOR SPONSORED WORKSHOPS

EXHIBITING COMPANIES will host free education sessions for attendees that will introduce new products and services, build skills with specific tools and techniques, and highlight innovative applications for existing instrumentation. Visit www.acs.org/denver2015 to register for workshops.

SUNDAY, MARCH 22

Characterizing Structure & Chemistry of Functional Nanomaterials. ***Sponsor:*** FEI Co., 3:30 to 6:00 PM, Colorado Convention Center, Room 103. The development of technologies for efficient resource usage, energy conversion, transportation, or environmental protection relies heavily on advances in developing new and improved nanostructures and nanomaterials. Characterization on length scales down to subnanometer and focus on structural evolution with the link to the nanomaterial's performance play a crucial role in obtaining detailed knowledge about the relationship between structure, unique property, and function in these systems of reduced dimensions. In this workshop, we will profile use cases in catalyst development and polymer engineering and take you through different electron microscopy characterization methods and routines that will enable you to get more insights into structure and chemistry of your functional nanomaterials.

MONDAY, MARCH 23

Spectroscopy Simplified: How To Run a Research FTIR. ***Sponsor:*** Thermo Scientific, 9:30 AM to noon, Colorado Convention Center, Exhibit Halls A/F, Exhibitor Workshop Room 1. This workshop will demonstrate the power and flexibility of the Thermo Scientific Nicolet iS50 FTIR spectrometer system and its unique capabilities to simplify its operation down to the touch of a button. The Nicolet iS50 research FTIR spectrometer system was designed to meet the needs of a dynamic research laboratory, providing the capability to configure the system with a number of spectral ranges, beam paths, and accessories. With this versatility, most users will assume the software will then be complicated to operate, requiring dedicated operators to maximize the productivity of the system. Yet with the unique touchpoint operation of the iS50, most system capabilities can be used with just the push of a button.

Innovative Technologies To Engage Your Student's Learning Experience. ***Sponsor:*** McGraw-Hill Higher Education, 9:30 AM to noon, Colorado Convention Center, Room 103.

9:30 AM— ***Flipping the Classroom.*** Presenter: Danaè Quirk Dorr, Minnesota State University, Mankato. The flipped classroom model has become one of the hottest topics in the higher education space in recent years thanks to a real improvement in technology and an overall change in scholarly mind-set. Learn about strategies and tools available to help you flip.

11:00 AM— ***Teaching Organic Chemistry in the 21st Century: The Rewards of Technology.*** Presenters: Philip A. Janowicz, California State University, Fullerton, and Michael Lewis, St. Louis University. Organic chemistry students are performing better using online homework. Janowicz will talk more in depth about his study on ACS exam scores for students who completed online homework versus those who completed written homework. Lewis will discuss how to flip an organic chemistry classroom.

Driving Separations Success. ***Sponsor:*** Waters Corp., 9:30 AM to noon, Colorado Convention Center, Exhibit Halls A/F, Exhibitor Workshop Room 2.

9:45 AM— ***Part 1: Meeting the Challenges of Food Quality Control Using UPLC.*** Focusing on UPLC for food testing using optical (non-MS) detectors and MS detectors, this session will cover applications including quality and nutrition: sweeteners, soft drink additives, amino acids, dairy (whey proteins, sugars, vitamins, preservatives), and safety: PAHs and aflatoxins.

11:00 AM— ***Part 2: Driving LC Success: Technical Seminar: Systematic Protocol.*** This technical seminar will teach a systematic protocol that can alleviate challenges in method development. This generic protocol will lead you toward successful and robust chromatographic separations.

SciFinder Training Session System with the Touch of a Button. ***Sponsor:*** CAS, 12:30 to 3:00 PM, Colorado Convention Center, Exhibit Halls A/F, Exhibitor Workshop Room 1. Come learn about how SciFinder brings data to your lab, as well as details and tips for refining and using your results with powerful features such as relevance ranking, experimental procedure information, and SciPlanner.

Protecting Our Natural Resources with GC/MS & LC/MS from Thermo Fisher Scientific. ***Sponsor***: Thermo Scientific, 12:30 to 3:00 PM, Colorado Convention Center, Exhibit Halls A/F, Exhibitor Workshop Room 2. Our natural resources are a precious commodity, and keeping them clean and pure can be a daunting task. This workshop will highlight two technologies from Thermo Fisher that are used to help ensure that the world is a cleaner, safer, and healthier place.

12:30 PM— Learn how you can access the next evolution of GC/MS/MS technology to achieve more at faster speeds. This means more capacity, more information, more compounds, and more results per unit time for higher levels of productivity and efficiency in analytical workflows.

1:45 PM— Significant advances in triple-quadrupole technologies have resulted in two state-of-the-art, next-generation instruments. See details of the groundbreaking advances "from an ion's view," and hear about transformations in your targeted quantitative workflows.

Innovative Technologies To Engage Your Students' Learning Experience. ***Sponsor:*** McGraw-Hill Higher Education, 12:30 to 3:00 PM, Colorado Convention Center, Room 103.

1:00 PM— ***Moving Beyond Traditional Homework with ALEKS.*** Presenter: Tracy McGill, Emory University. Are you struggling to find which adaptive online learning system is right for you? McGill will share why ALEKS for Chemistry is the perfect choice for her and her students. ALEKS uses adaptive questioning to quickly and accurately determine exactly what a student knows and doesn't know in a course.

2:30 PM— ***Revolutionizing the Lab Experience: LearnSmart Labs for General Chemistry.*** Presenters: Deborah Exton, University of Oregon, and Jimmy Reeves, University of North Carolina, Wilmington. LearnSmart Labs provides an adaptive, interactive, and personal-

ized lab experience that encourages students to theorize and experiment like scientists do. In the realistic LearnSmart Labs environment, students can practice the scientific method, safely develop and test hypotheses, and think critically about their findings before ever setting foot in a physical lab.

Online Homework with Targeted Instructional Feedback Leads to Improved Student Learning Outcomes. ***Sponsor:*** Sapling Learning, 3:30 to 6:00 PM, Colorado Convention Center, Room 103. Sapling Learning delivers online homework that engages students and empowers educators. Still, homework is only one piece of a full course solution. In this workshop, hear about the various ways that Sapling Learning provides or enables educators to select the best course materials for them. Whether you use a printed textbook, lecture slides, open educational resources, or some combination thereof, you can learn how to provide a unified learning experience for your students. You'll learn about the suite of options from Sapling Learning and our partners and how to incorporate them into a seamless learning experience. Our discussion will include used textbooks and instructor-generated content, and you will hear from faculty who are successfully implementing these varied resources. Each attendee will receive a free copy of the eTextbook "Chemistry," by John Olmsted and Greg Williams.

TUESDAY, MARCH 24

SciFinder Training Session System with the Touch of a Button. ***Sponsor:*** CAS, 9:30 AM to noon, Colorado Convention Center, Exhibit Halls A/F, Exhibitor Workshop Room 1. See SciFinder Training for Monday, 12:30 to 3:00 PM.

A Survey of Accelerated Materials Research Using Raman Microscopy & Imaging. ***Sponsor:*** Thermo Scientific, 9:30 AM to noon, Colorado Convention Center, Exhibit Halls A/F, Exhibitor Workshop Room 2. Raman spectroscopy is essential to competitive academic research in many applied scientific disciplines, including materials science, life sciences research, and chemical and biological engineering. Advances in Raman microscopy and imaging have made the technique accessible to a wide variety of researchers, regardless of expertise or field of study.

A case study showing how one leading research university has transformed its approach to research, including obtaining results faster, increasing the number and quality of publications, and improving funding successes, will be shared. See examples of current research using advanced Raman microscopy, which has been designed for greater accessibility and significantly enhanced productivity than previously possible.

Analysis of Polymers by Vibrational Spectroscopy & Microscopy. ***Sponsor:*** Bruker, 12:30 to 3:00 PM, Colorado Convention Center, Exhibit Halls A/F, Exhibitor Workshop Room 2. The latest advances in FTIR and Raman instrumentation and applications will be reviewed, with a thorough discussion of the following topics: polymers identification and classification, additives and contaminations, fast reaction monitoring, defects analysis using vibrational microscopy, chemical imaging, and depth profiling.

Compact Mass Spectrometry: A Swiss Army Knife Approach to Chemistry Challenges. ***Sponsor:*** Advion, 9:30 AM to noon, Colorado Convention Center, Room 103. Chemists ask many questions that each require a different approach. Advion offers a compact mass spectrometer that couples to any range of techniques to provide chemists with a complete answer to the questions they ask. This workshop will show examples using a direct sample analysis approach valuable to reaction monitoring, compound identification, natural product analysis, and food safety. Attendees who wish to learn more about an affordable mass spectrometer that does not require sample prep, has an easy user interface (including TLC and Direct Sample Analysis Probe), and offers answers in less than a minute are encouraged to attend.

Intelligent Real-Time Reaction Monitoring in the Fume Hood Using Benchtop NMR. ***Sponsor:*** Thermo Scientific, 12:30 to 3:00 PM, Colorado Convention Center, Exhibit Halls A/F, Exhibitor Workshop Room 1. Teaching reaction kinetics, thermodynamics, and pathways is a standard part of any undergraduate organic chemistry curriculum. Having hands-on access for the student to measure reaction mechanics in real time in the laboratory may give them insights not previously available in the classroom alone. This workshop will demonstrate a new capability of the Thermo Scientific picoSpin NMR spectrometer to intelligently measure reaction pathways from a reactor in real time. Watch products form in increasing concentration, right next to the apparatus.

Advances in Atomic & Molecular Spectroscopy. ***Sponsor:*** Agilent Technologies, 12:30 to 3:00 PM, Colorado Convention Center, Room 103. Recent innovation in FTIR, atomic spectroscopy, and elemental analysis (including ICP/MS) technology has allowed for more sensitive, accurate, and flexible measurements of organic and inorganic materials. This workshop will focus on two main techniques, FTIR and atomic spectroscopy/spectrometry.

12:30 to 1:30 PM— ***Innovations in FTIR: How New Technology Is Changing Infrared Analysis***

1:45 to 2:45 PM— ***New Elemental Analysis Solutions and Advanced Applications Using Next-Generation MP/AES, ICP/OES, ICP/MS, and ICP/QQQ***

Chromatography & Mass Spectrometry Tips, Tricks & Advanced Techniques. ***Sponsor:*** Agilent Technologies, 3:30 to 6:00 PM, Colorado Convention Center, Room 103. Stay up to date on the latest technology and applications using HPLC, LC/MS, GC, and GC/MS. This workshop will focus on implementing 2-D HPLC and other advanced HPLC techniques in your lab, ion mobility qTOF for advanced molecular analysis, and improving GC/MS capability using some new tips and tricks.

3:30 to 4:15 PM— ***Demystifying 2-D HPLC: Techniques You Can Use Tomorrow***

4:15 to 5:00 PM— ***Advantages of Ion Mobility qTOF for Characterization of Large Biological Molecules***

5:00 to 5:45 PM— ***GC/MS: Advanced Topics and Helpful Tips & Tricks***

WEDNESDAY, MARCH 25

New Developments in Isothermal Titration Calorimetry from MicroCal. ***Sponsor:*** Malvern Instruments, 9:30 AM to noon, Colorado Convention Center, Room 103. Measurements and characterization of binding interactions between proteins and low-molecular-weight (LMW) ligands are fundamental for drug discovery. Among the most recognized challenges in characterizing binding interactions are the need to (1) accurately assess a wide span of binding affinities (K_d) and (2) accurately rank and characterize LMW ligands based on affinity, mechanism of action, and energetics of interaction. Reliable interpretation of binding data can be complicated by the presence of inactive protein fractions or inaccurate assessment of protein concentration. Assessment of these data can be further hampered by inherent uncertainty in the concentration of compound stocks. This uncertainty results from inaccurate measurement, limited solubility, or potential chemical heterogeneity of the compounds, such as the presence of enantiomers and isomers. Isothermal titration calorimetry (ITC) directly measures heat released or absorbed in a binding event, providing means for studying protein-small molecule interactions in solution without the need for labeling or immobilization.

This workshop will present the new developments in highly sensitive MicroCal ITC instrumentation and data analysis. We will discuss the improvements in data quality that enable increased confidence when analyzing challenging data with low heats when sample is precious or low concentrations are required to accurately quantitate low-nanomolar-affinity interactions. We will present the new developments in MicroCal ITC software that allow automated data analysis, minimizing analysis time and user subjectivity in assessing data quality.

Designing Inhibitors with MOE Structure-Based Drug Design Tools. ***Sponsor:*** Chemical Computing Group, 3:30 to 6 PM, Colorado Convention Center, Room 103. This workshop covers the application of in silico structure-based drug design (SBDD) tools for the rational design of Tarceva-based EGFR kinase inhibitors. Starting with raw PDB protein-ligand 3-D structures, all the steps required to initiate and advance an SBDD study are covered: preparing PDB structures for modeling, binding pocket visualization, protein-ligand contact analysis, and the use of SAR for in situ modeling (modifying and optimizing ligands in the binding pocket) to design new compounds. Advanced topics such as pharmacophore query generation, protein-ligand docking, protein alignments for binding-site comparison, and in situ combinatorial synthesis will also be covered.

ACS EXCELLENCE

Spring 2015

The ACS Publications Magazine

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Questions or comments for the Editor
j_graham@acs.org

Meet the new Editors-in-Chief

Thomas F. Hofmann, Ph.D.

JOURNAL OF AGRICULTURAL AND FOOD CHEMISTRY

Thomas F. Hofmann is professor and chair of Food Chemistry and Molecular Sensory Science and Vice President for Research & Innovation at the Technische Universität München in Germany.

Q: How does research in your journal's area affect people's everyday lives?

TH: Primary agriculture and food production are facing limiting factors for key resources like land, water, energy, and inputs. On the other hand, the world faces a double burden of undernutrition and obesity. New procedures and products originating from sustainable agriculture to be used as food, feed, green biomaterials, or biofuel as well as new energy-efficient engineering solutions designed to deliver affordable, safe, nutritional, and tasty foods and beverages will have to be developed to better serve the coming needs of society and to create economic impact along the value chain. New knowledge on the chemistry and biochemistry involved is key for success and that's why the *Journal of Agricultural and Food Chemistry* is on the spot! I will do my very best to maintain *JAFC* as the premier journal publishing these scientific innovations.

Go to pubs.acs.org/jafc for more information

Sharon Hammes-Schiffer, Ph.D.

CHEMICAL REVIEWS

Sharon Hammes-Schiffer is Swanlund Professor of Chemistry at the University of Illinois at Urbana-Champaign.

Q: What are you most looking forward to about this new position?

SHS: I am looking forward to enhancing the topical diversity, visibility, and educational impact, while also retaining the comprehensive and accessible nature of the review articles in this journal. I plan to pursue several initiatives that will help achieve these goals. From a personal perspective, I am looking forward to interacting with chemists from all disciplines and learning about exciting new areas of chemistry.

Q: How does research in your journal's area affect people's everyday lives?

SHS: This journal serves as an educational tool for students and scientists entering new fields. The articles have both short-term and long-term impact. My own son, who is a junior chemical engineering major at Princeton, just told me that he used a *Chemical Review* from 1997 as the main source for his presentation on phage display for a course. My students have also used *Chemical Reviews* to learn about new topics.

Go to pubs.acs.org/cr for more information

Paul J. Chirk, Ph.D.

ORGANOMETALLICS

Paul J. Chirik is the Edward S. Sanford Professor at Princeton University.

Q: How did you first become interested in your journal's area of focus?

PC: My interest in organometallic chemistry began during my freshman year at Virginia Tech. I was fascinated by Professor Joseph Merola's work on iridium compounds that seemed to be able to activate and break some of the strongest bonds in chemistry. Despite my inexperience, he allowed me to work in his lab, gave me my own project, and the rest is history.

Q: What are you most looking forward to about this new position?

PC: I am looking forward to having *Organometallics* serve as the focal point for a vibrant, diverse, and collegial community. As Editor-in-Chief, I hope to meet new organometallic chemists from around the globe, learn about their science, and capture the best of it in the journal. I am also looking forward to maintaining the great tradition of excellence established by my predecessors, Dietmar Seyferth and John Gladysz.

Q: What's something about your journal's focus area that most people don't understand?

PC: Most people don't realize that organometallic compounds operate "behind the scenes" to enable our quality of life. In addition to helping discover new medicines, organometallic compounds are responsible for making plastics that are ubiquitous in our daily lives, serve as precursors for electronics, and are even found in the body, such as vitamin B-12.

Go to pubs.acs.org/organometallics for more information

David L. Sedlak, Ph.D.

Environmental Science & Technology

Environmental Science & Technology LETTERS

David L. Sedlak is Malozemoff Professor in Mineral Engineering, Co-director of Berkeley Water Center, and Director of the Institute for Environmental Science and Engineering at the University of California, Berkeley.

Q: How did you first become interested in your journal's area of focus?

DS: I first became aware of the field of environmental chemistry as I became interested in addressing problems associated with contamination of groundwater and soil at hazardous waste sites. As my awareness of the topic grew, I became aware of *Environmental Science & Technology* and its role as the leading journal in the field. *ES&T* was the journal where I published my first paper in 1990 and I have been publishing there ever since.

Q: What are your goals as Editor-in-Chief?

DS: We are proud of our reputation as the most read and most cited journal covering the environment. But bibliographic indicators will not save the planet. As Editor-in-Chief, I will work with the editorial team to leverage our standing as the leading environmental research journal to become the authoritative voice for advancing solutions to the environmental challenges facing society.

Go to pubs.acs.org/est and pubs.acs.org/estlett for more information

Kai Rossen, Ph.D.

Organic Process Research & Development

Kai Rossen is group leader at Sanofi in Germany.

Q: How does research in your journal's area affect people's everyday lives?

KR: *Organic Process Research & Development* has a very concrete and relevant influence on the lives of people. Unfortunately, this is seen only when things go wrong and an accident at a plant injures people or waste from a plant is polluting the environment. This context makes it very difficult to have a discussion with the public, as a perception is created that is simply wrong: the physician is saving the life of the patient, while the chemist in the pharmaceutical industry that gives the physicians the tools to do so is not seen as positive. I am aware that technical journals speak primarily to a closed audience and don't tend to reach the public, but it is important to tell the positive and relevant examples of our work to get the message of our positive contributions for the well-being of mankind across also to the general public.

Q: What are your goals as Editor-in-Chief?

KR: This is very simple: try to convey the excitement for the type of work ongoing in the pharmaceutical, agrochemical, flavor and fragrance, and fine-chemical and chemical industries, and its relationship with exciting new developments in various fields of science and engineering, to a new and younger generation of scientists from all over the world.

Go to pubs.acs.org/oprd for more information

Francoise Winnik, Ph.D.

Langmuir

Francoise Winnik is Professor, Faculty of Pharmacy and Department of Chemistry at the University of Montreal, Canada; Principal Investigator, International Center for Materials Nanoarchitectonics at the National Institute for Materials Science in Tsukuba, Japan; and Finnish Distinguished Professor at the University of Helsinki, Finland.

Q: What are your goals as Editor-in-Chief?

DS: *Langmuir* is a multidisciplinary journal. Its authors and readers are spread throughout the world. It is time to strengthen the ties of *Langmuir* with its readers, particularly outside North America, by increasing the number of non-North American members of the Board and by selecting Senior Editors worldwide. In addition, it is important to recognize outstanding research as it appears in *Langmuir*. Immediacy is key. Instant recognition by a journal creates a permanent bond between the author and the journal. Excellent articles published in *Langmuir* must be promoted among ACS readers and beyond. A related objective, probably even more important, will be to reach out to scientists who are no longer submitting their manuscripts to *Langmuir* and to those who have not published in *Langmuir* so far.

Go to pubs.acs.org/langmuir for more information

New Editor-in-Chief looks ahead

Bibiana Campos-Seijo seeks to make the best even better

When asked what challenges she faces for the upcoming year, Bibiana Campos-Seijo, Ph.D., admits that it will be a challenge to improve upon the number-one magazine in the chemical sciences. "We're already doing excellent work," she says. "But we can do even better."

Campos-Seijo took the helm in December 2014 as editor-in-chief of *Chemical & Engineering News* (C&EN) and VP of C&EN Media Group. She plans to continue and expand the magazine's outreach in the year ahead.

First, she's hoping to lead the redesign of both the print and web magazine. Both projects are in their early stages. She also wants to improve C&EN's impact on social media and develop more high-quality multimedia content, including videos, webinars, and Google Hangouts.

"Researchers depend on us to curate science from around the world and deliver it in an intuitive, user-friendly way."

—Dr. Bibiana Campos-Seijo

She wants to create a cohesive "family of products" among all C&EN content. "Many of our members read our print magazine, but don't know about our digital channels," Campos-Seijo says. "Others may read us online, but don't know how our different products relate. We want to take a close look at all of our content and make sure products complement one another and share a consistent look and feel."

Campos-Seijo also champions what she calls an "entrepreneurial" approach to journalism. "Researchers depend on us to curate science from around the world and deliver it in an intuitive, user-friendly way." This means listening and adapting not just to the types of content readers want to see, but how they want it presented. A priority for the website redesign will be to implement responsive design, which will ensure a good experience across all devices.

All of this is part of C&EN's "digital-first" approach designed to keep readers informed on the latest research news. Although C&EN's print magazine is published weekly, new content hits its website (cen.acs.org) every day. Campos-Seijo says that while there's no typical day at C&EN, daily editorial meetings are what make always-current web content possible.

Bibiana Campos -Seijo, Ph.D.

Making chemistry more accessible to all

Campos-Seijo also recognizes that she is leading C&EN at a critical time. Science awareness and interest are entering the mainstream in new and surprising ways: go to a restaurant, and you might see a dish inspired by molecular gastronomy. Turn on the television and watch entertainers like Bill Nye the Science Guy make science fun. Actor Alan Alda is helping researchers better communicate their work to the public. And traveling science festivals and workshops are teaching kids about everything from climate science to computer code.

"In other words, science is quite hot right now," Campos-Seijo says.

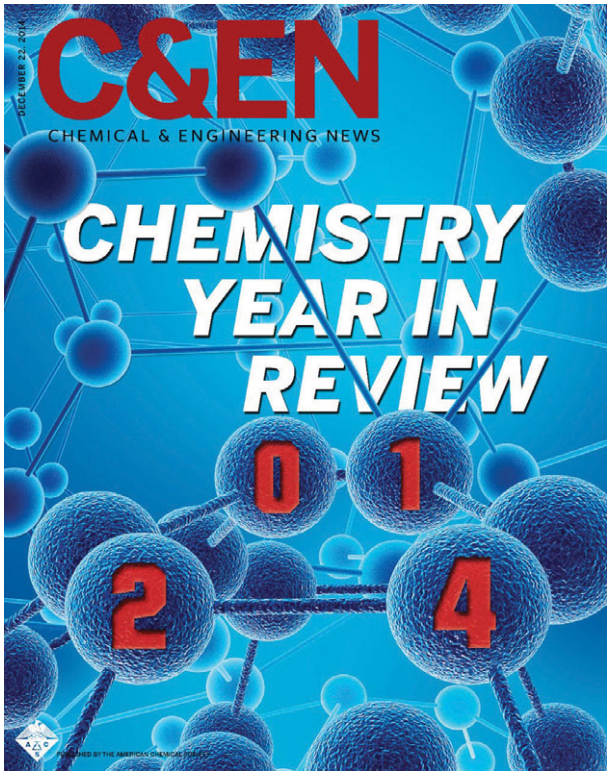
Quenching the world's thirst for science is part of C&EN's mission, and part of her role as editor-in-chief, Campos-Seijo says. "It's important for us to communicate not just with ACS members, but also nonmembers. We're ambassadors for

"Chemistry and science are not geographically limited. They're universal."

—Dr. Bibiana Campos-Seijo

“Working for C&EN is an ambition I’ve had for a long time.”

—Dr. Bibiana Campos-Seijo



chemistry. So we need to be out there talking to people and finding out what issues people care about and what support they need.”

To wit: in 2014, C&EN produced “From the SCENEs,” weekly stories based on papers in ACS journals; a webinar on the chemistry of cocktails; and the “Chemistry in Pictures” blog, all designed to reach people with different levels of chemistry knowledge. While C&EN’s primary audience remains the chemical sciences community, new and upcoming initiatives are designed for accessibility and broad appeal.

A perfect fit

Campos-Seijo (who goes by “Bibi”) was raised in Galicia, in northwest Spain. She holds a B.Sc. in chemistry from Spain’s University of Santiago de Compostela and England’s Manchester Metropolitan University and a Ph.D. in chemistry from Manchester Metropolitan.

She worked as a technical editor and in scientific publishing after earning her degree. In 2009, she became editor of *Chemistry World*, the magazine of the UK’s Royal Society of Chemistry. “This was sort of a natural progression for me,” Campos-Seijo says. “I’ve known and admired ACS and C&EN for many years. Working for C&EN is an ambition I’ve had for a long time.”

Campos-Seijo replaces Rudy Baum. Her experience makes her a perfect match for the new position. Having worked for both societies and commercial organizations, she understands the importance of building relationships with members and advertisers alike.

Campos-Seijo, along with her husband and children, relocated to ACS’ Washington, D.C. headquarters in November 2014. One challenge the family faces in their new home, she says, has been the switch to American English. “I think it was George Bernard Shaw who said that the U.S. and Britain are two countries divided by a common language,” she laughs. “We’re definitely finding that to be true.”

“It’s important for us to communicate not just with ACS members, but also nonmembers. We’re ambassadors for chemistry.”

—Dr. Bibiana Campos-Seijo

The language of science

While words and phrases may differ, Campos-Seijo points out that the issues facing scientists across countries and cultures are more alike than different.

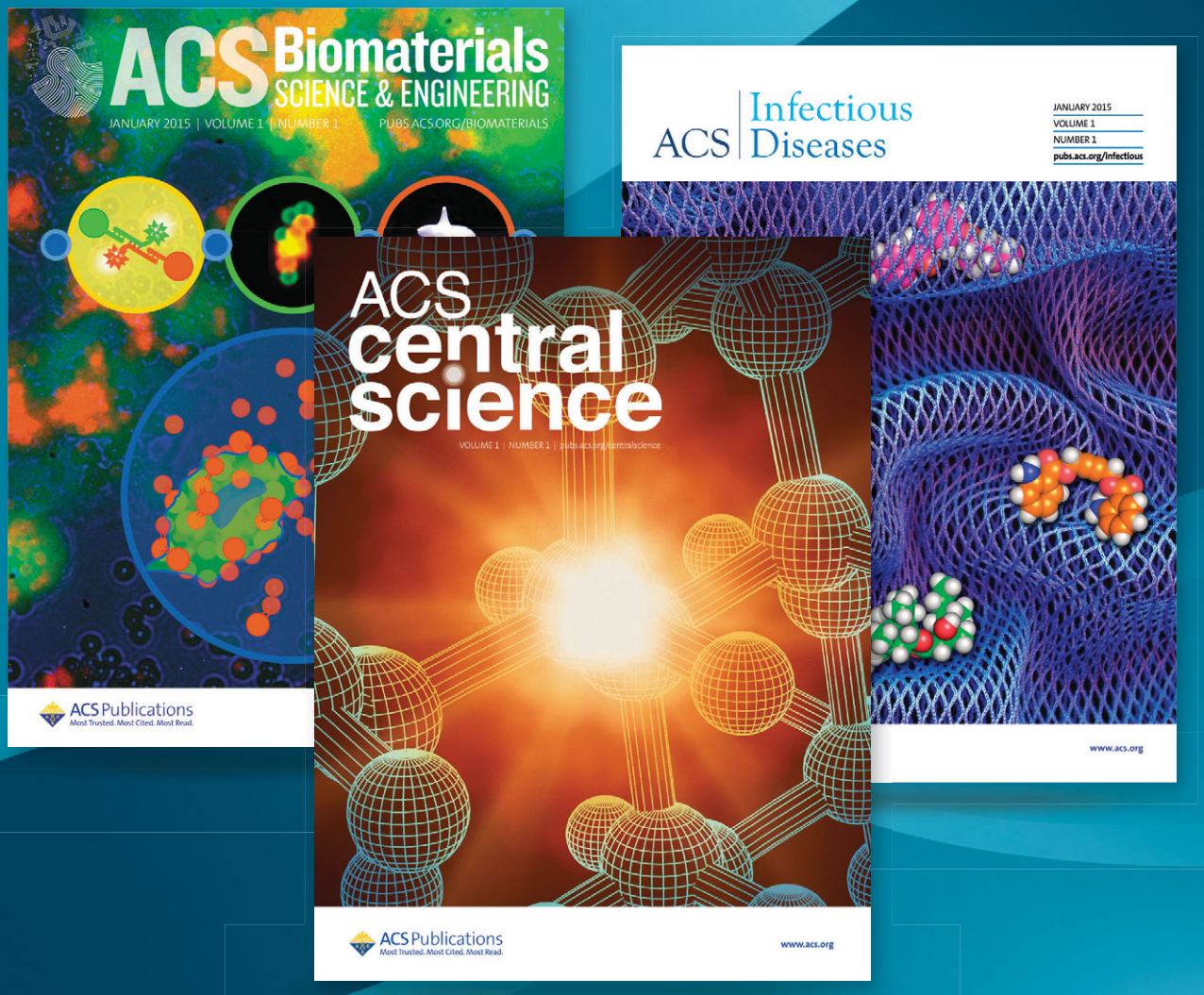
“We live in a global industry,” she says. “Scientists can collaborate more easily than ever before. As a publication, I think there’s a lot we can learn from this.” She looks forward to helping C&EN remain a bridge for science enthusiasts of all kinds—members and non-members, professionals and the public—all around the world.

“Chemistry and science are not geographically limited,” Campos-Seijo says. “They’re universal.”

C&EN
CHEMICAL & ENGINEERING NEWS

Go to cen.acs.org

INTRODUCING THE CLASS OF 2015



ACS Publications
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SCIENCE ROCK STAR

Seeks your greatest hits in research

Exceptional research

ACS Central Science takes center stage—while giving your exceptional research limitless possibilities to influence and inspire.

In December, ACS Publications began accepting submissions for *ACS Central Science*, a groundbreaking new journal that promises to elevate the prominence of chemistry as the discipline to which all other areas of science are linked.

ACS central science

This open access, multidisciplinary journal will showcase ultra-high-quality primary research in chemistry and allied fields, including biomedicine, energy science, nanotechnology, materials science, and earth and planetary science. Every month, issues will include a complement of thought-provoking review and opinion articles, commentaries, and interviews. Only 100–200 articles will be published each year, making the journal fiercely selective.

"With *ACS Central Science*, we have an opportunity to create a journal that not only offers exciting primary research articles, but that can also reach out and deliver the message that chemistry is the central science to the public at large," says journal Editor-in-Chief Carolyn Bertozzi, Ph.D. "We want to get people thinking about the connections between chemistry and other fields."

As ACS Publications' first completely open access journal, *ACS Central Science* is the centerpiece of the Society's efforts to redefine how the most innovative research is shared with the world. But this isn't just about improving access

< First, let's set the record straight.

Carolyn Bertozzi did not play guitar in the hard-rock-rap band "Rage Against the Machine." However, she did play keyboards in a band called "Bored of Education" while at Harvard with Tom Morello, who later went on to form and play guitar in "Rage Against the Machine," one of the most popular and influential bands of the 1990s. In the tweet above, the two former bandmates were reunited, raising hopes that the band might re-form at a future ACS National Meeting! All of us at ACS Publications are glad Dr. Bertozzi chose to rock our new journal, *ACS Central Science*.

should have no limits

to research. ACS Publications is also planning a host of supporting activities to elevate chemistry's visibility with the general public.

Improving access to research

Accessibility for the public is a key goal for *ACS Central Science*. The editorial team hopes to accomplish this through the journal's open access status and engaging front-end material.

As Bertozzi notes, "This is beneficial to the research community, but think about what it means to the general public.

"What if you're a high school science teacher and you want to assign high-level research to your students? Now you can."

The journal will also have a substantive front section, such as the news and views included in the cleverly titled "First Reactions," that will include feature stories, reviews, commentary, interviews, and more, all designed to complement the original research. The aim is to create readable, engaging content that puts the research in context.

"With First Reactions, we will provide succinct, accessible analysis of the research," says Kevin Davies, Ph.D., Vice President of Business Development for ACS Publications. "We want to help readers 'get behind the scenes' of research and hear from other scientists in the field about what it means. It will have a magazine-like format that accompanies the journal's research matter."

ACS Central Science will tap C&EN writers and social media platforms, including Twitter, Reddit, and Google+, to promote content and to showcase researchers. Publishing in *ACS Central Science* will give authors the visibility and prestige of publishing in a world-class, open access research journal, while offering access to the promotional powerhouse of the world's largest scientific society.

Removing barriers to publishing open access

As a key component to ACS Publications' open access initiatives, *ACS Central Science* does not levy any article processing fees on authors. Authors whose papers are selected for publication in *ACS Central Science* receive an ACS AuthorChoice license for immediate open availability at no charge.

> **"We want to get people thinking about the connections between chemistry and other fields."**
>
> —Dr. Carolyn Bertozzi

As an open access journal, all *ACS Central Science* content will be accessible by anyone at any time, free of subscription charges. Yet the publication will still offer the same exceptionally high quality standards and rigorous peer review that are a signature of all ACS Publications journals.

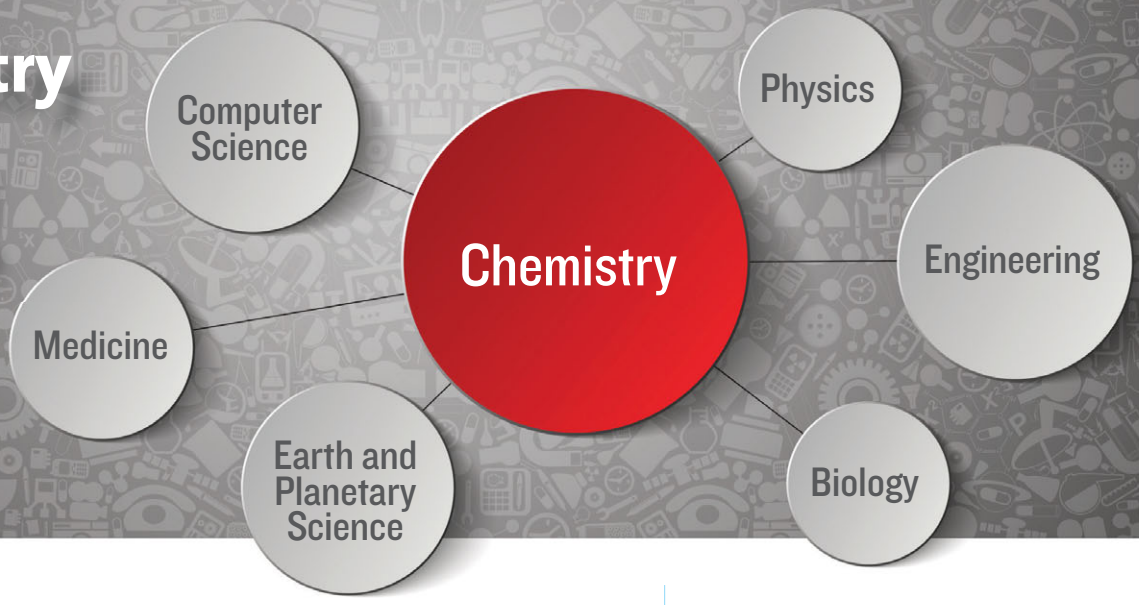
> **"We want to help readers 'get behind the scenes' of research and hear from other scientists in the field about what it means."**
>
> —Dr. Kevin Davies

The editorial staff is also committed to creating a positive experience for authors.

"We are committed to fast decision-making and turnaround," says Bertozzi. "We are all active researchers who understand the frustrations that can come with the peer-review process. We are going to provide constructive peer reviews, limit the number of reviews, and make decisions quickly and decisively. That's not unique to *ACS Central Science*. ACS Publications as a whole is committed to this."

> **"We are committed to fast decision-making and turnaround."**
>
> —Dr. Carolyn Bertozzi

Chemistry is the Central Science



"We envision *ACS Central Science* as the primary venue for reporting the most important advances in chemistry and in allied fields wherein chemical concepts and tools play a major role."

—Dr. Carolyn Bertozzi

Engaging the global community

The multidisciplinary nature of the journal demands an editorial team that has a global perspective, both in terms of research interests and geographical location. The selection of Bertozzi as Editor-in-Chief is instrumental to fulfilling this vision, Davies says.

"Carolyn is passionate about the interaction of chemistry and other research disciplines and understands the importance of open access," observes Davies. "She's going to be a dynamic leader for the journal. She wants to build a journal of great international reputation, to make it a must-read journal of not just research but also of engaging, accessible material."

Initially, five Senior Editors will help Bertozzi guide the direction of *ACS Central Science*. All active researchers, the Senior Editors represent an impressive array of research backgrounds and achievements.

"I wanted people who are very broad in their expertise and research activities and are highly respected in the community," notes Bertozzi. "Because they will shape the journal's contents, I wanted people who would be good stewards of the whole enterprise. We also needed global diversity. We wanted people who are in regions that are rich with top-notch science."

"I wanted people who are very broad in their expertise and research activities and are highly respected in the community."

—Dr. Carolyn Bertozzi

The journal's editorial advisory board is a globally diverse group of active researchers who are top scientists in their fields. The board's international and scientific diversity reflects the broad range of sciences that will be covered in the journal, which will ensure a fair and expeditious review of all material.

"World-class chemistry and related sciences are happening all over the globe," Davies notes. "Our intention is that the board will reflect the geographic strength of science around the world."

Coming soon...

ACS Central Science opened for submissions in December, and the initial response has been extremely positive. Articles will be published on the journal's website shortly after they are accepted. The first issue is expected to be published in Q1 2015.

For updates, visit the *ACS Central Science* website and follow the journal on Twitter at @ACSCentSci.

Bertozzi's vision for the journal, as well as submission procedures and a profile of the Senior Editors, can also be found on the *ACS Central Science* website.

Go to **pubs.acs.org/centralscience**

MEET THE EDITORIAL TEAM

EDITOR-IN-CHIEF

Carolyn Bertozzi
Howard Hughes Medical Institute
University of California, Berkeley
Departments of Chemistry and
Molecular and Cell Biology

Dr. Bertozzi's work spans a wide range of technologies and approaches at the interface of chemistry and biology. Her research focuses on creating new platform technologies for the development of medicines and diagnostics that will improve human health; for probing natural biology; and to develop road maps for creating synthetic life forms to serve human needs.

She is the T. Z. and Irmgard Chu Distinguished Professor of Chemistry, and Professor of Chemistry and Molecular and Cell Biology at University of California, Berkeley; Professor of Molecular and Cellular Pharmacology at University of California, San Francisco; Senior Faculty Scientist at Lawrence Berkeley National Laboratory; and a Howard Hughes Medical Institute Investigator.

She has served as Co-Director of the Berkeley Nanosciences and Nanoengineering Institute (BNNI) since 2011 and as Co-Director of the UC Berkeley Chemical Biology Graduate Program since 2001. She is co-founder and Chair of the Scientific Advisory Board of Redwood Bioscience and serves in a variety of other advisory roles, including the Research Advisory Board for GlaxoSmithKline and the Broad Institute Board of Scientific Counselors.

In April, Dr. Bertozzi will move her lab to Stanford University, where she will be Professor of Chemistry and, by courtesy, of Chemical and Systems Biology. Dr. Bertozzi will be a founding scientist of Stanford ChEM-H (Chemistry, Engineering & Medicine for Human Health), a new initiative chaired by Chaitan Khosla, which draws together faculty from diverse disciplines with the goal of improving lives.

SENIOR EDITORS

Christopher Chang
Howard Hughes Medical Institute
University of California Berkeley
Departments of Chemistry and
Molecular and Cell Biology

Dr. Chang's research is at the interface of inorganic chemistry, organic chemistry, and chemical and molecular biology. His research interests include molecular imaging and catalysis applied to neuroscience, stem cells, cancer, infectious diseases, renewable energy, and green chemistry.

Ben G. Davis
University of Oxford
Chemistry Research Laboratory

Dr. Davis' research covers organic chemistry and several disciplines within biology. His interests include synthesis and methodology, inhibitor/probe/substrate design, biocatalysis, enzymology, biosynthetic pathway determination, protein engineering, drug delivery, glycobiology, and molecular imaging.

Monica Olvera de la Cruz
Northwestern University
Department of Materials Science
and Engineering

In Dr. Olvera de la Cruz's research, she has developed theoretical models to determine the thermodynamics, statistics, and dynamics of macromolecules in complex environments including multicomponent solutions of heterogeneous synthetic and biological molecules, and molecular electrolytes.

David A. Tirrell
California Institute of Technology
Chemistry and Chemical Engineering

Dr. Tirrell's research covers biopolymers and polymers. Specifically, his research uses organic, biological, and materials chemistry to make new macromolecular systems of controlled architecture and novel function.

Dongyuan Zhao
Fudan University
Laboratory of Advanced Materials
Department of Chemistry

Dr. Zhao's research covers materials science generally, with a focus on the design, synthesis, assembly, growth, and properties of materials, including MOFs and nanomaterials.

Are you out of compliance

Here's how ACS Publications helps you go open access and meet funder requirements with our expanded ACS AuthorChoice and innovative ACS Author Rewards programs

Your research is groundbreaking. Your article has been accepted by your journal of choice. So, your work as an author is done, right? Not quite.

Does your article need to be open access? Requirements for open access are not uniform across funding agencies and institutions. That's why today's authors need to know the rules, not just for their funders and institutions, but also for their co-authors.

The world is embracing open access, putting more published, peer-reviewed research articles within the public's reach. While this is a positive development, it also means authors are often tasked with additional responsibilities to ensure they are in compliance with their funders' open access requirements.

As of January 2014, ACS has moved to the forefront of the open access world by offering new options to help authors negotiate this changing landscape. ACS AuthorChoice and ACS Author Rewards are designed to help authors efficiently and affordably satisfy the open access requirements of their funders and institutions.

ACS AuthorChoice: Your fast and affordable way to make articles open access

With the expanded ACS AuthorChoice program, ACS Publications helps authors meet open access requirements by offering more flexible options, money-saving discounts, and timesaving services that simplify compliance.

For a one-time fixed fee, the ACS AuthorChoice program enables authors to make the final published article freely accessible and can choose:

- **Immediate open availability upon publication**
- **Open availability 12 months after publication (ACS AuthorChoice+12)**
- **Creative Commons licenses**

Significant discounts are available for ACS members and authors at subscribing institutions.

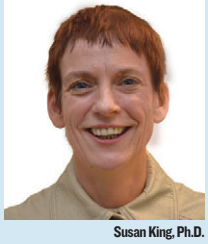
Authors always have the option of self-depositing the accepted manuscript (the post-peer review version, accepted by the journal, prior to additional editing and production enhancement by ACS Publications) to meet open access requirements. The accepted manuscript is available through the ACS Paragon Plus system and there is no cost or fee for this option.

ACS in harmony with CHORUS initiative

CHORUS, the Clearinghouse for the Open Research of the United States, offers a suite of services and best practices that provide a sustainable solution for agencies and publishers to deliver public access to published articles reporting on funded research in the United States. The first initiative of CHOR, Inc., a US 501(c)(3) non-profit organization, CHORUS leverages widely used technology to facilitate a simple compliance process, optimized search and dashboard services, and multi-party archiving and preservation capabilities.

Susan King, Ph.D., Senior Vice President of the Journals Publishing Group at ACS, is helping to lead the effort as the Chair of the CHOR, Inc. Board of Directors. In addition, Dan O'Brien, Assistant Director of Publishing Technology, and Dave Martinsen, Ph.D., Senior Scientist, Digital Strategy at ACS, participate in the CHORUS Technical Working Group. Once again, ACS Publications is at the forefront, working with publishers and agencies to create a sustainable solution for researchers to publish their work.

Utilized by the U.S. Department of Energy (DOE) in their PAGES (Public Access Gateway for Energy & Science) discovery service, CHORUS links users to published research on participating publishers' websites. ACS Authors have options to use ACS Author Rewards and ACS AuthorChoice to enable public availability of their final published article on the ACS Publications platform with related essential context, tools, and information, either immediately or 12 months after publication.



Susan King, Ph.D.

"Our participation in CHORUS is just one more way that ACS strives to make open access compliance as easy and streamlined as possible, while helping authors broaden their exposure in the scientific and public communities," says Dr. King.

CHORUS

with your funders?

ACS AuthorChoice makes the final published article, also known as the Version of Record, freely available. This is the professionally edited and typeset version of the article, with enhanced functionality, as it appeared in the ACS journal. Authors who choose ACS AuthorChoice also gain the advantages of ACS Certified Deposit.

ACS Certified Deposit: Assisting authors with managing deposits

ACS Certified Deposit is a program designed to help authors manage deposits of ACS AuthorChoice articles into repositories. Authors who participate in ACS AuthorChoice and ACS AuthorChoice+12, or who are selected for publication in *ACS Central Science* or ACS Editors' Choice, are eligible to receive ACS Certified Deposit at no charge. ACS also maintains long-term records verifying the deposit of an article in a repository, and will make those records available to the authors of an article published with ACS upon request.

For more information about ACS Certified Deposit or to submit a request, visit **http://pubs.acs.org/page/certified_deposit.html** or email **certifieddeposit@services.acs.org**.

ACS Author Rewards: Helping the scientific community transition to open access, while also thanking authors for their contributions

The ACS Author Rewards program is another of the four open access initiatives introduced by ACS Publications in January 2014. This $60 million direct-to-author open access stimulus program is designed to encourage authors to publish open access. Under this program, every corresponding author of a peer-reviewed article that was published in an ACS journal during 2014 received two ACS Author Rewards worth $750 each.

The rewards, provided as promotional codes, can be applied toward any ACS AuthorChoice license. They can be used individually on separate articles, combined, or transferred to a colleague.

Deposited into authors' ACS ChemWorx accounts in December 2014, the rewards are redeemable from January 1, 2015, to December 31, 2017.

Two free apps are available through ACS ChemWorx to help authors manage their open access options. The ACS AuthorChoice app guides authors through the process of making their articles open access. The ACS Author Rewards app allows authors to manage their rewards. Visit ACS ChemWorx at **https://hp.acschemworx.acs.org/**.

Four pillars of ACS Open Access

ACS AuthorChoice

< Expanded open access publishing options for authors and their sponsors.

ACS Author Rewards

< Credits to fund open access publishing options from ACS.

ACS Editors' Choice

< Free public access to research of interest to the global community.

ACS Central Science

< A new journal that's free to both readers and authors.

RESOURCES AVAILABLE FOR ADDITIONAL SUPPORT

ACS has an established reputation for supporting researchers with the publication process and has resources in place to assist with navigating these new open access options.

ACS Help Desk–The ACS Help Desk offers the extensive Knowledge Base, a compendium of more than 1,000 support references on a variety of topics. The Help Desk also offers 24x7, global support via live chat over the web, with Skype, and by telephone. To get support, call **1-800-227-9919** (toll free) or **1-202-872-4357** (international), or visit **https://help.acs.org**

ACS AuthorChoice–The ACS AuthorChoice webpages provide an informative overview of the program, helpful FAQs, pricing information, decision trees for selecting the best AuthorChoice option, and more. Go to **http://pubs.acs.org/page/4authors/authorchoice/index.html**

ACS Author Rewards–Visit the ACS Author Rewards webpages for more information about the program, helpful FAQs, and a guide to using the ACS Author Rewards app. Go to **http://pubs.acs.org/page/4authors/authorrewards/index.html**

3 Ways Researchers Can Boost Their Social Media Savvy

Social networks have become far more than just a way to stay close to family and friends. These digital communities are now a commonplace tool for scientists and publishers alike to collaborate, evaluate, and gain exposure to goings-on in their scientific communities.

How has social media transitioned from a fun distraction to a professional asset? For one, it gives researchers a channel they can use to engage with a range of stakeholders they may not have previously had direct access to, including editors, publishers, colleagues, professors, and lab mates. It is also an excellent way to network, as such platforms provide marketplaces in which even the most niche communities can be built; and in this environment, feedback can happen fast.

While consumption of research findings was once limited to the subscribers of a journal, digital networks now allow articles to achieve a broader reach at a faster pace. There are limitless opportunities for an article to go viral, and with open access becoming more and more prevalent throughout the scientific publishing landscape, the value and impact of social media is even more important.

So whether you're a researcher, author, or editor, a bit of social media savvy can pay off. Keep these tips in mind as you're building—or refining—your online presence.

1. Be present and participate

Whether gathering peer-reviewed articles or looking up a simple piece of information, most of today's research happens online. That's why you and your research need to be discoverable. Social media is an effective tool for optimizing this search engine visibility.

Your online presence—or lack thereof—affects how prominently your research appears in search results, which could limit your reach in the scientific community and beyond. Make sure you have an online profile and that your bio is updated and accurate on any associated academic institutions' websites. Good places to start are Google Scholar, Google+ (think SEO!), and LinkedIn.

Similarly, publishers often maintain social profiles to generate interest in their publications, share submission deadlines, and highlight emerging research.

"It can be too easy to get lost in a stream of technical jargon."

—Dr. Jillian Buriak

Twitter is a great resource for exposing people to your work, and a great channel to use to keep up with industry developments and your colleagues' latest research. Take advantage of Twitter's "list" functionality; create one that covers all relevant journals and publishers for your work. In turn, share your Twitter list with your own network, thus making yourself a resource for others in your field.

2. Be creative

Think beyond just posting links as you develop and engage with social media content. If you've just published a new article, use social media not only to promote the publication, but also to generate further discussion with fellow scientists, authors, and researchers. Engaging posts and interesting visuals will keep your profile fresh and those interested in your research intrigued.

Posts should:

- **Provide information**
- **Include a call to action**
- **Be grammatically correct**
- **Keep things positive**
- **Provide a link**
- **Include images or visuals**
- **Be mobile friendly**
- **Demonstrate that you are present**
- **Alternate formats**
- **Be customized**

Use Facebook posts to promote appearances at conferences and events, then tweet from the event to share updates and start conversations. By engaging in social media, you can meet new people and grow your network. Many events are now facilitating such interactions, with Meetups, event-specific hashtags, and even conference-specific apps.

Reddit is also a valuable resource for the scientist, but be careful not to post solely about your own content. This social media channel is a community in the strongest sense, and users expect true thought leadership. A great balance is Reddit's "Ask Me Anything (AMA)" format, which is an excellent way to respond to questions about your work. The community has an opportunity to get their questions answered, and you have the opportunity to go more in-depth.

3. Be methodical

Decide what you want to share, then determine the best way to share it. New social media tools are emerging on a daily basis, and old tools are constantly evolving. What does this mean for you? Always keep one eye on the bigger picture. Ask yourself: Who am I trying to reach? Is this platform the right fit for what I'm trying to communicate?

Twitter is a good forum to communicate opinions, post updates for conferences and meetings, and quickly disseminate information and easily digestible news. Conversely, a blogging platform, like WordPress, is more suited for longer articles and collections of links to published content.

Another advantage of social media is that it yields data you can use to make better decisions about your content. Consider signing up for free management systems like Tweetdeck or HootSuite, which will give you a bird's eye view of what is happening online. Do people respond more favorably to certain platforms or formats than others? Stay informed on new ways to engage and explore mediums that make sense for you.

Remember, you don't always have to reinvent the wheel. As many researchers have discovered, the LinkedIn for scientists is... LinkedIn.

Go to pubs.acs.org/page/follow.html

SOCIAL MEDIA IS NOT IMMATERIAL TO YOUR SUCCESS: TIPS FROM AN EDITOR

Dr. Jillian Buriak

"With only 140 characters, it's a challenge to express science in a way that is creative and attracts attention," says Jillian Buriak, Editor-in-Chief of *Chemistry of Materials* and a popular presence on social media.

"It can be too easy to get lost in a stream of technical jargon. Try thinking carefully about condensing your meaning into 5 to 10 words, and harness the power of commonly used hashtags (#graphene, #solar, #nano, #OA, #materials, for instance). If you want to catch the attention of someone in particular, top off the tweet with the Twitter handle of a scientist and/or their institutions. This encourages retweeting to further spread your message."

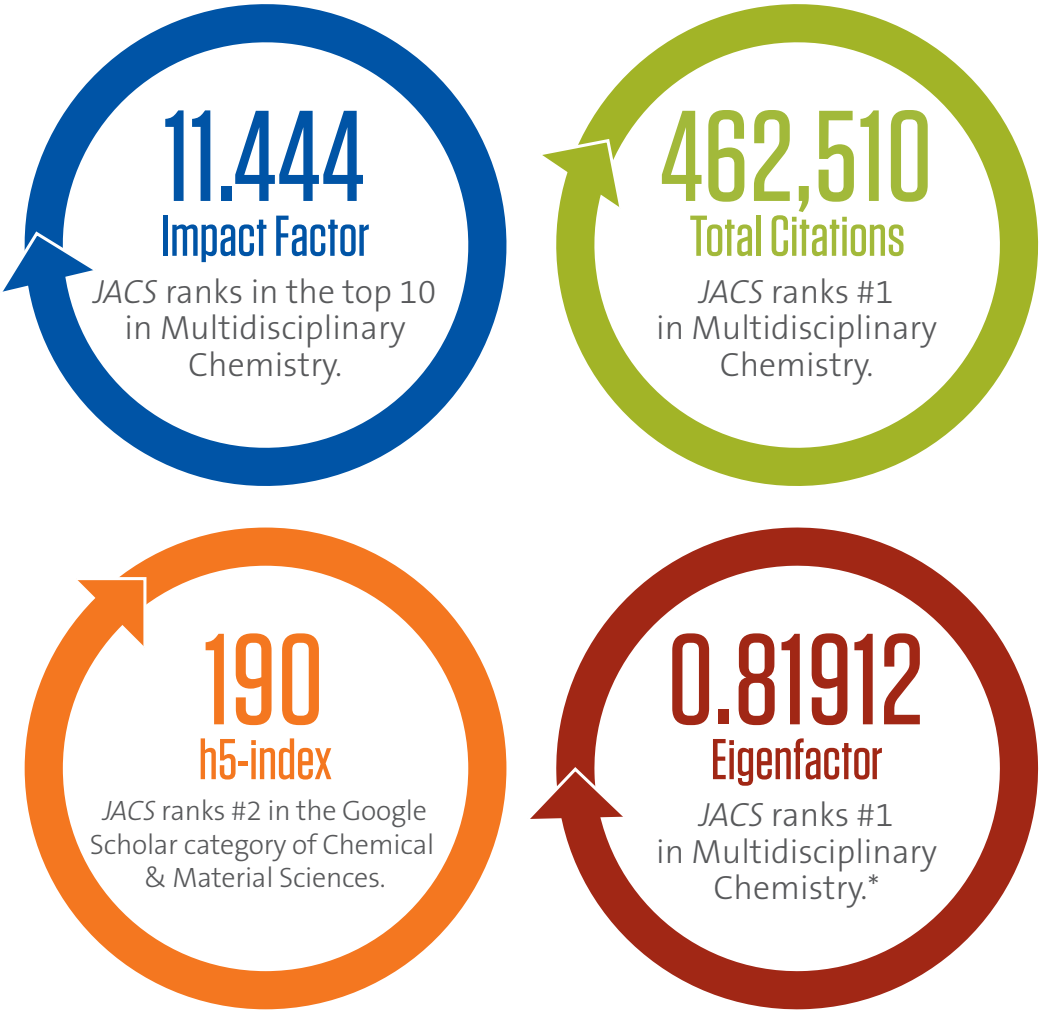
The Most Cited Journals

ACS Publications is a Leader in Chemistry & Related Areas of Science, as reported in the 2013 Journal Citation Reports® from ThomsonReuters

Journal Title	Total Citations	Impact Factor	Current Articles
Accounts of Chemical Research	47,005	24.348	279
ACS Applied Materials & Interfaces	16,373	5.900	1,781
ACS Catalysis	4,446	7.572	378
ACS Chemical Biology	4,711	5.356	314
ACS Chemical Neuroscience	1,259	4.210	153
ACS Combinatorial Science	685	3.401	87
ACS Macro Letters	1,847	5.242	231
ACS Medicinal Chemistry Letters	1,737	3.073	214
ACS Nano	58,446	12.033	1,178
Analytical Chemistry	102,654	5.825	1,638
Biochemistry	88,295	3.194	920
Bioconjugate Chemistry	14,074	4.821	209
Biomacromolecules	27,578	5.788	501
Chemical Research in Toxicology	11,018	4.19	191
Chemical Reviews	124,463	45.661	207
Chemistry of Materials	79,744	8.535	604
Crystal Growth & Design	24,937	4.558	664
Energy & Fuels	21,961	2.733	840
Environmental Science & Technology	105,646	5.481	1,689
Industrial & Engineering Chemistry Research	43,808	2.235	1,910
Inorganic Chemistry	90,888	4.794	1,646
Journal of Agricultural and Food Chemistry	82,432	3.107	1,506
Journal of Chemical & Engineering Data	16,833	2.045	460
Journal of Chemical Education*	7,338	1.001	359
Journal of Chemical Information and Modeling	11,630	4.068	296
Journal of Chemical Theory and Computation	14,415	5.310	553
Journal of Medicinal Chemistry	61,787	5.480	797
Journal of Natural Products*	20,791	3.947	336
The Journal of Organic Chemistry	98,978	4.638	1,397
Journal of Physical Chemistry A	57,303	2.775	1,470
Journal of Physical Chemistry B	121,463	3.377	1,720
Journal of Physical Chemistry C	96,606	4.835	3,113
Journal of Physical Chemistry Letters	13,562	6.687	677
Journal of Proteome Research	19,028	5.001	527
Journal of the American Chemical Society	462,510	11.444	2,840
Langmuir	113,157	4.384	1,887
Macromolecules	101,162	5.927	1,049
Molecular Pharmaceutics	8,173	4.787	450
Nano Letters	103,399	12.940	996
Organic Letters	80,234	6.324	1,584
Organic Process Research & Development	4,201	2.549	170
Organometallics	41,998	4.253	898

*co-publications

There are many ways to measure a journal...



Here's another way: Look at its editors. »»

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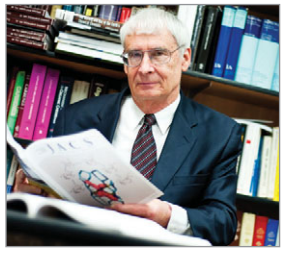

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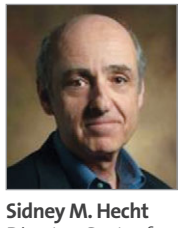

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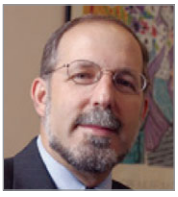

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C&EN

To start, *Chemical & Engineering News* (C&EN) is the weekly resource chemists count on to deliver the latest chemistry news from the worlds of research, business, education, government, and beyond. C&EN's online resources include C&EN Archives, a growing collection of full, cover-to-cover C&EN issues, with the previous year's issues added on a rolling basis each year. In addition, with C&EN Mobile, members of the ACS can now access all of the issues for no charge by entering their ACS ID. If you are not a member, individual issues of C&EN are available for purchase within the app.

ACS Publications

ACS Publications will introduce its newest journal, *ACS Central Science*, along with its Editor-in-Chief, Dr. Carolyn Bertozzi, at the ACS booth. *ACS Central Science* is the first completely open access journal from the ACS. This groundbreaking, highly selective journal, publishing only 100-200 papers in its first year, is now accepting submissions. Find out more at the ACS Publications booth or go to pubs.acs.org/centralscience. Stop by also to learn about *ACS Infectious Diseases* and *ACS Biomaterials Science & Engineering*, two new journals publishing their first issues in 2015.

On Monday, March 23rd at 12:00 noon MT, you can take part in an exciting live ACS Publications webinar at the booth's main stage. "Mastering the Art of Scientific Publication," the popular, new webinar series, will feature a panel of distinguished ACS journal editors giving tips and advice to help authors, with a Q&A period at the end of the event.

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All presenters should prepare for their presentation by verifying the following details: the status of your abstract at maps.acs.org (using your ACS ID to log in to the system); mode of presentation (oral or poster); and the time, length, and location of your presentation. Speakers should arrive in their presentation rooms at least 30 minutes before their scheduled speaking time. Poster presenters should set up their poster at least one hour before the start of their poster session. If you need to withdraw your presentation, please send a withdrawal notice to maps@acs.org and contact your symposium organizer immediately.

TECHNICAL SESSION EQUIPMENT. Each technical session meeting room will be equipped with the following: LCD projector, screen, podium, podium microphone or lapel microphone, and laser pointer. Speakers need to provide their own laptops or arrange for specialty equipment directly with their symposium organizer and/or division program chair. To request other specialty equipment (at the standard fee), contact an ACS Operations Office during the meeting.

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POSTER SESSIONS. All materials must be confined to a 4-foot-high by 8-foot-wide display board in the convention center and 4-foot-high by 6-foot-wide display board in hotels. Presenters must mount their poster one hour before the scheduled session start time. Poster numbers supplied by ACS will be in the upper corner of each poster board, and this number corresponds with the number assigned to each poster in the technical program. Pushpins will be available at the poster session. Presenters must remain with their posters for the duration of their scheduled session as indicated in the technical program. All posters must remain up until the session ends and then must be removed within one hour. ACS cannot assume responsibility for materials beyond these time limits.

SCI-MIX POSTER SESSION ONLY. Sci-Mix presenters may begin poster setup at 7:15 PM (45 minutes before the session begins). Each presenter may be accompanied by one assistant only, and both people are required to check in before entering the hall. After exiting, presenters will not be permitted to reenter the hall until the session begins at 8:00 PM.

ABSTRACTS & PREPRINTS

ONLINE TECHNICAL PROGRAM. The technical program for the 249th national meeting is now available at www.acs.org/denver2015. You can search by divisions or committees, symposia, speakers, or keywords from abstracts as well as presidential events and the multidisciplinary theme of "Chemistry of Natural Resources."

ABSTRACTS (USB FLASH DRIVE). Abstracts of all scientific sessions at the meeting can be purchased in USB flash drive (thumb drive) format through ACS Attendee Registration either online by Jan. 30 or on-site in Denver from March 22 to 26. The ACS member fee is $65 each; the nonmember fee is $90 each. Attendees can pick up their abstracts on-site at ACS Attendee Registration at the Colorado Convention Center. You can have a USB flash drive shipped to you if you place your order by Jan. 30, pay an $8.00 postage fee per item, and provide a valid street address within the U.S. or Canada. If you are not attending the meeting, you can purchase abstracts only from the ACS Office of Society Services, 1155—16th St., N.W., Washington, DC 20036; (800) 227-5558. Abstract USB flash drives and their shipping costs are nonrefundable.

PREPRINTS/GRAPHICAL ABSTRACTS. Preprints and graphical abstracts from the following divisions may be ordered directly from each division. You can purchase them via the information below or inquire about these products at the hospitality table for each division near their meeting rooms.

Energy & Fuels.
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Polymer Chemistry.
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Denver 2015

Interdivisional Poster Session & Mixer

Monday, March 23
Colorado Convention Center
Hall C from 8PM – 10PM

SCI-MIX

Sci-Mix is a national meeting wide social event with colleagues meeting each other in a relaxed atmosphere combined with serious scientific poster discussions. Speak informally with presenters as they represent the best of what their division has to offer in terms of science and presentation. It is free and all attendees are welcomed.

You can now access the Sci-Mix seesions on the free meeting mobile app. Download it today!

TECHNICAL PROGRAM SUMMARY

Presidential Events — PRES

Diane Grob Schmidt, Program Chair

Colorado Convention Center	S	M	Tu	W	Th
The Transnational Practice of Chemistry & Allied Sciences & Engineering: Study, Research & Careers without Borders**	A				
Nanotechnology: Delivering on the Promise**	P	D			
DOE Nanoscience Research Centers			A		
Particles at Fluid Interfaces* (COLL)	D	A			
Functionalization of Complex Nanosurfaces* (COLL)	D	D	A		
Basic Research in Colloids, Surfactants & Nanomaterials* (COLL)	D			A	D
Metallic Nanostructures for Optical & Electrochemical Sensing & Alternative Energy Conversion* (COLL)	DE	D	A	D	
Department, University & National Models for Faculty Development To Support Adoption of Evidence-Based Teaching* (CHED)	P				
Plasmonic Catalysis & Sensing* (COLL)	E	D	A	D	
Nanoscience* (INOR)	E		E	D	D
Fundamental Research in Colloids, Surfaces & Nanomaterials* (COLL)	E				
Transitioning between Academic Research into Practical Use: Solar Energy & Advanced Materials* (COMSCI)		A			
Electrical, Thermal & Mass Transport in Polymer Nanocomposites & Alloys* (POLY)		D	E		
Excellence in Graduate Polymer Research* (POLY)		D	E		
Advances in Formulations Science & Technology* (COLL)		P			
Nanoscience & Nanotechnology of Natural Resources* (MPPG)			A		
GSSPC: Designed by Nature, Developed by Science: Interdisciplinary Perspectives on Biocatalysis* (CHED)			D		

Presidential Events (continued) — PRES

Diane Grob Schmidt, Program Chair

Colorado Convention Center	S	M	Tu	W	Th
The Interface of Chemical & Biological Sciences International Disarmament Efforts* (IAC)			D		
Applied Nanotechnology for Food & Agriculture* (AGFD)			P	A	
Ask Dr. Safety: EH&S Support of Nanotechnology R&D* (CHAS)			A		

Multidisciplinary Program Planning Group — MPPG

R. Weber, Program Chair

Colorado Convention Center	S	M	Tu	W	Th
Chemistry of Natural Resources Plenary CNR	P				
The Fred Kavli Innovations in Chemistry Lecture CNR		P			
The Kavli Foundation Emerging Leader in Chemistry Lecture		P			
Nanoscience & Nanotechnology of Natural Resources** CNR			A		
Green Chemistry & the Environment* (ENVR)	D	A		E	
Catalysis for Unconventional Energy Sources* (ENFL)	D	A			
Nanomaterials for Solar Energy Conversion & Storage* (ENFL)	D	D	D	D	A
Uranium in Seawater* (I&EC)	D	D			
Environmental Reactivity of Organic Micropollutants & Their Transformation Products in Receiving Waters* (ENVR)	D			E	
Assessing Toxicity of Environmental Contaminants* (ENVR)	D			E	
Biogenically Enhanced Recovery & Bioremediation in Fossil Fuel Reservoirs* (ENVR)	D			E	
Negative Carbon Emission Technologies: BECCS (Bio-Energy with Carbon Capture & Storage)* (ENFL)	D				

Multidisciplinary Program Planning Group (continued) MPPG

R. Weber, Program Chair

Colorado Convention Center	S	M	Tu	W	Th
Understanding the Geochemical Interactions of Organic Compounds in the Subsurface* (GEOC)	D				
Nanotechnology: Delivering on the Promise* (PRES)	P	D			
Environmental Chemistry & Health Impacts of Fine & Ultrafine Particulate Matter* (ENVR)		A		E	
Enhanced Extraction & Utilization of Unconventional Energy Sources: Hydrofracking, EOR & Novel Approaches* (ENFL)		A			
Biomass to Fuel & Products* (SOCED)		A			
Geochemistry & Reactive Transport in Nano-Pore Geomaterials* (GEOC)		A			
Transitioning between Academic Research into Practical Use: Solar Energy & Advanced Materials* (COMSCI)		A			
Modern Analytical Approaches for the Characterization of Natural Organic Matter in the Environment* (ENVR)		D	A	E	
Hydraulic Fracturing Impacts on Water, Soil & Air Quality* (ENVR)		D	D		
Chemical Technology in Antiquity* (HIST)		D			
Solutions to Metals Contamination of Water* (ENVR)		P	D	E	
Chemistry in the Marine Boundary Layer* (ENVR)		P		E	
DOE Nanoscience Research Centers: National Resources for the Nanoscience Community* (PRES)			A		
C1 Chemistry* (ENFL)			D	D	A
Iron Oxides: Formation, Structure, Reactivity & Applications* (GEOC)			D	D	
Molecular Catalyst for Solar Fuels* (INOR)			DE	A	
Advances in Analytical Chemistry for Discovering Emerging Contaminants in the Natural Environment* (ENVR)			D	E	

Multidisciplinary Program Planning Group (continued) MPPG

R. Weber, Program Chair

Colorado Convention Center	S	M	Tu	W	Th
Chemistry of the Energy Water Nexus: Focus on Fracking* (INOR)			D		
12th International Symposium on Heavy Oil Upgrading, Production & Characterization* (ENFL)				D	A
Surface Physicochemical Processes in Engineered & Natural Systems* (ENVR)				D	A
Computational Pyrolysis & Upgrading of Bio-Oils* (COMP)				D	
Analytical Chemistry of Natural Resources* (ANYL)				D	
Trace Materials in Air, Soil & Water* (ENVR)				D	
Water Sustainability in Oil & Gas Exploration: Treatment Issues* (ENVR)				DE	
Water Our Most Critical Resource* (AGFD)				P	A
ACS Award for Affordable Green Chemistry: Honoring John Frye, Todd Werpy & Alan Zacher* (CELL)				P	
Water Recycling in Domestic Use, Energy Extraction & Agricultural Use* (ENVR)				E	A
Bioavailability & Biogeochemical Interactions Affecting Remediation of Hazardous Substances in the Environment* (ENVR)				E	A
Environmental Chemistry: Pedagogical Models & Practices* (ENVR)				E	A

*Cosponsored symposium with primary organizer shown in parentheses; located with primary organizer.
**Primary organizer of a cosponsored symposium.

CNR: Chemistry of Natural Resources

A = AM AE = AM/EVE P = PM D = AM/PM
E = EVE DE = AM/PM/EVE PE = PM/EVE

Division of Agricultural & Food Chemistry — AGFD

K. Deibler, Program Chair

Colorado Convention Center	S	M	Tu	W	Th
Undergraduate Symposium**	A				
Vitamin D: Past, Present & Future for Animals & Humans	P				
Graduate Student Symposium**	P				
Agricultural & Food Chemistry General Papers		D	A	P	
Medicinal & Aromatic Crops: Production, Phytochemistry & Utilization**		D			
Sci-Mix		E			
Phenolic & Polyphenolic Chemistry in Food Processing**			D		
Applied Nanotechnology for Food & Agriculture**			P	A	
Agricultural & Food Chemistry General Posters			P		
Water Our Most Critical Resource** CNR				P	A
Nanotechnology: Delivering on the Promise* (PRES)	P	D			
Undergraduate Research Posters* (CHED)		P			
Ask Dr. Safety: EH&S Support of Nanotechnology R&D* (CHAS)			A		

Division of Agrochemicals — AGRO

P. Rice, Program Chair

Located with Primary Sponsor	S	M	Tu	W	Th
Environmental Reactivity of Organic Micropollutants & Their Transformation Products in Receiving Waters* (ENVR)	D			E	
Assessing Toxicity of Environmental Contaminants* (ENVR)	D			E	
Nanotechnology: Delivering on the Promise* (PRES)	P	D			
Medicinal & Aromatic Crops: Production, Phytochemistry & Utilization* (AGFD)		D			
Advances in Analytical Chemistry for Discovering Emerging Contaminants in the Natural Environment* (ENVR)			D	E	
Phenolic & Polyphenolic Chemistry in Food Processing* (AGFD)			D		

Division of Agrochemicals (continued) — AGRO

P. Rice, Program Chair

Located with Primary Sponsor	S	M	Tu	W	Th
Surface Physicochemical Processes in Engineered & Natural Systems* (ENVR)				D	A
Microalgae: A Renewable Energy Source & a Sustainable Solution for the Environment* (ENVR)				D	
Water Recycling in Domestic Use, Energy Extraction & Agricultural Use* (ENVR)				E	A

Division of Analytical Chemistry — ANYL

D. Duckworth, Program Chair

Embassy Suites Denver – Downtown Convention Center	S	M	Tu	W	Th
Environmental Analytical Chemistry: A Tool for Introducing Research	P				
Advances in Bioanalytical Chemistry		D	D		
Advances in Analytical Separations		D			
Sci-Mix		E			
Advances in Mass Spectrometry			A		
Active Learning in the Undergraduate Analytical Chemistry Curriculum			P		
General Analytical Posters			E		
Advances in Electrochemistry				A	
Analytical Chemistry of Natural Resources**				D	
Frank H. Field & Joe L. Franklin Award for Outstanding Achievement in Mass Spectrometry: Honoring Hilkka I. Kenttämaa**				P	
Nakanishi Prize: Honoring Fred W. McLafferty					A
Advances in Analytical Spectroscopy					P
Macromolecular & Nanoparticle Separation Science* (POLY)	D	D	DE		
Nanotechnology: Delivering on the Promise* (PRES)	P	D			
Modern Analytical Approaches for the Characterization of Natural Organic Matter in the Environment* (ENVR)		D	A	E	
Undergraduate Research Posters* (CHED)		P			

Division of Analytical Chemistry (continued) ANYL

D. Duckworth, Program Chair

Embassy Suites Denver – Downtown Convention Center	S	M	Tu	W	Th
DOE Nanoscience Research Centers: National Resources for Nanoscience Community* (PRES)			A		
Advances in Analytical Chemistry for Discovering Emerging Contaminants in the Natural Environment* (ENVR)			D	E	
GSSPC: Designed by Nature, Developed by Science: Interdisciplinary Perspectives on Biocatalysis* (CHED)			D		
The Interface of Chemical & Biological Sciences International Disarmament Efforts* (IAC)			D		

Division of Biochemical Technology BIOT

M. Lazzara, A. Kantardjieff, Program Chairs

Grand Hyatt Denver	S	M	Tu	W	Th
David Perlman Memorial Lectureship	A				
Downstream Processes CNR	D	D	D	D	D
Upstream Processes	D	D	D	D	D
Biomolecular & Biophysical Processes	D	D	D	D	D
Emerging Technologies	D	D	D		
Colorado Biotechnology CNR	D	P			
Biosimilars & Follow-On Biologics		A	A		
Marvin J. Johnson Award in Microbial & Biochemical Technology		A			
Sci-Mix		E			
BIOT Young Investigator Award			A		
Biofuels & Sustainable Energy CNR			P	D	D
Alan S. Michaels Award in the Recovery of Biological Products			P		
Poster Session			E		
Biotechnology & Bioengineering Awards Presentation & Gaden Award				A	
Quality-by-Design for Biopharmaceuticals				D	
Biotechnology & Bioengineering Daniel I. C. Wang Award				P	

Division of Biochemical Technology (continued) BIOT

M. Lazzara, A. Kantardjieff, Program Chairs

Grand Hyatt Denver	S	M	Tu	W	Th
WCC Rising Stars Awards Symposium* (WCC)		D			
Undergraduate Research Posters* (CHED)		P			
Phenolic & Polyphenolic Chemistry in Food Processing* (AGFD)			D		

Division of Biological Chemistry BIOL

C. Crews, V. Bandarian, Program Chairs

Hyatt Regency Denver at Colorado Convention Center	S	M	Tu	W	Th
Young Investigators in Biological Chemistry	A				
Complex Enzymatic Transformations	P				
Alfred Bader Award in Bioinorganic or Bioorganic Chemistry: Honoring Michael A. Marletta	E				
Current Topics in Biological Chemistry	E				
The Chemistry & Biology of Non-Natural Nucleic Acids		A			
New Approaches to Investigating Chromatin Modifying Enzymes: Structure & Function		P			
Putting Chemical Biology in Context			A		
ACS Chemical Biology Award Symposium			P		
In Vivo We Trust: Small Molecule Phenotypic Screening in Animals				A	
Graduate Student & Postdoctoral Symposium				P	
Interfacial Biomolecular Recognition* (COLL)	E		A	D	D

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Division of Biological Chemistry (continued) BIOL

C. Crews, V. Bandarian, Program Chairs

Hyatt Regency Denver at Colorado Convention Center	S	M	Tu	W	Th
Undergraduate Research Posters* (CHED)		P			
GSSPC: Designed by Nature, Developed by Science: Interdisciplinary Perspectives on Biocatalysis* (CHED)			D		

Division of Business Development & Management BMGT

K. Allen, J. Bryant, Program Chairs

Embassy Suites Denver – Downtown Convention Center	S	M	Tu	W	Th
ACS Award in Industrial Chemistry: Honoring Thomas J. Colacot**		D			
The Transnational Practice of Chemistry & Allied Sciences & Engineering: Study, Research & Careers without Borders* (PRES)	A				
Earning ACS Awards: An Interactive Symposium on Constructing Successful Award Nominations* (PROF)	P				
Forensic Toxicology of Marijuana* (SOCED)		A			
Innovations in Macromolecular Network Chemistry* (POLY)		P	E	P	D

Division of Carbohydrate Chemistry CARB

E. Rozners, Program Chair

Colorado Convention Center	S	M	Tu	W	Th
Wolfrom Award Symposium	A				
Isbell Award & Gin New Investigator Award Symposium	P				
Glycomimetic Compounds: An Untapped Source of Novel Therapeutics		D			
Sci-Mix		E			
Protein Glycosylation: Simulation, Synthesis, Characterization & Application			D		
General Posters			E		

Division of Carbohydrate Chemistry (continued) CARB

E. Rozners, Program Chair

Colorado Convention Center	S	M	Tu	W	Th
Nanotechnology: Delivering on the Promise* (PRES)	P	D			
General Posters* (CELL)	E				
Frontiers in Glycoscience* (CELL)		D	D		

Division of Catalysis Science & Technology CATL

V. Schwartz, Program Chair

Colorado Convention Center	S	M	Tu	W	Th
Theoretical & Experimental Synergies at the Frontiers of Renewable Energy Catalysis CNR	D	A	P	A	A
Electrocatalysis & Photocatalysis CNR	D	D			
Honoring Jens Rostrup-Nielsen	D	P	D		
New Catalysis through Ligand Design	D				
George A. Olah Award in Hydrocarbon or Petroleum Chemistry: Honoring Jingguang G. Chen		D	A		
Surface Chemistry & Catalysis on Oxides		D	D	D	
Gabor A. Somorjai Award for Creative Research in Catalysis: Honoring Maurice Brookhart		P			
Sci-Mix		E			
Catalytic Materials & Technologies for Upgrading of CO_x & Natural Gas CNR			D	D	D
General Poster Session			E		
Novel Catalytic Materials for Renewable Fuels/Chemicals CNR				D	D
General Papers				P	D
Catalysis for Unconventional Energy Sources* (ENFL)	D	A			
E.V. Murphree Award in Industrial & Engineering Chemistry: Honoring Joseph R. Zoeller* (I&EC)			D		
GSSPC: Designed by Nature, Developed by Science: Interdisciplinary Perspectives on Biocatalysis* (CHED)			D		
Elucidation of Mechanisms & Kinetics on Surfaces* (COLL)				D	

Division of Cellulose & Renewable Materials — CELL

C. Frazier, Program Chair

Colorado Convention Center	S	M	Tu	W	Th
Functional Lignocellulosics & Nanotechnology CNR	D	D	A	D	
Cellulose in Solid State & Solution: Structure, Chemistry & Reaction Mechanisms: Anselme Payen Award Honoring Thomas Rosenau CNR	D	D	D	A	
Lignin Biosynthesis, Characterization & Modifications CNR	D	D			
Application of Computational Chemistry to Biomass Chemistry & Utilization CNR	D	P			
Advances in Lignocellulosic Materials & Chemistry: A Tribute to W.G. Glasser CNR	DE	A			
General Posters** CNR	E				
Frontiers in Glycoscience** CNR		D	D		
Sci-Mix		E			
Renewable Resources for Materials & Energy: Recent Research & Developments in Ibero-America CNR			A	D	A
Smart & Responsive Composites from Renewable Building Blocks** CNR			A	D	
Cellulose Dissolution: New Solvents & Mechanisms CNR				D	A
ACS Award for Affordable Green Chemistry: Honoring John Frye, Todd Werpy & Alan Zacher** CNR				P	
Research on Renewable Materials: US & EU Perspectives CNR					D
Conservation Science of Cellulosic Materials: Recent Developments CNR					D
Biomass to Fuel & Products* (SOCED)		A			
Polymeric Biomaterials* (PMSE)		P	D	D	A
Sustainability in the 21st Century: Optimizing Complex Interdependent Systems* (SOCED)		P			

Division of Chemical Education — CHED

W. Jones, I. Levy, A. Marsh, Program Chairs

Sheraton Denver Downtown Hotel	S	M	Tu	W	Th
Current Practice & Research Using ACS Exams	A				
Undergraduate Research Papers**	D	D			
Chemistry Education Research	D		P	D	
NMR Spectroscopy in the Undergraduate Curriculum	D				
From Cornerstone to Capstone: Culminating Experiences in the Undergraduate Chemistry Curriculum that Foster Integration & Application of Foundational Knowledge	D				
High School Program**	D				
Department, University & National Models for Faculty Development to Support Adoption of Evidence-Based Teaching**	P				
General Posters	E				
Integrating Chemistry & Polymer Science Research into the Classroom**		A			
Research at Community Colleges: Strategies for Enhancing Student Transfer & Success		A			
Experiments for Physical Chemistry Laboratory		D			
ACS Award for Achievement in Research for the Teaching & Learning of Chemistry: Honoring Vickie M. Williamson**		D			
Chemistry Education: International & Multi-Cultural Perspectives		D			
Undergraduate Research Posters**		P			
ACS Award for Encouraging Disadvantaged Students in Chemistry: Honoring Catherine H. Middlecamp**		P			
Online Course Development & the Effects on the On-Campus Classroom		P			
Sci-Mix		E			

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Division of Chemical Education (continued) CHED

W. Jones, I. Levy, A. Marsh, Program Chairs

Sheraton Denver Downtown Hotel	S	M	Tu	W	Th
STRETCH Your Students' Polymer Knowledge by Putting Some BOUNCE into Your Curriculum**		E			
Successful Student Chapters		E			
Chemistry Education Research: Graduate Student Research Forum			A		
ACS-CEI Award for Incorporating Sustainability into Chemistry Education**			A		
Citizens First: Communicating Climate Science to the Public** CNR			A		
George C. Pimentel Award in Chemical Education: Honoring I. Dwaine Eubanks**			D		
GSSPC: Designed by Nature, Developed by Science: Interdisciplinary Perspectives on Biocatalysis**			D		
NSF Programs that Support Undergraduate Education			D		
Overcoming Obstacles in Student Learning in Physical Chemistry			P		
Perspectives on Climate Change Literacy & Education: Local to International			P		
General Papers			E		A
Instructors & Researchers: Advancing Graduate Education in Chemistry				A	
Process-Oriented Guided Inquiry Learning (POGIL)				A	
Using Technology in the Undergraduate Laboratory				A	
Computational Chemistry in the Undergraduate Curriculum: What Is Working & How Do We Assess It?**				D	
Green Chemistry: Theory & Practice**				D	
Undergraduate Research in Chemistry: Expanding Opportunities & Broadening Participation				P	
Nanotechnology in Undergraduate Education & Research				P	
Research on Learning in the Laboratory				P	
Undergraduate Symposium* (AGFD)	A				

Division of Chemical Education (continued) CHED

W. Jones, I. Levy, A. Marsh, Program Chairs

Sheraton Denver Downtown Hotel	S	M	Tu	W	Th
Growing Opportunities for Research Abroad: An Undergraduate Perspective of International Research Experiences* (IAC)	D				
Graduate Student Symposium* (AGFD)	P				
Diversifying STEM: Uniting through Our Differences for a Brighter Scientific Future* (CMA)		A			
Environmental Chemistry: Pedagogical Models & Practices* (ENVR)				E	A

Division of Chemical Health & Safety CHAS

D. Decker, F. Wood-Black, J. Pickel, Program Chairs

Embassy Suites Denver – Downtown Convention Center	S	M	Tu	W	Th
Legalized Marijuana & Health & Safety**		P			
Sci-Mix		E			
Safety in Undergraduate Teaching**			P		
Ask Dr. Safety: EH&S Support of Nanotechnology R&D**			A		
Nanotechnology: Delivering on the Promise* (PRES)	P	D			

Division of Chemical Information CINF

E. Bolstad, Program Chair

Colorado Convention Center	S	M	Tu	W	Th
Getting to the Best Reaction: Tools for Finding a Needle in a Haystack	A				
Defining "Value" in Scholarly Communications: Evolving Ways of Evaluating Impact on Science	P				
Research Results: Reproducibility, Reporting, Sharing & Plagiarism		D	A		
Sci-Mix		E			
Molecular & Structural 2D & 3D Chemical Fingerprinting: Computational Storing, Searching & Comparing Molecular & Chemical Structures			P		

Division of Chemical Information (continued) — CINF

E. Bolstad, Program Chair

Colorado Convention Center	S	M	Tu	W	Th
Development & Use of Data Format Standards for Cheminformatics				D	
Drug Discovery* (COMP)	D	D	D	D	

Division of Chemical Toxicology — TOXI

A. C. Bryant-Friedrich, Program Chair

Located with Primary Sponsor	S	M	Tu	W	Th
Forensic Toxicology of Marijuana* (SOCED)		A			

Division of Chemistry & the Law — CHAL

K. Bianco, J. Hasford, Program Chairs

Embassy Suites Denver – Downtown Convention Center	S	M	Tu	W	Th
Strengthening Your Patent Rights in Light of Recent Federal Circuit Court Decisions	A				
Hot Topics in Chemical and Pharmaceutical Patent Law	P				
A Patent Litigation Primer		A			
Anti-Doping: A Unique Combination of Chemistry and the Law		P			
Sci-Mix		E			
Fundamental Concepts in Protecting Chemical Technologies			A		
Legal and Business Considerations for Chemical Technologies			P		
Patenting Chemical Inventions				A	
Intellectual Property and Natural Resources: What Can I Protect and How?				P	
The Many Faces of CHAL: Where Chemistry Meets the Law					A
The Interface of Chemical & Biological Sciences International Disarmament Efforts* (IAC)			D		

Division of Colloid & Surface Chemistry — COLL

R. Nagarajan, Program Chair

Marriott City Center Denver	S	M	Tu	W	Th
Particles at Fluid Interfaces**	D	A			
Biomembrane Synthesis, Structure, Mechanics & Dynamics	D	D	A	D	
Molecular Engineering of Peptide Assembly	D	D	A		
Functionalization of Complex Nanosurfaces**	D	D	A		
Basic Research in Colloids, Surfactants & Nanomaterials**	D			A	D
Metallic Nanostructures for Optical & Electrochemical Sensing & Alternative Energy Conversion**	DE	D	A	D	
ACS Award in Colloid & Surface Chemistry: Honoring Paul S. Weiss	P	D	D		
Plasmonic Catalysis & Sensing	E	D	A	D	
Interfacial Biomolecular Recognition**	E		A	D	D
Fundamental Research in Colloids, Surfaces & Nanomaterials**	E				
Advances in Formulations Science & Technology**		P			
Sci-Mix		E			
Natural Resource Capture, Storage & Energy Conversion				D	D
Elucidation of Mechanisms & Kinetics on Surfaces**				D	
Chemical Processes at Environmental Interfaces* (ENVR)	D	A		E	
Role of Membrane in Amyloid-Formation & the Pathogenicity of Amyloid Disease* (PHYS)	D	D	P		
Nanotechnology: Delivering on the Promise* (PRES)	P	D			
WCC Rising Stars Awards Symposium* (WCC)		D			
Molecular-Scale Processes Controlling Reactivity at Mineral-Water Interfaces* (GEOC)			D	D	

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Division of Computers in Chemistry — COMP

E. Esposito, S. Wildman, Program Chairs

Colorado Convention Center	S	M	Tu	W	Th
Molecular Mechanics**	D	A		A	
Computational Design, Discovery & Optimization of Organic Semiconductor Materials**	D	A			
Drug Discovery**	D	D	D	D	
Electronic Structure Methods for Highly Polarizable Systems**	D	D			
Quantum Chemistry**	P	P	P	D	
ACS Award for Research at an Undergraduate Institution: Honoring George C. Shields		P	D		
ACS Award for Computers in Chemical & Pharmaceutical Research: Honoring David A. Case**		P	D		
Sci-Mix		E			
Computational Study of Water			A	A	
Materials Science			D		
The Chemical Computing Group Excellence Award for Graduate Students			E		
The OpenEye Outstanding Junior Faculty Award			E		
Poster Session			E		
NVIDIA GPU Award			E		
Computational Pyrolysis & Upgrading of Bio-Oils** CNR				D	
Symposium Organizer Selections				P	
Membranes				P	
Modeling Excited States of Complex Systems* (PHYS)	D	D	P	D	A
Role of Membrane in Amyloid-Formation & the Pathogenicity of Amyloid Disease* (PHYS)	D	D	P		
Computational Chemical Dynamics: Advancing Our Understanding of Chemical Processes in Gas-Phase, Biomolecular & Condensed-Phase Systems* (PHYS)	D	D		D	A
Modeling Complex Biomolecules: From Structure to Dynamics & Function* (PHYS)	D	D		D	A
Undergraduate Research Posters* (CHED)		P			
Phenolic & Polyphenolic Chemistry in Food Processing* (AGFD)			D		

Division of Energy & Fuels — ENFL

A. Park, Program Chair

Colorado Convention Center	S	M	Tu	W	Th
Catalysis for Unconventional Energy Sources** CNR	D	A			
Nanomaterials for Solar Energy Conversion & Storage** CNR	D	D	D	D	A
Materials & Interfaces in Lithium Batteries & Beyond	D	D	D	D	A
Hybrid Functional Porous Materials for Sustainable Energy: Carbon, MOF & Conductive Polymers	D	D			
Negative Carbon Emission Technologies: BECCS (Bio-Energy with Carbon Capture & Storage)** CNR	D				
Chemistry of Energy & Fuels	D				
Enhanced Extraction & Utilization of Unconventional Energy Sources: Hydrofracking, EOR & Novel Approaches** CNR		A			
ENFL Distinguished Researcher Award: Honoring James Burrington		D	A		
Two-Dimensional Materials for Energy & Fuel		P	D	D	A
Sci-Mix		E			
C1 Chemistry**			D	D	A
Advances in the Chemistry of Energy & Fuels			P		
12th International Symposium on Heavy Oil Upgrading, Production & Characterization** CNR				D	A
Nanotechnology: Delivering on the Promise* (PRES)	P	D			
Biomass to Fuel & Products* (SOCED)		A			
Sustainability in the 21st Century: Optimizing Complex Interdependent Systems* (SOCED)		P			
DOE Nanoscience Research Centers: National Resources for the Nanoscience Community* (PRES)			A		
Energy & Materials* (POLY)			DE	D	D
Computational Pyrolysis & Upgrading of Bio-Oils* (COMP)				D	

Division of Environmental Chemistry — ENVR

S. Al-Abed, Program Chair

Colorado Convention Center	S	M	Tu	W	Th
Chemical Processes at Environmental Interfaces** CNR	D	A		E	
Green Chemistry & the Environment** CNR	D	A		E	
Environmental Reactivity of Organic Micropollutants & Their Transformation Products in Receiving Waters** CNR	D			E	
Assessing Toxicity of Environmental Contaminants** CNR	D			E	
Biogenically Enhanced Recovery & Bioremediation in Fossil Fuel Reservoirs** CNR	D			E	
Environmental Chemistry & Health Impacts of Fine & Ultrafine Particulate Matter** CNR		A		E	
Modern Analytical Approaches for the Characterization of Natural Organic Matter in the Environment** CNR		D	A	E	
Hydraulic Fracturing Impacts on Water, Soil & Air Quality** CNR		D	D		
Solutions to Metals Contamination of Water** CNR		P	D	E	
Dispersion of Nanoparticles & Its Implication for Interfacial, Biological & Environmental Processes		P	D		
Chemistry in the Marine Boundary Layer** CNR		P		E	
Sci-Mix		E			
Advances in Analytical Chemistry for Discovering Emerging Contaminants in the Natural Environment** CNR			D	E	
Environmental Implications of Nano: Release from Consumer Products & Advances in Nanometrology				AE	
Surface Physicochemical Processes in Engineered & Natural Systems** CNR				D	A
Microalgae: A Renewable Energy Source & a Sustainable Solution for the Environment** CNR				D	
Trace Materials in Air, Soil & Water** CNR				D	
Water Sustainability in Oil & Gas Exploration: Treatment Issues** CNR				DE	
Water Recycling in Domestic Use, Energy Extraction & Agricultural Use** CNR				E	A

Division of Environmental Chemistry (continued) — ENVR

S. Al-Abed, Program Chair

Colorado Convention Center	S	M	Tu	W	Th
Bioavailability and Biogeochemical Interactions Affecting Remediation of Hazardous Substances in the Environment** CNR				E	A
Environmental Chemistry: Pedagogical Models & Practices** CNR				E	A
General Posters				E	
Undergraduate Research Posters* (CHED)		P			
GSSPC: Designed by Nature, Developed by Science: Interdisciplinary Perspectives on Biocatalysis* (CHED)			D		
Elucidation of Mechanisms & Kinetics on Surfaces* (COLL)				D	

Division of Fluorine Chemistry — FLUO

V. Petrov, Program Chair

Embassy Suites Denver – Downtown Convention Center	S	M	Tu	W	Th
ACS Award for Creative Work in Fluorine Chemistry: Honoring Véronique Gouverneur**	D				
Sci-Mix		E			
ACS Award for Creative Research & Applications of Iodine Chemistry: Honoring Karl O. Christe**			D		

Division of Geochemistry — GEOC

S. Kerisit, Program Chair

Colorado Convention Center	S	M	Tu	W	Th
Coupled Cycling of Biogeochemical Critical Elements & Contaminants CNR	D	A			

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Division of Geochemistry (continued) GEOC

S. Kerisit, Program Chair

Colorado Convention Center	S	M	Tu	W	Th
Understanding the Geochemical Interactions of Organic Compounds in the Subsurface** CNR	D				
Geochemistry & Reactive Transport in Nano-Pore Geomaterials** CNR		A			
2015 Geochemistry Division Medal Symposium		P			
Sci-Mix		E			
Iron Oxides: Formation, Structure, Reactivity & Applications** CNR			D	D	
Molecular-Scale Processes Controlling Reactivity at Mineral-Water Interfaces** CNR			D	D	
Honoring Donald Sparks, 2015 Geochemistry Medal Recipient			P	D	D
Precipitation, Dissolution & Adsorption under Confinement					D
WCC Rising Stars Awards Symposium* (WCC)		D			
Undergraduate Research Posters* (CHED)		P			

Division of History of Chemistry HIST

S. Rasmussen, Program Chair

Sheraton Denver Downtown Hotel	S	M	Tu	W	Th
HIST Tutorial & General Papers	P				
Chemical Technology in Antiquity** CNR		D			
Sci-Mix		E			
Modern Chemical Warfare: History, Chemistry, Toxicology, Morality			D		
Nanotechnology: Delivering on the Promise* (PRES)	P	D			
George C. Pimentel Award in Chemical Education: Honoring I. Dwaine Eubanks* (CHED)			D		

Division of Industrial & Engineering Chemistry I&EC

P. Smith, Program Chair

Embassy Suites Denver – Downtown Convention Center	S	M	Tu	W	Th
Uranium in Seawater** CNR	D	D			
ACS Award in Separations Science & Technology: Honoring Richard D. Noble	D				
Sci-Mix		E			
E.V. Murphree Award in Industrial & Engineering Chemistry: Honoring Joseph R. Zoeller**			D		
General Posters			E		
General Papers				D	
Nanotechnology: Delivering on the Promise* (PRES)	P	D			
ACS Award in Industrial Chemistry: Honoring Thomas J. Colacot* (BMGT)		D			
GSSPC: Designed by Nature, Developed by Science: Interdisciplinary Perspectives on Biocatalysis* (CHED)			D		

Division of Inorganic Chemistry INOR

S. Koch, N. Radu, Program Chairs

Colorado Convention Center	S	M	Tu	W	Th
Environmental & Energy-Related Inorganic Chemistry CNR	A		E	P	
Organometallic Chemistry	AE		E	D	A
Chemistry of Materials	AE			P	D
Chemical Approaches to Spintronics Research	D	P	A		
ACS Award in Organometallic Chemistry: Honoring William J. Evans	D	P	A		
ACS Award in Inorganic Chemistry: Honoring John T. Groves	D	P			
Earth-Abundant Materials for Sustainable Hydrogen Production & Storage CNR	D		E		
Harry Gray Award for Creative Work in Inorganic Chemistry by a Young Investigator: Honoring Emily A. Weiss**	D				
Undergraduate Research at the Frontiers of Inorganic Chemistry	DE	P	D		
2015 Priestley Medalist: Honoring Jacqueline K. Barton	DE	P	D		

Division of Inorganic Chemistry (continued) INOR

S. Koch, N. Radu, Program Chairs

Colorado Convention Center	S	M	Tu	W	Th
ACS Award in the Chemistry of Materials: Honoring Mark E. Thompson	P				
Division of Inorganic Chemistry Celebration of the Gabor A. Somorjai Award: Honoring Maurice Brookhart	P				
Lanthanide & Actinide Chemistry	PE			P	P
ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry: Honoring Kim R. Dunbar**	E	P	D	A	
Bioinorganic Chemistry	E	P	E		A
Coordination Chemistry	E		E	A	D
Nanoscience**	E		E	D	D
Inorganic Spectroscopy	E			P	
ACS National Awards in Inorganic Chemistry: Plenary Session		A			
F. Albert Cotton Award in Synthetic Inorganic Chemistry: Honoring Jaqueline L. Kiplinger**		P	D		
Interactions of Metal Complexes with Proteins or Nucleic Acids		P	DE	A	
Division of Inorganic Chemistry Celebration of the Alfred Bader Award in Bioinorganic or Bioorganic Chemistry: Honoring Michael A. Marletta		P			
Sci-Mix		E			
Chemistry of the Energy Water Nexus: Focus on Fracking** CNR			D		P
Molecular Catalysts for Solar Fuels**			DE	A	
Soluble Inorganic Semiconductors: Synthesis, Properties & Applications			DE		
Solid-State Inorganic Chemistry			PE	A	
Inorganic Catalysts			PE	P	A
Electrochemistry			E	P	
Main Group Chemistry			E		A
Department, University & National Models for Faculty Development To Support Adoption of Evidence-Based Teaching* (CHED)	P				

Division of Inorganic Chemistry (continued) INOR

S. Koch, N. Radu, Program Chairs

Colorado Convention Center	S	M	Tu	W	Th
WCC Rising Stars Awards Symposium* (WCC)		D			
Undergraduate Research Posters* (CHED)		P			
ACS Award for Creative Research & Applications of Iodine Chemistry: Honoring Karl O. Christe* (FLUO)			D		

Division of Medicinal Chemistry MEDI

W. Young, Program Chair

Colorado Convention Center	S	M	Tu	W	Th
Applications of Positron Emission Tomography in Drug Discovery	A				
Targeting the Microbiome	A				
General Oral Session	D			D	
Young Investigators in Medicinal Chemistry**	P				
Biased Agonism: An Emerging Paradigm in GPCR Drug Discovery	P				
General Poster Session	E			E	
Approaches To Targeting RNA with Small Molecules		A			
Innate Potential: Advances in Non-Biologic Modulation of Innate Immune Targets		A			
Recent Advances in Targeting the Nav1.7 Sodium Channels		A			
Honoring Richard Gibbs		P			
Modulators of the Nuclear Receptor RORc		P			
New Models for Drug Discovery: Public, Private & Non-Profit		P			
Sci-Mix		E			
E. B. Hershberg Award for Important Discoveries in Medicinally Active Substances: Honoring Ruth R. Wexler**			A		

Division of Medicinal Chemistry (continued) — MEDI

W. Young, Program Chair

Colorado Convention Center	S	M	Tu	W	Th
Observations from Recent Drug Launches: The Rules of Today May Not Apply Tomorrow			A		
Why You Should Have Paid Attention in P-Chem: Thermodynamics in Drug Discovery			A		
Smissman Award: Honoring Dennis Liotta			P		
The Role of Rings in Drug Design			P		
Advances in the Treatment of Fibrotic Diseases				A	
Small Molecule Approaches to Autism Spectrum Disorder Therapy				A	
First Time Disclosures				P	
MEDI Award Symposium				P	
Drug Discovery* (COMP)	D	D	D	D	
Medicinal & Aromatic Crops: Production, Phytochemistry & Utilization* (AGFD)		D			
Undergraduate Research Posters* (CHED)		P			
Phenolic & Polyphenolic Chemistry in Food Processing* (AGFD)			D		
GSSPC: Designed by Nature, Developed by Science: Interdisciplinary Perspectives on Biocatalysis* (CHED)			D		

Division of Nuclear Chemistry & Technology — NUCL

J. Braley, D. Hobart, Program Chairs

Embassy Suites Denver – Downtown Convention Center	S	M	Tu	W	Th
Glenn T. Seaborg Award for Nuclear Chemistry: Honoring Heino Nitsche	D	D			
Nuclear Forensics	P	D			
50th Anniversary of the NUCL Division			D	D	
Convergence of Theory & Experiment in Heavy Element Chemistry				D	A
Uranium in Seawater* (I&EC)	D	D			
Chemical Tales of Success: Helpful Tips for Younger Chemists* (YCC)			A		

Division of Organic Chemistry — ORGN

M. McIntosh, R. Broene, Program Chairs

Colorado Convention Center	S	M	Tu	W	Th
Materials, Devices & Switches	A				
New Reactions & Methodology	D	D	A	A	
Asymmetric Reactions & Syntheses	D				
Nanomaterials	P				
Development of Direct C-H Functionalization Processes towards the Synthesis of Biologically Active Compounds	P				
Ronald Breslow Award for Achievement in Biomimetic Chemistry: Honoring Eric T. Kool	P				
Asymmetric Reactions & Syntheses; Chemistry of Fullerenes, Carbon Nanotubes & Graphene; Materials, Devices & Switches; Nanomaterials; Physical Organic Chemistry: Calculations, Mechanisms, Photochemistry & High-Energy Species; Total Synthesis of Complex Molecules	E				
Elias J. Corey Award for Outstanding Original Contribution in Organic Synthesis by a Young Investigator: Honoring Jin-Quan Yu		A			
Miniaturization in Chemistry: Sub-Nanoscale Synthesis, Analysis & Application		A			
Physical Organic Chemistry: Calculations, Mechanisms, Photochemistry & High-Energy Species		D	A		
Molecular Recognition & Self-Assembly		D			
Synthetic Biology Applied to Natural & Unnatural Product Pathways		P			
Herbert C. Brown Award for Creative Research in Synthetic Methods: Honoring Gary A. Molander		P			
Sci-Mix		E			
ACS Award for Creative Invention: Honoring Jotham W. Coe			A		
ACS Award for Creative Work in Synthetic Organic Chemistry: Honoring F. Dean Toste			A		
Biologically-Related Molecules & Processes			D		

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Division of Organic Chemistry (continued) ORGN

M. McIntosh, R. Broene, Program Chairs

Colorado Convention Center	S	M	Tu	W	Th
Metal-Mediated Reactions & Syntheses			P	D	
Green Chemistry: Reactions in Alternative Media			P		
James Flack Norris Award in Physical Organic Chemistry: Honoring Charles L. Perrin			P		
Ernest Guenther Award in the Chemistry of Natural Products: Honoring Thomas R. Hoye			P		
Biologically Related Molecules & Processes; Chemistry of Natural Resources; Metal-Mediated Reactions & Syntheses; Molecular Recognition & Self-Assembly; Peptides, Proteins & Amino Acids CNR			E		
National Fresenius Award: Honoring Abigail G. Doyle**				A	
Total Synthesis of Complex Molecules				A	
Heterocycles & Aromatics				D	
ACS Award for Creative Invention: Honoring Jotham W. Coe				P	
Peptides, Proteins & Amino Acids				P	
Heterocycles & Aromatics; New Reactions & Methodology				E	
Department, University & National Models for Faculty Development To Support Adoption of Evidence-Based Teaching* (CHED)	P				
WCC Rising Stars Awards Symposium* (WCC)		D			
GSSPC: Designed by Nature, Developed by Science: Interdisciplinary Perspectives on Biocatalysis* (CHED)			D		

Division of Physical Chemistry PHYS

E. Sibert, Program Chair

Colorado Convention Center	S	M	Tu	W	Th
Atmospheric Chemistry: Transformations of Matter in the Troposphere	D	D	P	D	A
Modeling Excited States of Complex Systems**	D	D	P	D	A
Role of Membrane in Amyloid-Formation & the Pathogenicity of Amyloid Disease**	D	D	P		
Computational Chemical Dynamics: Advancing Our Understanding of Chemical Processes in Gas-Phase, Biomolecular & Condensed-Phase Systems**	D	D		D	A
Modeling Complex Biomolecules: From Structure to Dynamics & Function**	D	D		D	A
Carbon in the Galaxy: The Formation of Complex Organics from the Outflow of Carbon Stars & Their Evolution	D	D		D	A
Probing Nano-Plasmonic Phenomena at the Single Molecule, Single Electron & Single Photon Level	D	D		D	A
Design of Materials & Chemical Processes: The Genomic Approach	D	D		D	
Sci-Mix		E			
PHYS Award Symposium			A		
Physical Electrochemistry of Electrocatalytic Processes			P	D	A
Ahmed Zewail Prize in Molecular Sciences			P		
Physical Chemistry Poster Session				E	
Molecular Mechanics* (COMP)	D	A		A	
Computational Design, Discovery & Optimization of Organic Semiconductor Materials* (COMP)	D	A			
Electronic Structure Methods for Highly Polarizable Systems* (COMP)	D	D			
Quantum Chemistry* (COMP)	P	P	P	D	
WCC Rising Stars Awards Symposium* (WCC)		D			
ACS Award for Computers in Chemical & Pharmaceutical Research: Honoring David A. Case * (COMP)		P	D		
Computational Chemistry in the Undergraduate Curriculum: What Is Working & How Do We Assess It?* (CHED)				D	

Division of Polymer Chemistry — POLY

M. Jeffries-El, D. Boday, T. White, Program Chairs

Sheraton Denver Downtown Hotel	S	M	Tu	W	Th
Putting Renewable Polymers To Work	D	A	E		
Macromolecular & Nanoparticle Separation Science**	D	D	DE		
Next Generation Smart Materials**	D	D	E	D	D
General Topics: New Synthesis & Characterization of Polymers	D		AE	E	
Celebrating the Fifth Year Anniversary of Polymer Chemistry (RSC)	D				
Electrical, Thermal & Mass Transport in Polymer Nanocomposites & Alloys**		D	E		
Excellence in Graduate Polymer Research**		D	E		
Innovations in Macromolecular Network Chemistry**		P	E	P	D
Sci-Mix		E			
Carl S. Marvel Creative Polymer Chemistry Award in Honor of Todd Emrick			D		
Energy & Materials**			DE	D	D
Undergraduate Research in Polymer Science**			DE		
Polymer Composites & High Performance Materials			PE	D	D
Interacting with the Immune System Using Polymeric Systems			E	D	D
POLY/PMSE Plenary Lecture & Awards Reception**				E	
Nanotechnology: Delivering on the Promise* (PRES)	P	D			
Integrating Chemistry & Polymer Science Research into the Classroom* (CHED)		A			
Undergraduate Research Posters* (CHED)		P			
STRETCH Your Students' Polymer Knowledge by Putting Some BOUNCE into Your Curriculum* (CHED)		E			
Joint PMSE/POLY Poster Session* (PMSE)			E		

Division of Polymeric Materials: Science & Engineering — PMSE

A. Tsou, Q. Lin, C. Stafford, M. Becker, Program Chairs

Sheraton Denver Downtown Hotel	S	M	Tu	W	Th
Design Principles of Functional Macromolecular Materials	D	D	A		
Stimulus-Responsive Assemblies & Materials	D	D	D		
Advances in X-ray & Neutron Scattering Techniques for Elucidating Polymer Morphology	D	D	D		
Graphene & Carbon Nanotubes: Synthesis, Devices & Applications	D	D			
Nanostructured Porous Polymers: Synthesis, Properties & Applications	D	D			
ACS Award in Applied Polymer Science: Honoring Geoffrey W. Coates	D				
General Papers/New Concepts in Polymeric Materials	P	D		D	A
Cooperative Research Award: Honoring Andy Tsou & Benjamin Hsiao		A			
Polymeric Biomaterials**		P	D	D	A
Sci-Mix		E			
Nanoscale Spectroscopic & Microscopic Characterization			D	D	
Polymer Modeling: Structure, Dynamics & Function			D	D	
ACS Award in Polymer Chemistry: Honoring Nikos Hadjichristidis			D	D	
Drug Delivery & Drug Device Combination Products			P	D	A
Joint PMSE/POLY Poster Session**			E		
Macromolecular & Nanoparticle Separation Science* (POLY)	D	D	DE		
Next Generation Smart Materials* (POLY)	D	D	E	D	D
Integrating Chemistry & Polymer Science Research into the Classroom* (CHED)		A			
WCC Rising Stars Awards Symposium* (WCC)		D			
Innovations in Macromolecular Network Chemistry* (POLY)		P	E	P	D

*Cosponsored symposium with primary organizer shown in parentheses; located with primary organizer.
**Primary organizer of a cosponsored symposium.

CNR: Chemistry of Natural Resources

A = AM AE = AM/EVE P = PM D = AM/PM
E = EVE DE = AM/PM/EVE PE = PM/EVE

Division of Polymeric Materials: Science & Engineering (continued) PMSE

A. Tsou, Q. Lin, C. Stafford, M. Becker, Program Chairs

Sheraton Denver Downtown Hotel	S	M	Tu	W	Th
Undergraduate Research Posters* (CHED)		P			
STRETCH Your Students' Polymer Knowledge by Putting Some BOUNCE into Your Curriculum* (CHED)		E			
Smart & Responsive Composites from Renewable Building Blocks* (CELL)			A	D	
Energy & Materials* (POLY)			DE	D	D
POLY/PMSE Plenary Lecture & Awards Reception* (POLY)				E	

Division of Professional Relations PROF

R. D. Libby, Program Chair

Hyatt Regency Denver at Colorado Convention Center	S	M	Tu	W	Th
Native American Women Chemists of Color**	A				
Earning ACS Awards: An Interactive Symposium on Constructing Successful Award Nominations**	P				
ACS Award for Encouraging Women into Careers in the Chemical Sciences: Honoring E. Ann Nalley**		A	A		
Chemical Angel Network: Chemists Investing in Chemical Companies**		P			
Proposing & Administering a Successful REU Program			P		
Hands-On STEM Enrichment Programs for Persons with Disabilities				P	
Growing Opportunities for Research Abroad: An Undergraduate Perspective of International Research Experiences* (IAC)	D				
Best Practices for Success with SBIR & STTR Grants* (SCHB)	P				
Starting a Successful Research Program at a Predominantly Undergraduate Institution* (YCC)	P				
Diversifying STEM: Uniting through our Differences for a Brighter Scientific Future* (CMA)		A			

Division of Professional Relations (continued) PROF

R. D. Libby, Program Chair

Hyatt Regency Denver at Colorado Convention Center	S	M	Tu	W	Th
Kathryn C. Hach Award for Entrepreneurial Success: Honoring Terry L. Brewer* (SCHB)		A			
Excellence in Graduate Polymer Research* (POLY)		D	E		
WCC Rising Stars Awards Symposium* (WCC)		D			

Rubber Division RUBB

T. R. DeLapa, Program Chair

Located with Primary Sponsor	S	M	Tu	W	Th
STRETCH Your Students' Polymer Knowledge by Putting Some BOUNCE into Your Curriculum* (CHED)		E			

Division of Small Chemical Businesses SCHB

J. Sabol, Program Chair

Embassy Suites Denver – Downtown Convention Center	S	M	Tu	W	Th
Best Practices for Success with SBIR & STTR Grants**	P				
Entrepreneurs' Poster Session**	P				
Kathryn C. Hach Award for Entrepreneurial Success: Honoring Terry L. Brewer**		A			
Water Is the Next Oil: Small Businesses Percolating to the Top** CNR		P			
Sci-Mix		E			
Nanotechnology: Delivering on the Promise* (PRES)	P	D			

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E = EVE DE = AM/PM/EVE PE = PM/EVE

Division of Small Chemical Businesses (continued) SCHB

J. Sabol, Program Chair

Embassy Suites Denver – Downtown Convention Center	S	M	Tu	W	Th
Earning ACS Awards: An Interactive Symposium on Constructing Successful Award Nominations* (PROF)	P				
Chemical Angel Network: Chemists Investing in Chemical Companies* (PROF)		P			
Chemical Tales of Success: Helpful Tips for Younger Chemists* (YCC)			A		

Committee on Chemical Safety C C S

E. Howson, Program Chair

Located with Primary Sponsor	S	M	Tu	W	Th
Nanotechnology: Delivering on the Promise* (PRES)	P	D			
Legalized Marijuana & Health & Safety* (CHAS)		P			
Safety in Undergraduate Teaching* (CHAS)			P		
Ask Dr. Safety: EH&S Support of Nanotechnology R&D* (CHAS)			A		

Committee on Chemistry & Public Affairs CCPA

S. Butts, Program Chair

Located with Primary Sponsor	S	M	Tu	W	Th
Nanotechnology: Delivering on the Promise* (PRES)	P	D			
DOE Nanoscience Research Centers: National Resources for the Nanoscience Community* (PRES)			A		

Committee on Corporation Associates CORP

D. Mason, Program Chair

Located with Primary Sponsor	S	M	Tu	W	Th
Nanotechnology: Delivering on the Promise* (PRES)	P	D			

Committee on Divisional Activities D A C

M. J. Morello, Program Chair

Located with Primary Sponsor	S	M	Tu	W	Th
Frontiers in Glycoscience* (CELL)		D	D		

Committee on Environmental Improvement C E I

C. Middlecamp, Program Chair

Located with Primary Sponsor	S	M	Tu	W	Th
Green Chemistry & the Environment* (ENVR)	D	A		E	
Uranium in Seawater* (I&EC)	D	D			
Assessing Toxicity of Environmental Contaminants* (ENVR)	D			E	
DOE Nanoscience Research Centers: National Resources for the Nanoscience Community* (PRES)			A		
ACS-CEI Award for Incorporating Sustainability into Chemistry Education* (CHED)			A		
Citizens First: Communicating Climate Science to the Public* (CHED)			A		
Green Chemistry: Theory & Practice* (CHED)				D	
Water Sustainability in Oil & Gas Exploration: Treatment Issues* (ENVR)				DE	

Committee on Minority Affairs C M A

J. Sarquis, Program Chair

Hyatt Regency Denver at Colorado Convention Center	S	M	Tu	W	Th
Diversifying STEM: Uniting through Our Differences for a Brighter Scientific Future**		A			
Native American Women Chemists of Color* (PROF)	A				
ACS Award for Encouraging Disadvantaged Students in Chemistry: Honoring Catherine H. Middlecamp* (CHED)		P			

Committee on Science — COMSCI

D. Crans, Program Chair

Colorado Convention Center	S	M	Tu	W	Th
Transitioning between Academic Research into Practical Use: Solar Energy & Advanced Materials**		A			
The Transnational Practice of Chemistry & Allied Sciences & Engineering: Study, Research & Careers without Borders* (PRES)	A				
Nanotechnology: Delivering on the Promise* (PRES)	P	D			

International Activities Committee — IAC

H.N. Cheng, Program Chair

Hyatt Regency Denver at Colorado Convention Center	S	M	Tu	W	Th
Growing Opportunities for Research Abroad: An Undergraduate Perspective of International Research Experiences**	D				
The Interface of Chemical & Biological Sciences International Disarmament Efforts**			D		
The Transnational Practice of Chemistry & Allied Sciences & Engineering: Study, Research & Careers without Borders* (PRES)	A				
Nanotechnology: Delivering on the Promise* (PRES)	P	D			

Senior Chemists Committee — SCC

G. Heinze, Program Chair

Located with Primary Sponsor	S	M	Tu	W	Th
STRETCH Your Students' Polymer Knowledge by Putting Some BOUNCE into Your Curriculum* (CHED)		E			

Society Committee on Education — SOCED

D. Swartling, Program Chair

Sheraton Denver Downtown Hotel	S	M	Tu	W	Th
Forensic Toxicology of Marijuana** CNR		A			
Biomass to Fuel & Products** CNR		A			
Sustainability in the 21st Century: Optimizing Complex Interdependent Systems** CNR		P			
The Transnational Practice of Chemistry & Allied Sciences & Engineering: Study, Research & Careers without Borders* (PRES)	A				
Undergraduate Research Papers* (CHED)	D	D			
High School Program* (CHED)	D				
Nanotechnology: Delivering on the Promise* (PRES)	P	D			
Excellence in Graduate Polymer Research* (POLY)		D	E		
Undergraduate Research Posters* (CHED)		P			

Women Chemists Committee — WCC

K. Woznack, A. Debaillie, Program Chairs

Colorado Convention Center	S	M	Tu	W	Th
WCC Rising Stars Awards Symposium**		D			
Native American Women Chemists of Color* (PROF)	A				
Harry Gray Award for Creative Work in Inorganic Chemistry by a Young Investigator: Honoring Emily A. Weiss* (INOR)	D				
ACS Award for Creative Work in Fluorine Chemistry: Honoring Véronique Gouverneur* (FLUO)	D				
ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry: Honoring Kim R. Dunbar* (INOR)	E	P	D	A	

Women Chemists Committee (continued) W C C

K. Woznack, A. Debaillie, Program Chairs

Colorado Convention Center	S	M	Tu	W	Th
ACS Award for Encouraging Women into Careers in the Chemical Sciences: Honoring E. Ann Nalley* (PROF)		A	A		
ACS Award for Achievement in Research for the Teaching & Learning of Chemistry: Honoring Vickie M. Williamson* (CHED)		D			
F. Albert Cotton Award in Synthetic Inorganic Chemistry: Honoring Jaqueline L. Kiplinger* (INOR)		P	D		
ACS Award for Encouraging Disadvantaged Students in Chemistry: Honoring Catherine H. Middlecamp* (CHED)		P			
E. B. Hershberg Award for Important Discoveries in Medicinally Active Substances: Honoring Ruth R. Wexler* (MEDI)			A		
National Fresenius Award: Honoring Abigail G. Doyle * (ORGN)				A	
Frank H. Field & Joe L. Franklin Award for Outstanding Achievement in Mass Spectrometry: Honoring Hilkka I. Kenttämaa* (ANYL)				P	

Younger Chemists Committee Y C C

T. Matos, A. Gavrilenko, Program Chairs

Hyatt Regency Denver at Colorado Convention Center	S	M	Tu	W	Th
Starting a Successful Research Program at a Predominantly Undergraduate Institution**	P				
Chemical Tales of Success: Helpful Tips for Younger Chemists**			A		
Growing Opportunities for Research Abroad: An Undergraduate Perspective of International Research Experiences* (IAC)	D				
Young Investigators in Medicinal Chemistry* (MEDI)	P				
Best Practices for Success with SBIR & STTR Grants* (SCHB)	P				
Entrepreneurs' Postor Session* (SCHB)	P				

Younger Chemists Committee (continued) Y C C

T. Matos, A. Gavrilenko, Program Chairs

Hyatt Regency Denver at Colorado Convention Center	S	M	Tu	W	Th
Kathryn C. Hach Award for Entrepreneurial Success: Honoring Terry L. Brewer* (SCHB)		A			
Excellence in Graduate Polymer Research* (POLY)		D	E		
Water Is the Next Oil: Small Businesses Percolating to the Top* (SCHB)		P			
Environmental Chemistry: Pedagogical Models & Practices* (ENVR)				E	A

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CNR: Chemistry of Natural Resources

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E = EVE DE = AM/PM/EVE PE = PM/EVE

How to Read the Technical Program

1. **Search for the Division—** listed in alphabetical order

3. **Locate the session name**

4. **Locate the time or poster #**

CHAS

Division of Chemical Health and Safety

D.M. Decker, F. K. Wood-Black and J. M. Pickel, *Program Chairs*

MONDAY AFTERNOON

Section A

Embassy Suites Denver–Downtown Convention Center

Silverton Ballroom 1

Legalized Marijuana & Health & Safety

Cosponsored by CCS

N. R. Langerman, R. W. Phifer, *Organizers, Presiding*

1:30 Introductory Remarks.

1:40 CHAS **1.** Taking care of Mary Jane's workers. J. Lieberman

2:10 CHAS **2.** Safety considerations in the development of sensible workplace drug testing

Note: *Times represent the start of oral presentations and numbers represent poster numbers.*

2. **Locate the day**

5. **Locate the venue and room for each session**

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Amy (Vocals)

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ACS looks forward to welcoming you to this very special event, Monday, March 23, from 3:00 p.m. to 4:00 p.m. in the Colorado Convention Center Room 601. New members will network with other Rockstars of Chemistry, such as award winners, published authors, and notable scientists. Light refreshments will be served. Guests will receive reserved seating for the Kavli Lecture Series.

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CHEMISTRY OF NATURAL RESOURCES

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PRES

Presidential Events

D. G. Schmidt, *Program Chair*

SUNDAY MORNING

Section A

Colorado Convention Center
Mile High Ballroom 3A

The Transnational Practice of Chemistry and Allied Sciences and Engineering: Study, Research and Careers without Borders

Building a Global Technical Workforce

Cosponsored by BMGT, COMSCI, IAC and SOCED

J. L. Benham, S. Hill, B. Miller, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 PRES **1.** Global landscape: Chemistry-related transnational mobility and global talent innovation. **J.L. Benham**

8:30 PRES **2.** Building a global technical workforce. **T. Connelly**

9:00 PRES **3.** Science in diplomacy and global relations: "Good guys only win if they work together". **D. Hupaylo**

Section A

Colorado Convention Center
Mile High Ballroom 3A

The Transnational Practice of Chemistry and Allied Sciences and Engineering: Study, Research and Careers without Borders

Attracting and Preparing Chemists for the Global Chemical Enterprise

Cosponsored by BMGT, COMSCI, IAC and SOCED

J. L. Benham, S. Hill, B. Miller, *Organizers, Presiding*

10:00 PRES **4.** School of pharmaceutical science and technology of Tianjin University: A demo project as an international center of excellence in Chin. **J.S. Siegel**

10:30 PRES **5.** From international/multinational ventures to transnational/global chemistry: Lowering activation barriers across national borders. **L. Echegoyen**

11:00 PRES **6.** Chemistry in a global economy: Can our curriculum meet the challenge? **J.S. Francisco**

11:30 PRES **7.** Connecting the dots: Interdisciplinary relationships case study in 21st century global workforce. **A. Phillips Diaz**

12:00 Concluding Remarks.

Basic Research in Colloids, Surfactants & Nanomaterials Metal Nanomaterials

Sponsored by COLL, Cosponsored by PRES

Functionalization of Complex Nanosurfaces

Sponsored by COLL, Cosponsored by PRES

Metallic Nanostructures for Optical & Electrochemical Sensing & Alternative Energy Conversion

Sponsored by COLL, Cosponsored by PRES

Particles at Fluid Interfaces

Sponsored by COLL, Cosponsored by PRES

SUNDAY AFTERNOON

Section A

Colorado Convention Center
Mile High Ballroom 3A

Nanotechnology: Delivering on the Promise

Research & Development

Cosponsored by AGFD, AGRO, ANYL, CARB, CCPA, CCS, CHAS, COLL, COMSCI, CORP, ENFL, HIST, I&EC, IAC, MPPG, PMSE, POLY, SCHB and SOCED

D. G. Schmidt, *Organizer*
L. J. Doemeny, C. Geraci, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 PRES **8.** Nanotechnology: Delivering the promise — R&D. **C.A. Mirkin**

2:05 PRES **9.** NSF: Building foundational knowledge and infrastructure for nanotechnology. **M. Roco**

2:35 PRES **10.** National Institutes of Health: The impact of nanotechnology in biology and medicine. **L. Henderson**

3:05 Intermission.

3:15 PRES **11.** Nanoscience and technology for energy. **H. Kung**

3:45 PRES **12.** Nanomaterials and nanomanufacturing with an emphasis on national security. **L. Sloter**

4:15 Keynote Address. **L. Whitman**

5:00 Discussion.

Basic Research in Colloids, Surfactants & Nanomaterials

Metal Oxide Nanomaterials

Sponsored by COLL, Cosponsored by PRES

Department, University, and National Models for Faculty Development to Support Adoption of Evidence-Based Teaching

Sponsored by CHED, Cosponsored by INOR, ORGN and PRES

Functionalization of Complex Nanosurfaces

Sponsored by COLL, Cosponsored by PRES

Metallic Nanostructures for Optical & Electrochemical Sensing & Alternative Energy Conversion

Sponsored by COLL, Cosponsored by PRES

Particles at Fluid Interfaces

Sponsored by COLL, Cosponsored by PRES

SUNDAY EVENING

Fundamental Research in Colloids, Surfaces & Nanomaterials

Sponsored by COLL, Cosponsored by PRES

Metallic Nanostructures for Optical & Electrochemical Sensing & Alternative Energy Conversion

Sponsored by COLL, Cosponsored by PRES

Nanoscience

Sponsored by INOR, Cosponsored by PRES

MONDAY MORNING

Section A

Colorado Convention Center
Mile High Ballroom 3A

Nanotechnology: Delivering on the Promise

Opportunities and Challenges for Health, Safety and the Environment

Cosponsored by AGFD, AGRO, ANYL, CARB, CCPA, CCS, CHAS, COLL, COMSCI, CORP, ENFL, HIST, I&EC, IAC, MPPG, PMSE, POLY, SCHB and SOCED

D. G. Schmidt, *Organizer*
L. J. Doemeny, C. Geraci, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 PRES **13.** Innovation trends, policies, and practices. **T. Earles**

9:05 PRES **14.** The regulatory void. **L. Bergeson**

9:35 PRES **15.** Adaptive governance. **V. Murashov**

10:05 Intermission.

10:20 PRES **16.** Sustainability and life cycle issues. **J.T. Morris**

10:50 PRES **17.** What is responsible development of nanotechnology? **A. Lin**

11:20 Discussion.

Electrical, Thermal, & Mass Transport in Polymer Nanocomposites & Alloys Barrier and Separation Behavior

Sponsored by POLY, Cosponsored by PRES

Excellence in Graduate Polymer Research

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

Functionalization of Complex Nanosurfaces

Sponsored by COLL, Cosponsored by PRES

Metallic Nanostructures for Optical & Electrochemical Sensing & Alternative Energy Conversion Sensing, Electronics, & Photophysics

Sponsored by COLL, Cosponsored by PRES

Particles at Fluid Interfaces

Sponsored by COLL, Cosponsored by PRES

Plasmonic Catalysis and Sensing

Sponsored by COLL, Cosponsored by PRES

Transitioning between Academic Research

into Practical Use: Solar-Energy and Advanced Materials

Sponsored by COMSCI, Cosponsored by MPPG‡ and PRES

MONDAY AFTERNOON

Section A

Colorado Convention Center
Mile High Ballroom 3A

Nanotechnology: Delivering on the Promise

Bridging the Gap to a Thriving US Marketplace

Cosponsored by AGFD, AGRO, ANYL, CARB, CCPA, CCS, CHAS, COLL, COMSCI, CORP, ENFL, HIST, I&EC, IAC, MPPG, PMSE, POLY, SCHB and SOCED

D. G. Schmidt, *Organizer*
L. J. Doemeny, C. Geraci, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 PRES **18.** Nanomaterials in the marketplace. **M. Philbert**

2:00 PRES **19.** University tech transfer issues. **M. Liehr**

2:30 PRES **20.** Nanotech market forecasting. **B. Giles**

3:00 Intermission.

3:15 PRES **21.** Regulation: Facilitating advancement or serving as a barrier – a shared responsibility. **T.L. Medley**

3:45 PRES **22.** Nanomanufacturing, nanomarkets, and applications. **A. Malshe**

4:15 Discussion.

Advances in Formulations Science & Technology

Sponsored by COLL, Cosponsored by PRES

Electrical, Thermal, & Mass Transport in Polymer Nanocomposites & Alloys Energy, Electrical and Thermal

Sponsored by POLY, Cosponsored by PRES

Excellence in Graduate Polymer Research

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

Functionalization of Complex Nanosurfaces

Sponsored by COLL, Cosponsored by PRES

Metallic Nanostructures for Optical & Electrochemical Sensing & Alternative Energy Conversion Spectroelectrochemistry, Imaging, & Surface

Sponsored by COLL, Cosponsored by PRES

Plasmonic Catalysis and Sensing

Sponsored by COLL, Cosponsored by PRES

TUESDAY MORNING

Section A

Colorado Convention Center
Room 506

DOE Nanoscience Research Centers

National Resources for the Nanoscience Community

Cosponsored by ANYL, CCPA, CEI, ENFL and MPPG

M. V. Buchanan, *Organizer*
G. Maracas, *Organizer, Presiding*

8:30 Introductory Remarks.

8:40 PRES **23.** User opportunities at the Center for Nanophase Materials Sciences: From materials-by-design to neutron nanoscience. **H.M. Christen**

9:10 PRES **24.** Molecular foundry: A knowledge-based user facility for nanoscale science. **J. Neaton**

9:40 PRES **25.** Hybrid nanomaterials and tailoring nanoscale interactions at the Center for Nanoscale Materials. **A. Roelofs**

10:10 Intermission.

10:30 PRES **26.** Nanomaterials integration: A pathway to technological innovation. **N.D. Shinn, Q. Jia**

11:00 PRES **27.** Center for Functional Nanomaterials and its unique capabilities for research on nanomaterials by design and *in operando*. **E. Mendez**

11:30 Concluding Remarks.

Ask Dr. Safety: EH&S Support of Nanotechnology R&D

Sponsored by CHAS, Cosponsored by AGFD, CCS and PRES

Functionalization of Complex Nanosurfaces

Sponsored by COLL, Cosponsored by PRES

GSSPC: Designed by Nature, Developed by Science: Interdisciplinary Perspectives on

Biocatalysis

Sponsored by CHED, Cosponsored by ANYL, BIOL, CATL, ENVR, I&EC, MEDI, ORGN and PRES

Metallic Nanostructures for Optical & Electrochemical Sensing & Alternative Energy Conversion

Biosensing, Energy Conversion & Catalysts

Sponsored by COLL, Cosponsored by PRES

Nanoscience and Nanotechnology of Natural Resources

Sponsored by MPPG, Cosponsored by PRES

Plasmonic Catalysis and Sensing

Sponsored by COLL, Cosponsored by PRES

The Interface of Chemical and Biological

Sciences International Disarmament Efforts

Sponsored by IAC, Cosponsored by ANYL, CHAL, CPRC and PRES

TUESDAY AFTERNOON

Applied Nanotechnology for Food & Agriculture

Sponsored by AGFD, Cosponsored by PRES

GSSPC: Designed by Nature, Developed by Science: Interdisciplinary Perspectives on Biocatalysis

Sponsored by CHED, Cosponsored by ANYL, BIOL, CATL, ENVR, I&EC, MEDI, ORGN and PRES

The Interface of Chemical and Biological Sciences International Disarmament Efforts

Sponsored by IAC, Cosponsored by ANYL, CHAL, CPRC and PRES

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TUESDAY EVENING

Electrical, Thermal, & Mass Transport in Polymer Nanocomposites & Alloys
Sponsored by POLY, Cosponsored by PRES

Excellence in Graduate Polymer Research
Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

WEDNESDAY MORNING

Applied Nanotechnology for Food & Agriculture
Sponsored by AGFD, Cosponsored by PRES

Basic Research in Colloids, Surfactants & Nanomaterials Amphiphilic Systems
Sponsored by COLL, Cosponsored by PRES

Metallic Nanostructures for Optical & Electrochemical Sensing & Alternative Energy Conversion

Biosensing, Catalysts, & Electrochemistry
Sponsored by COLL, Cosponsored by PRES

Nanoscience
Sponsored by INOR, Cosponsored by PRES

Plasmonic Catalysis and Sensing
Sponsored by COLL, Cosponsored by PRES

WEDNESDAY AFTERNOON

Metallic Nanostructures for Optical & Electrochemical Sensing & Alternative Energy Conversion

Fabrication for Biosensing, Energy Conversion & Catalysts
Sponsored by COLL, Cosponsored by PRES

Nanoscience

Metals
Sponsored by INOR, Cosponsored by PRES

Plasmonic Catalysis and Sensing
Sponsored by COLL, Cosponsored by PRES

THURSDAY MORNING

Basic Research in Colloids, Surfactants & Nanomaterials
Sponsored by COLL, Cosponsored by PRES

Nanoscience
Sponsored by INOR, Cosponsored by PRES

THURSDAY AFTERNOON

Basic Research in Colloids, Surfactants & Nanomaterials
Sponsored by COLL, Cosponsored by PRES

Nanoscience Semiconductors
Sponsored by INOR, Cosponsored by PRES

MPPG

Multidisciplinary Program Planning Group

R. Weber, *Program Chair*

SUNDAY MORNING

Assessing Toxicity of Environmental

Contaminants
Sponsored by ENVR, Cosponsored by AGRO, CEI and MPPG‡

Biogenically Enhanced Recovery and Bioremediation in Fossil Fuel Reservoirs
Sponsored by ENVR, Cosponsored by MPPG‡

Catalysis for Un-conventional Energy Sources

Fuel Cell, Solar Cell and Solar Fuel
Sponsored by ENFL, Cosponsored by CATL and MPPG‡

Earth-Abundant Materials for Sustainable Hydrogen Production and Storage
Sponsored by INOR, Cosponsored by MPPG

Environmental Reactivity of Organic Micropollutants and Their Transformation Products in Receiving Waters
Sponsored by ENVR, Cosponsored by AGRO and MPPG‡

Green Chemistry and the Environment
Sponsored by ENVR, Cosponsored by CEI and MPPG

Nanomaterials for Solar Energy Conversion & Storage
Sponsored by ENFL, Cosponsored by MPPG‡

Negative Carbon Emission Technologies: BECCS (Bio-Energy with Carbon Capture & Storage)
Sponsored by ENFL, Cosponsored by MPPG‡

Understanding the Geochemical Interactions of Organic Compounds in the Subsurface
Sponsored by GEOC, Cosponsored by MPPG‡

Uranium in Seawater The Chemistry
Sponsored by I&EC, Cosponsored by CEI, MPPG‡, and NUCL

SUNDAY AFTERNOON

Section A

Colorado Convention Center
Bellco Theatre

Chemistry of Natural Resources Plenary

R. S. Weber, *Organizer, Presiding*

3:00 Introductory Remarks.

3:05 MPPG **1.** Fundamentals of gas hydrates and their role in energy transportation and storage. **C.A. Koh**

3:45 MPPG **2.** Four horsemen of the advanced biofuels apocalypse: Sustainability, technology, profitability, and politics. **P.F. Bryan**

4:25 MPPG **3.** Water in the Anthropocene: too much, too little, too dirty. **P. Kareiva**

5:05 Discussion.

Assessing Toxicity of Environmental Contaminants
Sponsored by ENVR, Cosponsored by AGRO, CEI and MPPG‡

Biogenically Enhanced Recovery and Bioremediation in Fossil Fuel Reservoirs
Sponsored by ENVR, Cosponsored by MPPG‡

Catalysis for Un-conventional Energy Sources

Biofuel and CO_2 Utilization
Sponsored by ENFL, Cosponsored by CATL and MPPG‡

Earth-Abundant Materials for Sustainable Hydrogen Production and Storage
Sponsored by INOR, Cosponsored by MPPG

Environmental Reactivity of Organic

Micropollutants and Their Transformation Products in Receiving Waters
Sponsored by ENVR, Cosponsored by AGRO and MPPG‡

Green Chemistry and the Environment
Sponsored by ENVR, Cosponsored by CEI and MPPG

Nanomaterials for Solar Energy Conversion & Storage
Sponsored by ENFL, Cosponsored by MPPG‡

Nanotechnology: Delivering on the Promise Research & Development
Sponsored by PRES, Cosponsored by AGFD, AGRO, ANYL, CARB, CCPA, CCS, CHAS, COLL, COMSCI, CORP, ENFL, HIST, I&EC, IAC, MPPG, PMSE, POLY, SCHB and SOCED

Negative Carbon Emission Technologies: BECCS (Bio-Energy with Carbon Capture & Storage)
Sponsored by ENFL, Cosponsored by MPPG‡

Understanding the Geochemical Interactions of Organic Compounds in the Subsurface
Sponsored by GEOC, Cosponsored by MPPG‡

Uranium in Seawater

The Sorbents
Sponsored by I&EC, Cosponsored by CEI, MPPG‡, and NUCL

MONDAY MORNING

Biomass to Fuel and Products
Sponsored by SOCED, Cosponsored by CELL, ENFL and MPPG

Catalysis for Un-conventional Energy Sources

Novel Catalysts
Sponsored by ENFL, Cosponsored by CATL and MPPG‡

Chemical Technology in Antiquity
Sponsored by HIST, Cosponsored by MPPG‡

Enhanced Extraction & Utilization of Unconventional Energy Sources: Hydrofracking, EOR and Novel Approaches
Sponsored by ENFL, Cosponsored by MPPG‡

Environmental Chemistry and Health Impacts of Fine and Ultrafine Particulate Matter
Sponsored by ENVR, Cosponsored by MPPG

Geochemistry and Reactive Transport in Nano-Pore Geomaterials
Sponsored by GEOC, Cosponsored by MPPG‡

Hydraulic Fracturing Impacts on Water, Soil and Air Quality

Groundwater Impacts
Sponsored by ENVR, Cosponsored by MPPG‡

Modern Analytical Approaches for the Characterization of Natural Organic Matter in the Environment

Use of Mass Spectrometry and Other Methods to Characterize NOM in Diverse Environments
Sponsored by ENVR, Cosponsored by ANYL and MPPG

Nanomaterials for Solar Energy Conversion & Storage
Sponsored by ENFL, Cosponsored by MPPG‡

Nanotechnology: Delivering on the Promise Opportunities and Challenges for Health, Safety and the Environment
Sponsored by PRES, Cosponsored by AGFD, AGRO, ANYL, CARB, CCPA, CCS, CHAS, COLL, COMSCI, CORP, ENFL, HIST, I&EC, IAC, MPPG, PMSE, POLY, SCHB and SOCED

Transitioning between Academic Research into Practical Use: Solar-Energy and Advanced Materials
Sponsored by COMSCI, Cosponsored by MPPG‡ and PRES

Uranium in Seawater

Sorbents and Analysis
Sponsored by I&EC, Cosponsored by CEI, MPPG‡ and NUCL

MONDAY AFTERNOON

Section A

Colorado Convention Center
Bellco Theatre

The Kavli Foundation Emerging Leader in Chemistry Lecture

R. S. Weber, *Organizer, Presiding*

4:00 Introductory Remarks.

4:05 MPPG **4.** Radical frontiers in catalysis. **T. Betley**

Section A

Colorado Convention Center
Bellco Theatre

The Fred Kavli Innovations in Chemistry Lecture

R. S. Weber, *Organizer, Presiding*

5:30 Introductory Remarks.

5:35 MPPG **5.** Us vs. them: Distinguishing humans from microbes with carbohydrate. **L.L. Kiessling**

Chemical Technology in Antiquity
Sponsored by HIST, Cosponsored by MPPG‡

Chemistry in the Marine Boundary Layer
Sponsored by ENVR, Cosponsored by MPPG

Hydraulic Fracturing Impacts on Water, Soil and Air Quality

Surface Water Impacts/Fluid Chemistry
Sponsored by ENVR, Cosponsored by MPPG‡

Modern Analytical Approaches for the Characterization of Natural Organic Matter in the Environment

Extraction Techniques to Isolate NOM and Characterization of Pyrogenic Organic Matter (Biomass Burning)
Sponsored by ENVR, Cosponsored by ANYL and MPPG

Nanomaterials for Solar Energy Conversion & Storage
Sponsored by ENFL, Cosponsored by MPPG‡

Nanotechnology: Delivering on the Promise

Bridging the Gap to a Thriving US Marketplace
Sponsored by PRES, Cosponsored by AGFD, AGRO, ANYL, CARB, CCPA, CCS, CHAS, COLL, COMSCI, CORP, ENFL, HIST, I&EC, IAC, MPPG, PMSE, POLY, SCHB and SOCED

Solutions to Metals Contamination of Water
Sponsored by ENVR, Cosponsored by MPPG‡

Uranium in Seawater

Analysis and Toxicity/Cost
Sponsored by I&EC, Cosponsored by CEI, MPPG‡, and NUCL

TUESDAY MORNING

Section A

Colorado Convention Center
Mile High Ballroom 3A

Nanoscience and Nanotechnology of Natural Resources
Cosponsored by PRES

P. Alivisatos, P. S. Weiss, *Organizers, Presiding*

9:00 Introductory Remarks.

9:05 MPPG **6.** Your anion is my plasmonic nanostructure: Discovering molecular plasmonics. **N.J. Halas**

9:35 MPPG **7.** Silicon nanostructures for new energy applications. **S. Lee**

10:05 MPPG **8.** Design of colloidal heterostructures for photocatalytic hydrogen generation. **A. Rogach**

10:35 MPPG **9.** Dimensionality matters: Dimensionality effects on optoelectronic behavior of semiconductor nanocrystals. **U. Banin**

11:05 MPPG **10.** Nanomaterials design for programmed multi- and staged release. **P.T. Hammond**

11:35 Concluding Remarks.

Advances in Analytical Chemistry for Discovering Emerging Contaminants in the Natural Environment
Sponsored by ENVR, Cosponsored by AGRO, ANYL and MPPG

C1 Chemistry

Methane Activation
Sponsored by ENFL, Cosponsored by MPPG‡

DOE Nanoscience Research Centers National Resources for the Nanoscience Community
Sponsored by PRES, Cosponsored by ANYL, CCPA, CEI, ENFL and MPPG

Iron Oxides: Formation, Structure, Reactivity and Applications

Formation and Transformation
Sponsored by GEOC, Cosponsored by MPPG‡

Hydraulic Fracturing Impacts on Water, Soil and Air Quality

Air & Water Quality
Sponsored by ENVR, Cosponsored by MPPG‡

TECHNICAL PROGRAM

Modern Analytical Approaches for the Characterization of Natural Organic Matter in the Environment

NMR and Photochemical Analysis of NOM
Sponsored by ENVR, Cosponsored by ANYL and MPPG

Molecular Catalysts for Solar Fuels
Sponsored by INOR, Cosponsored by MPPG

Nanomaterials for Solar Energy Conversion & Storage
Sponsored by ENFL, Cosponsored by MPPG‡

Solutions to Metals Contamination of Water
Sponsored by ENVR, Cosponsored by MPPG‡

TUESDAY AFTERNOON

Advances in Analytical Chemistry for Discovering Emerging Contaminants in the Natural Environment
Sponsored by ENVR, Cosponsored by AGRO, ANYL and MPPG

C1 Chemistry

Methane Activation
Sponsored by ENFL, Cosponsored by MPPG‡

Chemistry of the Energy Water Nexus: Focus on Fracking
Sponsored by INOR, Cosponsored by MPPG‡

Hydraulic Fracturing Impacts on Water, Soil and Air Quality Treatment and Regulations
Sponsored by ENVR, Cosponsored by MPPG‡

Iron Oxides: Formation, Structure, Reactivity and Applications

Formation and Transformation
Sponsored by GEOC, Cosponsored by MPPG‡

Molecular Catalysts for Solar Fuels
Sponsored by INOR, Cosponsored by MPPG

Nanomaterials for Solar Energy Conversion & Storage
Sponsored by ENFL, Cosponsored by MPPG‡

Solutions to Metals Contamination of Water
Sponsored by ENVR, Cosponsored by MPPG‡

WEDNESDAY MORNING

12th International Symposium on Heavy Oil Upgrading, Production & Characterization
Sponsored by ENFL, Cosponsored by MPPG‡

Analytical Chemistry of Natural Resources

Environmental Analysis: Analytical Methods for Natural Resource Assessment and Protection
Sponsored by ANYL, Cosponsored by MPPG‡

C1 Chemistry

CO_2 Conversion
Sponsored by ENFL, Cosponsored by MPPG‡

Computational Pyrolysis & Upgrading of Bio-Oils

Bonding and Kinetics
Sponsored by COMP, Cosponsored by MPPG

Iron Oxides: Formation, Structure, Reactivity and Applications

Biotic and Abiotic Redox Reactions
Sponsored by GEOC, Cosponsored by MPPG‡

Molecular Catalysts for Solar Fuels
Sponsored by INOR, Cosponsored by MPPG

Nanomaterials for Solar Energy Conversion & Storage
Sponsored by ENFL, Cosponsored by MPPG‡

Surface Physicochemical Processes in Engineered and Natural Systems
Sponsored by ENVR, Cosponsored by AGRO and MPPG‡

Trace Materials in Air, Soil, and Water
Sponsored by ENVR, Cosponsored by MPPG‡

Water Sustainability in Oil and Gas Exploration: Treatment Issues
Sponsored by ENVR, Cosponsored by CEI and MPPG‡

WEDNESDAY AFTERNOON

12th International Symposium on Heavy OilUpgrading, Production & Characterization

Characterization
Sponsored by ENFL, Cosponsored by MPPG‡

ACS Award for Affordable Green Chemistry: Symposium in Honor of John Frye, Todd Werpy, and Alan Zacher
Sponsored by CELL, Cosponsored by MPPG

Analytical Chemistry of Natural Resources Instrumentation and Methods
Sponsored by ANYL, Cosponsored by MPPG‡

C1 Chemistry

Syngas Chemistry
Sponsored by ENFL, Cosponsored by MPPG‡

Computational Pyrolysis & Upgrading of Bio-Oils

Reaction Engineering
Sponsored by COMP, Cosponsored by ENFL‡ and MPPG

Iron Oxides: Formation, Structure, Reactivity and Applications

Environmental Applications
Sponsored by GEOC, Cosponsored by MPPG‡

Nanomaterials for Solar Energy Conversion & Storage
Sponsored by ENFL, Cosponsored by MPPG‡

Surface Physicochemical Processes in Engineered and Natural Systems
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Trace Materials in Air, Soil, and Water
Sponsored by ENVR, Cosponsored by MPPG‡

Water Our Most Critical Resource
Sponsored by AGFD, Cosponsored by MPPG

Water Sustainability in Oil and Gas Exploration: Treatment Issues
Sponsored by ENVR, Cosponsored by CEI and MPPG‡

WEDNESDAY EVENING

Advances in Analytical Chemistry for Discovering Emerging Contaminants in the Natural Environment
Sponsored by ENVR, Cosponsored by MPPG

Assessing Toxicity of Environmental Contaminants
Sponsored by ENVR, Cosponsored by MPPG‡

Bioavailability and Biogeochemical Interactions Affecting Remediation of Hazardous Substances in the Environment
Sponsored by ENVR, Cosponsored by MPPG‡

Biogenically Enhanced Recovery and Bioremediation in Fossil Fuel Reservoirs
Sponsored by ENVR, Cosponsored by MPPG‡

Chemistry in the Marine Boundary Layer
Sponsored by ENVR, Cosponsored by MPPG

Environmental Chemistry: Pedagogical Models and Practices
Sponsored by ENVR, Cosponsored by CHED, MPPG‡ and YCC

Environmental Chemistry and Health Impacts of Fine and Ultrafine Particulate Matter
Sponsored by ENVR, Cosponsored by MPPG

Environmental Reactivity of Organic Micropollutants and Their Transformation Products in Receiving Waters
Sponsored by ENVR, Cosponsored by AGRO and MPPG‡

Modern Analytical Approaches for the Characterization of Natural Organic Matter in the Environment
Sponsored by ENVR, Cosponsored by ANYL and MPPG

Solutions to Metals Contamination of Water
Sponsored by ENVR, Cosponsored by MPPG‡

Water Recycling in Domestic Use, Energy Extraction, and Agricultural Use
Sponsored by ENVR, Cosponsored by AGRO and MPPG‡

Water Sustainability in Oil and Gas Exploration: Treatment Issues
Sponsored by ENVR, Cosponsored by CEI and MPPG‡

THURSDAY MORNING

12th International Symposium on Heavy Oil Upgrading, Production & Characterization

Characterization
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ACS Award for Affordable Green Chemistry: Symposium in Honor of John Frye, Todd Werpy, and Alan Zacher
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Analytical Chemistry of Natural Resources Instrumentation and Methods
Sponsored by ANYL, Cosponsored by MPPG‡

C1 Chemistry

Syngas Chemistry
Sponsored by ENFL, Cosponsored by MPPG‡

Computational Pyrolysis & Upgrading of Bio-Oils Reaction Engineering
Sponsored by COMP, Cosponsored by ENFL‡ and MPPG

Iron Oxides: Formation, Structure, Reactivity and Applications

Environmental Applications
Sponsored by GEOC, Cosponsored by MPPG‡

Nanomaterials for Solar Energy Conversion & Storage
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Surface Physicochemical Processes in Engineered and Natural Systems
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Trace Materials in Air, Soil, and Water
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Water Our Most Critical Resource
Sponsored by AGFD, Cosponsored by MPPG

Water Sustainability in Oil and Gas Exploration: Treatment Issues
Sponsored by ENVR, Cosponsored by CEI and MPPG‡

AGFD

Division of Agricultural And Food Chemistry

K. Deibler, *Program Chair*

SOCIAL EVENTS:

AGFD Reception, 6:00 PM: Tues

BUSINESS MEETINGS:

AGFD Membership Planning Meeting, 12:00 PM: Sun

AGFD Division Executive Committee Meeting, 5:00 PM: Sun

AGFD Future Programs Planning Meeting, 12:00 PM: Mon

SUNDAY MORNING

Section B

Colorado Convention Center
Room 112

Undergraduate Symposium
Cosponsored by CHED

C. J. Brine, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 AGFD **1.** Microwave-assisted green synthesis of silver nanoparticles for the assessment of total antioxidant capacity in fruits. **S. Bukovsky-Reyes**, J.E. Owens

9:05 AGFD **2.** Metabolite fingerprinting of *Punica granatum* L. by HPLC with UV/DAD and ESI-MS^n detection. **S.F. Groothuis**, F.P. Prencipe, S. Benvenuti, F. Pellati

9:35 AGFD **3.** Production of stilbenoids in hairy root cultures of muscadine grape: Effect of methyl jasmonate and cyclodextrin. **T. Knapp**, L. Nopo-Olazabal, F. Medina-Bolivar

10:05 Intermission.

10:20 AGFD **4.** Evaluation, optimization, and utilization of SOP 218.7 for the determination of Cr VI in drinking water. **J. Bautista**, J. Weigand, M. Hart, G.D. Claycomb

10:50 AGFD **6.** Determining volatile acidity in wines through acetic acid gas detection tubes. **M. Bee**, G.L. Sacks, P. Howe

11:20 AGFD **7.** Alkylresorcinols: Purification from wheat bran and quantification in wholegrain wheat breads. **N. Stone**, Y. Zhu, P. Wang, S. Sang

SUNDAY AFTERNOON

Section A

Colorado Convention Center
Room 113

Vitamin D: Past, Present & Future for Animals & Humans

Kenneth A. Spencer Award

M. Appell, B. Burton-Freeman, E. Hellmuth, L. Howard, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 AGFD **8.** Progress and future investigations in understanding the role of vitamin D in canine and feline health and disease. **D. Thamm**, K.A. Selting

1:30 AGFD **9.** Vitamin D and immunity: Advancing human and animal health through vitamin D research in cattle. **C. Nelson**

1:55 AGFD **10.** Toward a physiological referent for the vitamin D requirement. **R.P. Heaney**

2:20 Discussion.

2:30 Intermission.

2:45 AGFD **11.** Vitamin D in the prevention and treatment of cancer. **B.W. Hollis**

3:10 AGFD **12.** LC-MS/MS offers new insights into vitamin D metabolism in humans and knockout animal models. **G. Jones**

3:35 AGFD **13.** Tribute to Ronald L. Horst. **D.C. Beitz**

4:00 Panel Discussion.

Section B

Colorado Convention Center
Room 112

Graduate Student Symposium
Cosponsored by CHED

C. J. Brine, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 AGFD **14.** Detection and quantification of melamine in dairy products using molecularly-imprinted polymers-surface enhanced Raman spectroscopic biosensors. **Y. Hu**, X. Lu

1:35 AGFD **15.** Novel method for debittering table olives. **R. Johnson**, A.E. Mitchell

2:05 AGFD **16.** Of terroir and tannins: The role of pathogenesis-related proteins in red wine astringency. **L.F. Springer**, G.L. Sacks

2:35 Intermission.

2:50 AGFD **17.** Acute oral toxicity and nephrotoxicity mechanism(s) of selected fatty acid esters of 3-MCPD. **M. Liu**, G. Huang, J. Liu, B. Gao, L.L. Yu

3:20 AGFD **18.** Influence of gingerols and their metabolites on the human immune system. **C.E. Schoenknecht**, P.H. Schieberle

3:50 AGFD **19.** Inexpensive, portable paper-fluidic device for use in food safety and agricultural applications. **C.K. Koo**, S.R. Nugen

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Nanotechnology: Delivering on the Promise

Research & Development

Sponsored by PRES, Cosponsored by AGFD, AGRO, ANYL, CARB, CCPA, CCS, CHAS, COLL, COMSCI, CORP, ENFL, HIST, I&EC, IAC, MPPG, PMSE, POLY, SCHB and SOCED

MONDAY MORNING

Section A

Colorado Convention Center

Room 113

Medicinal & Aromatic Crops: Production, Phytochemistry, & Utilization

Cosponsored by AGRO and MEDI

C. L. Cantrell, V. Jeliazkov, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 AGFD **20.** Production of essential oils for the personal care industry: Quality and regulatory issues. **B. Schmidt**

9:00 AGFD **21.** Green extraction of natural products: From innovations to industrial applications. **F. Chemat**

9:25 AGFD **22.** Dual utilization of medicinal and aromatic crops: For plant chemicals and biofuels. **V. Jeliazkov**, C.L. Cantrell, N. Stewart, B. Joyce, E. Jeliazkova

9:50 AGFD **23.** Selected aspects of environmental protection in the processing of coal-monitoring and revitalization in relation to the isolation, identification and utilization of isolated organic compounds. **I. Salamon**, J. Sandor, J. Mitra

10:15 Intermission.

10:30 AGFD **24.** Breeding of German chamomile, *Matricaria recutita* L., with the high content of /-/- α- bisabolol. **I. Salamon**, **S. Mudroncekova**, J. Fejer

10:55 AGFD **25.** Biosynthesis of amphetamine-like alkaloids in *Catha edulis* and *Ephedra* spp., two distantly related taxa. **E. Lewinsohn**, J. Hagel, R. Krizevski, E. Bar, R.A. Groves, A. Levy, K. Kilpatrick, Y. Zhang, N. Dudai, C.W. Sensen, S. Ben Shabat, S. Yaron, M. Frederic, P.J. Facchini

11:20 AGFD **26.** Saline water management strategy on growth and tuber yield of *Helianthus tuberosus* (L.) cv. Stampede. **J.F. Ferreira**, N. Dias, X. Liu, D. Suarez

Section B

Colorado Convention Center

Room 112

Agricultural & Food Chemistry General Papers

Health and Nutrition in Food Chemistry

K. Deibler, *Organizer, Presiding*

8:00 AGFD **27.** Innovative tactic toward rapid isolation of unique bioactive sphingoids from dietary natural resources. **S. B.**, K. Monde

8:20 AGFD **28.** Common juniper (*Juniperus communis* L.) and its qualitative and quantitative characteristics of essential oil in Albania. **I. Salamon**, **A. Ibraliu**, S. Mudroncekova, J. Fejer

8:40 AGFD **29.** Treatment with soluble phenolic antioxidants significantly improves antioxidant capacity of insoluble wheat bran. **E. Doğan**, V. Gökmen

9:00 Intermission.

9:15 AGFD **30.** Study of the synergy between soluble and dietary fiber bound antioxidants. **E.E. Çelik**, V. Gökmen, L. Skibsted

9:35 AGFD **31.** Carotenoid content and composition in winter squash, (*Cucurbita maxima Duch.*) and (*Cucurbita moschata Duch.*): Variability associated with different cultigens, harvest dates, and storage times. **J. Noseworthy**

9:55 AGFD **32.** Effect of xanthan/enzymatically modified guar gum mixtures on the stability of oil-in-water emulsions. **P. Chityala**, H. Khouryieh, K. Williams

10:15 Intermission.

10:30 AGFD **33.** Rice (Oryza sativa L.) resistant starch and novel processing methods to increase resistant starch concentration. **S.A. James**, T. Pushparaj, D. Thavarajah, S. Premakumara, K. Abeysekara, S. Sotheeswaran

10:50 AGFD **34.** Fractionation and characterization of glabrous canary seed components for food and non-food applications. **E.M. Abdelaal**, P. Hucl, C. Patterson

11:10 AGFD **35.** Induced resistance in ash (*Fraxinus spp.*) against emerald ash borer: A proteomic investigation. **S. Chakraborty**, S. Opiyo, A. Hill, D. Cipollini, D.A. Herms, P. Bonello

Nanotechnology: Delivering on the Promise

Opportunities and Challenges for Health, Safety and the Environment

Sponsored by PRES, Cosponsored by AGFD, AGRO, ANYL, CARB, CCPA, CCS, CHAS, COLL, COMSCI, CORP, ENFL, HIST, I&EC, IAC, MPPG, PMSE, POLY, SCHB and SOCED

MONDAY AFTERNOON

Section A

Colorado Convention Center

Room 113

Medicinal & Aromatic Crops: Production, Phytochemistry, & Utilization

Cosponsored by AGRO and MEDI

C. L. Cantrell, V. Jeliazkov, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 AGFD **36.** Chemical composition and antimicrobial activity of crude extract preparations from the medicinal plant *Vexibia alopecuroides* (L.) Jakovl. **T. Kustova**, T. Karpenyuk, M. Jacob, C.L. Cantrell, S. Ross

1:30 AGFD **37.** β-Triketones from *Leptospermum scoparium* as natural herbicides Inhibiting *p*-hydroxyphenylpyruvate dioxygenase. **F. Dayan**, D. Owens, D. Nanayakkara

1:55 AGFD **38.** Cilantro essential oil and its major constituents as a source of new drugs against Leishmaniasis. M.A. Donega, **S. . Mello**, R.M. Moraes, S.K. Jain, B.L. Tekwani, C.L. Cantrell

2:20 AGFD **39.** Essential oils in prevention and treatment of human opportunistic fungal diseases. **T. Markovic**, V. Jeliazkov

2:45 Intermission.

3:00 AGFD **40.** Effects of plant-derived bioactive compounds on rumen fermentation, nutrient utilization, immune response, and productivity of ruminant animals. **A.N. Hristov**, J. Oh

3:25 AGFD **41.** Hairy roots and human health: Production and discovery of bioactive compounds. **F. Medina-Bolivar**, T. Yang, L. Fang, K. Mockaitis, N. Joshee

3:50 AGFD **42.** Bioactive constituents isolated from essential oils from plants in *Asteraceae* and *Apiaceae* families. **K.M. Meepagala**

4:15 AGFD **43.** Recent research and development of *Antrodia cinnamomea*: An endemic medicinal mushroom of Taiwan. **S. K J**, S. Wang

4:40 Concluding Remarks.

Section B

Colorado Convention Center

Room 112

Agricultural & Food Chemistry General Papers

K. D. Deibler, *Organizer, Presiding*

1:00 AGFD **44.** Bacteriophage-based scheme to enable rapid MALDI-TOF screening of samples for bacterial contaminants. **S.D. Alcaine**, L. Tilton, Z. Wang, S.R. Nugen

1:20 AGFD **45.** Quantification of plant sterols and plant stanols in phytosterol-enriched foods and dietary supplements. **C.T. Srigley**, E. Haile

1:40 AGFD **46.** Phytochemical composition and in vitro antimicrobial activity of selected essential oils on foodborne pathogens. **R. Tardugno**, F. Pellati, A. Serio, A. Paparella, S. Benvenuti

2:00 Intermission.

2:15 AGFD **47.** Determination of quantitative sodium mass transfer coefficient during osmotic processing of potatoes. **A. Kinchla**, T. Hinkley

2:35 AGFD **48.** Feline bitter receptors TAS2R38 and TAS2R43 have response profiles distinct from the human homologues. **J. Rucker**, M. Sandau, J. Goodman, A. Thomas, N. Rawson

2:55 AGFD **49.** Physics and chemistry of brewing better coffee. **C.H. Hendon**, L. Colonna-Dashwood, M. Colonna-Dashwood

3:15 Intermission.

3:30 AGFD **50.** Estimation of procyanidin/prodelphinidin and *cis/trans* flavanol ratios of condensed tannin fractions by ^{1}H-^{13}C HSQC NMR spectroscopy: Correlation with thiolysis. **W. Zeller**, A. Ramsay, H. Ropiak, C. Fryganas, I. Mueller-Harvey, R.H. Brown, C. Drake, J.H. Grabber

3:50 AGFD **51.** Impact by condensed tannins with different mean degrees of polymerization on protein precipitation. **W. Zeller**, M.L. Sullivan, I. Mueller-Harvey, J.H. Grabber, A. Ramsay, C. Drake, R.H. Brown

4:10 AGFD **52.** Determination of amygdalin in apple seeds, fresh apples, and processed apple juices. **I. Bolarinwa**

4:30 AGFD **5.** Withdrawn.

Nanotechnology: Delivering on the Promise

Bridging the Gap to a Thriving US Marketplace

Sponsored by PRES, Cosponsored by AGFD, AGRO, ANYL, CARB, CCPA, CCS, CHAS, COLL, COMSCI, CORP, ENFL, HIST, I&EC, IAC, MPPG, PMSE, POLY, SCHB and SOCED

MONDAY EVENING

Section A

Colorado Convention Center

Halls C/D

Sci-Mix

K. D. Deibler, *Organizer*

8:00 - 10:00

74, 77-78, 84, 92-97, 100, 103, 115, 118-120, 124-125. See subsequent listings.

TUESDAY MORNING

Section A

Colorado Convention Center

Room 113

Agricultural & Food Chemistry General Papers

Agricultural and the Environment

K. Deibler, *Organizer*

B. Park, *Presiding*

8:00 AGFD **53.** Highly sensitive colorimetric sensors for fumigants. **G. Sun**

8:20 AGFD **54.** Evaluation of biochar in three soil types for nutrient and water retention toward increased crop yield. **B.J. Winters**

8:40 AGFD **55.** Positive role of lignin in enzymatic hydrolysis of lignocellulosic biomass. **Y. Huang**, M. Tu

9:00 Intermission.

9:15 AGFD **56.** Green technologies for the generation of value added cotton. **S. Chang**, B. Condon, J. Smith

9:35 AGFD **57.** Withdrawn.

9:55 AGFD **58.** Phytotoxic and mosquito larvicidal constituents from *Ammi visnaga* seeds. **K.M. Meepagala**, J.J. Becnel

10:15 AGFD **59.** Mustard meal extract as a natural herbicide for liverwort control. **I.E. Popova**, J.S. Dubie, M.J. Morra

10:35 Intermission.

10:50 AGFD **60.** Phage amplification-based paper-fluidic device for the detection of generic *E. coli*. **S.D. Alcaine**, S.R. Nugen

11:10 AGFD **61.** Is tomato worth an electron? Bioelectrochemical treatment of waste residues from tomato processing Industry. **V. Gadhamshetty**, **A. Fogg**

11:30 AGFD **62.** Herbicide metabolism database. **J. Yao**, W. Xu, M. Lin, J. Hu, Q. Tang

Section B

Colorado Convention Center

Room 112

Phenolic & Polyphenolic Chemistry in Food Processing

Reactions/Properties

Cosponsored by AGRO, BIOT, COMP and MEDI

B. D. Guthrie, *Organizer, Presiding*

9:30 Introductory Remarks.

9:35 AGFD **63.** Understanding physical-chemical, biological (antioxidant) and optical properties of natural polyphenols at an atomistic-scale. **P. Trouillas**, M. Otyepka

9:55 AGFD **64.** Beyond ORAC: Dietary polyphenolics as metal-binding a98ntioxidants and food preservatives. **N.R. Perron**, H.C. Wang, J.L. Brumaghim

10:15 Intermission.

10:30 AGFD **66.** Carbonyl-scavenging ability of phenolic compounds: A second barrier defense against the damage caused by lipid oxidation and oxidative stress. **R. Zamora**, F.J. Hidalgo

10:50 AGFD **65.** Antiglycation activity of tannic acid in ovalbumin-glucose model system. **H. Akillioglu**, V. Gökmen

11:10 AGFD **67.** Phenolic acids: Precursors for desirable aroma-active compounds and the undesirable toxicologically relevant styrene in wheat beer. **M. Granvogl**, D. Langos, P.H. Schieberle

Ask Dr. Safety: EH&S Support of Nanotechnology R&D

Sponsored by CHAS, Cosponsored by AGFD, CCS and PRES

TUESDAY AFTERNOON

Section A

Colorado Convention Center

Room 113

Applied Nanotechnology for Food & Agriculture

Cosponsored by PRES

M. Appell, B. Park, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 AGFD **68.** Effect of nano size reduction on absorption and bioavailability of calcium from fortified milk powder in rats. **H. Mirhosseini**, A. Erfanian, M. Abd Manap, b. rasti, S. Bin Mustafae

1:35 AGFD **69.** Green synthesis and electrospray atmospheric pressure ionization mass spectral studies of hydrazinocurcumin: A potentially important derivative for intestinal absorption studies at the nanolevel. **B. Dayal**, A. Mehta, D. Kulkarni, A. Pandey, S. Li, M.A. Lea

2:05 AGFD **70.** Withdrawn.

2:35 Intermission.

Technical program information known at press time. The official technical program for the 249th ACS National Meeting is available at: www.acs.org/denver2015

2:50 AGFD **71.** Nanocompositions for enhancing shelf life and quality of fruits, vegetables, and flowers. **G. Paliyath**, P. Padmanabhan, S. Mihindukulasurya, J. G.J., I. El Sharkawy, S. Jayasankar, L. Lim, A. Sullivan, S. K.S., G. R, K. Gill

3:20 AGFD **72.** Investigation of materials for the removal of arsenic from foodstuffs. **T. Reed**, A.W. Apblett

3:50 AGFD **73.** Bionanosensor adjusting the farming cultural practices in emergent nations. **J. Reyes**, N.D. Becerra-Mora, Y. Moreno, C.L. Macias, N.A. Mariño, A. Kohli, P. Kohli

4:20 Concluding Remarks.

Section A

Colorado Convention Center

Room 113

Agricultural & Food Chemistry General Posters

K. Deibler, *Organizer, Presiding*

3:30 - 5:30

AGFD **74.** Thermal stability of food allergens and nonallergenic proteins: A comparative study. **Y. Wu**, T. Fu

AGFD **75.** Grain quality traits in a sorghum association mapping panel. **S. Bean**, T. Herald, J.D. Wilson, P. Gadgil, R.C. Kaufman, B.P. Ioerger

AGFD **76.** Factors related to reduced *in-vitro* protein digestibility in a diverse sorghum population. **S.L. Adrianos**, D.L. Blackwell, S. Bean, B.P. Ioerger, M. Tilley, T. Herald, P. Gadgil

AGFD **77.** Smell of the entrance to the heaven: Volatiles from the coffee berry blossom end and their potential applications in pest managements of coffee berry borer *Hypothenemus hampei* (Coleoptera: Curculionidae). **Y. Yu**, E. Jang, M. siderhurst

AGFD **78.** Influence of plant maturity on anthocyanin levels, phenolic composition, and antioxidant properties of purple basil (*Ocimum basilicum* L.). **K.R. McCance**, E.D. Niemeyer

AGFD **79.** Determination of the antioxidant properties of flavanones and flavanone glucuronide metabolites. **K.A. Costello**, E.D. Niemeyer

AGFD **80.** Withdrawn.

AGFD **81.** Chiral and achiral profiling of a pesticide formulation using ultraperformance convergence chromatography (UPC^2) with PDA and mass detection. **M. Twohig**, M. O'Leary, P.G. Alden

AGFD **82.** Effectiveness of flocculants on inorganic and metallic species removal during aerobic digestion of wastewater from poultry processing plant. **N. Lovanh**, J.H. Loughrin, K. Cook, K. Sistani, P. Silva

AGFD **83.** Novel structural modifications of plant oils. **A. Biswas**, H. Cheng

AGFD **84.** QSAR and density functional approaches to evaluate trichothecene toxicity and detection. **M. Appell**, W.B. Bosma

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AGFD **85.** Cross species amplification of thirteen distinct microsatellite loci in *Z. aquatica*. **B.J. Pinto**

AGFD **86.** Influence of biological fertilization on seed production of winter wheat. **D. Trifan**, M. Bularda

AGFD **87.** Sorption of organic dyes by straw biochar and its effective factor. **X. Ji**, L. Lyu, C. Yang

AGFD **88.** Detoxification with enzymes for tung meal. **R. Liu**

AGFD **89.** Distribution and enantiomeric profiles of organochlorine pesticides in surface sediments from Bering Sea, Chukchi Sea, and Arctic Ocean. **M. Jin**, B. Xue, S. Zhou

AGFD **90.** Enhanced anti-ultraviolet and thermal stability of a pesticide by modification of a volatile organic compound (VOC)-free vinyl-silsesquioxane in severe environments. **D. Lin**, X. Han, L. Hu

AGFD **91.** Antilipidemic actions of the dietary fiber extract of soybean residues in Kunming mice. **D. Lin**, Z. Tu

AGFD **92.** Advanced glycation endproducts may affect digestion and antigen processing of food allergens. **C.P. Mattison**, J. Dinter, M. Berberich, S. Chung, S. Reed, S. Le Gall, C.C. Grimm

AGFD **93.** Behavior of whey protein concentrates under extreme storage conditions. **M.H. Tunick**

AGFD **94.** Alternative hop processing. **C. Knuston**, B.E. Sturgeon

AGFD **95.** Mechanism behind the antibacterial properties of hop acid investigated with model cell membranes. **Y. Park**, A. Sostareccz

AGFD **96.** Determination of the presence of flavor- and aroma-affecting compounds in beer resulting from various yeast washing techniques. **D. Kazal**, W.H. Steel

AGFD **97.** Improving lag time in second-generation washed beer yeast. **W.H. Steel**

AGFD **98.** Changes of volatile compounds in Muscadine grape (*Vitis rotundiforlia*) during ripening. **B. Lee**, F. Chen

AGFD **99.** Vapor-infusion of wine flavor volatiles in specialty dark chocolate and analysis via GC-M. **S. Richards**, S. Bremer, K.L. Nuckles, C.R. Thurman, P.J. Iles, L.D. Giddings, M. Alvarez, N.R. Bastian

AGFD **100.** Volatile-organic component sensitive colorimetric chemosensor: Application for determination of apple quality. **Y. Kim**, S. Jin, G. Kim, J. Park

AGFD **101.** Withdrawn.

AGFD **102.** Effect of fat concentration and fermentation on thermal proprieties of milk bases. **Z. Bao**, J. Xiong, J. Ye

AGFD **103.** Production of lactic acid from cheese whey in controlled pH batch fermentation using *Lactobacillus plantarum* DSA 20174. **A.A. Ayad**, **D. Gad El-Rab**, **S. Ibrahim**

AGFD **104.** Mineral and trace element analysis of berry liquors from Northern Europe. **N.J. Ronkainen**, N.S. Olson, S. Mustaly

AGFD **105.** Roasting effects on phenolic content and free-radical scavenging activities of pulp pre-conditioned and fermented cocoa (*Theobroma cacao*) beans. **E. Afoakwa**, E. Ofosu-Ansah, J. Takrama, A.S. Budu

AGFD **106.** Synthesis and characterization of cationic starches and their application in preparation of fertilizer nanoparticles through four-Inlet vortex mixer. **Y. Shi**, S. Zhang, X. Jia, K. Chen, X. Guo

AGFD **107.** Multiplex real-time PCR detection and identification of food-borne pathogens *Salmonella enterica*, *Escherichia coli* and *Shigella flexneri*. **K.C. Sweetin**, **K.M. Elkins**

AGFD **108.** Multiplex real-time PCR detection and differentiation of food-borne pathogen *Bacillus cereus* and related *Bacillus* species. **J.D. Roussillon**, K.M. Elkins

AGFD **109.** Determination of heavy metals in tomatoes sauces. **M. Reyna Liriano**, R. Tremont

AGFD **110.** Mold population on freshly-harvested rice and factors affecting prevalence. **S. Thote**, G. Atungulu, H. Zhong

AGFD **111.** Fatty acid analysis of tilapia. **E.M. Crosier**, M.J. Yurkevicius, A.L. Rhyne, N.E. Breen

AGFD **112.** Comparison of the fatty acid profiles of wild caught and farm raised salmon. **M.J. Yurkevicius**, E.M. Crosier, D.L. Taylor, N.E. Breen, A.L. Rhyne

AGFD **113.** Antioxidant effect of porcine pancreatic phospholipase A2 and detection and pro-oxidative activity of ferryl-hemoglobin in washed cod muscle. **N. Tatiyaborworntham**, M.P. Richards

AGFD **114.** Effect of porcine pancreatic phospholipase A2 on trout hemoglobin-promoted lipid oxidation and heme partitioning in washed cod muscle. **N. Tatiyaborworntham**, M.P. Richards

AGFD **115.** Isolation and characterization of chitin from the mushroom *Pleurotus ostreatus* with possible application in biomedical and pharmaceutical application. **B. Calderon**

AGFD **116.** Methyglyoxal scavenging activity of deacetylasperulosidic acid. **S. Deng**, B. West, J. Jensen, C. Su

AGFD **117.** Dietary sources of iridoids inhibit advanced glycation end product formation. **B. West**, A. Bogdanov, S. Deng, C. Su, C. Jensen, Z. Zaynudinov

AGFD **118.** Exploration of curcumin, UV-Vis absorption, and degradation kinetics. **H. Goemann**, T. Roettgen, J.D. Alia

AGFD **119.** Role of polyphenols of *Artemisia nova* and *Artemisia wyomingensis* in sage grouse dietary preferences. **A.H. Nguyen**, J.S. Forbey, G.G. Frye, J.W. Connelly, C.Y. Dadabay

AGFD **120.** Antioxidant protection in human blood plasma of varying triglyceride content utilizing a ferric reduction assay. R. Chandra, **C. Chidi, K. Huerta-Ruiz-Garza**

AGFD **121.** Withdrawn.

AGFD **122.** Antioxidant activity assay based on rapid colorimetric measurement of gold nanoparticles. **J. Chou**, X. Li, Y. Yin, N. Indrisek, J. Merono

AGFD **123.** Chemical constituents and biological evaluation of leaves' essential oils of *Vitex agnus-castus L.* growing in the southern-west of Algeria. **K. Sekkoum**

AGFD **124.** Block ionomer complexes formed by carboxymethyl-dextran-*block*-poly(ethylene glycol) copolymer and α-lactalbumin. **J. Du**, O.G. Jones

AGFD **125.** Antioxidant activities of supercritical carbon dioxide and ethanol extracts of *Aronia melanocarpa* (black chokeberry) pomace. **J. Wenzel**, T. Dixon, E. Tucker, L. Wang, M. Ammerman, C. Samaniego

AGFD **126.** Digestibility, viscosity, and microstructural properties of waxy and non-waxy rice starches resulting from microwave heat-moisture treatment. **A. Anderson**

AGFD **127.** Beauvericin as virulence factor of entomopathogenic fungus Beauveria bassiana (BALS.) used on bark beetles attacking spruces. **S. Mudroncekova**, I. Salamon, M. Barta

AGFD **128.** Lyophilization technology for isolation of anthocyanins from fruits of the high bush blueberry (Vaccinium corymbosum L.). **I. Salamon**, R. Mariychuk, S. Mudroncekova, D. Grulova

AGFD **129.** Distribution of residues in various muscles of cattle following intramuscular administration of hormones. **S. Sklenka**, P.S. Chu, J. Ward, A. Chiesa, T. Johnson

AGFD **130.** Comparison of kinetic profile of two total antioxidant capacity assays. **C. Krzykwa**, S.P. Canete

AGFD **131.** Identification of toxic metal ions in water using a gold nanoparticle based colorimetric sensor array. **G. Sener**, L. Uzun, A. Denizli

AGFD **132.** Effect of different proportions of ethanol on the crystalline structure of bacterial celluloses. **J. Xiong**, Z. Wang, J. Ye

AGFD **133.** Teaching laboratory for food analysis: Titration and HPLC characterization of kombucha fermentation. **N. Lawton**, W. Hall, S. Tachibana

AGFD **134.** Polyphenol antioxidants in savory snacks: Are any there? **J. Goodman**, **J.A. Vinson**

AGFD **135.** Isoflavone metabolism leading by the human intestinal bacteria. **M. Kim**, J. Han

AGFD **136.** Analysis of aroma compounds in whiskey by DLLME-GC/MS. **J.E. Owens**, L.B. Zimmerman, M.A. Gardner, L. Lowe, D.A. Orban, C.N. Goolsby

AGFD **137.** Biosoprtion of various mushrooms. **W. Ryan**, C. Fowler, K. Yuan, D.J. Schauer

AGFD **138.** Active site analysis of lepidopteran Farnesyl diphosphate synthase: Implications in omologous juvenile hormone biosynthesis. S.E. Sen, **T. Horsfield**, A. Jones

AGFD **139.** Mercury analysis of tuna using a low-cost cold vapor spectroscopy apparatus. **J. Hernandez**

AGFD **140.** Analysis of lipid transfer proteins in Arabidopsis thaliana by means of epitope tags to decipher the role of LTP4's lipid in plant senescence. **J. Bautista**

AGFD **141.** Efforts toward the development of a titrimetric method for measuring biosorption capacity. **S. Ardon**, H. Duke, B. Stewart, T. Robertson, D.J. Schauer

AGFD **142.** Withdrawn.

AGFD **143.** Antioxidant and aldose reductase inhibitory activities of color-fleshed potatoes. **D. Kalita**, B. Shieh, H. Ali, D.V. LaBarbera, D.G. Holm, J.M. Petrash, S.S. Jayanty

Section B

Colorado Convention Center

Room 112

Phenolic & Polyphenolic Chemistry in Food Processing

Sources

Cosponsored by AGRO, BIOT, COMP and MEDI

B. D. Guthrie, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 AGFD **144.** Ultrasound-assisted extraction of phenolic compounds from hazelnut shells. **B. Yuan**, M.A. Hanna

1:25 AGFD **145.** Effects of pod storage and fermentation duration on total polyphenols, *o*-diphenols, and anthocyanin concentrations in cocoa (*Theobroma cacao*) beans. **E. Afoakwa**, J.E. Kongor, J. Takrama, A.S. Budu, H. Mensah-Brown

1:45 AGFD **146.** Effect of solvent composition on grafting gallic acid onto chitosan via carbodiimides. **P. Guo**, J.D. Anderson, J.J. Bozell, S. Zivanovic

2:25 AGFD **148.** Analysis of grape seed tannins by mass spectrometry (MALDI-TOF and ORBITRAP ESI-MS). **E. Salas**, N. Teixeira, S. Maia, J. Oliveira, N. Mateus, V. De Freitas

2:45 Concluding Remarks.

WEDNESDAY MORNING

Section A

Colorado Convention Center

Room 113

Applied Nanotechnology for Food & Agriculture

Cosponsored by PRES

M. Appell, B. Park, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 AGFD **149.** Potentiometric PVC membrane sensors and their analytical applications in pharmaceuticals analysis: One example potentiometric PVC membrane sensors determination of moxifloxacin in pharmaceutical dose form. **G.A. Mostafa**

9:05 AGFD **150.** Development of phage-conjugated magnetic nanoprobes for bacterial separation. **S.R. Nugen**, J. Chen

9:35 Intermission.

‡ *Cooperative Cosponsorship*

9:50 AGFD **151.** Label-free detection of *Salmonella typhimurium* with ssDNA aptamers. **B. Park**, B. Wang, Z. Lou, B. Xu, Y. Kwon

10:20 AGFD **152.** Integration of nanostructured dielectrophoretic device and surface-enhanced Raman probe for highly sensitive rapid bacteria detection. **F. Madiyar**, S. Bhana, L. Swisher, X. Huang, C.T. Culbertson, J. Li

10:50 Discussion.

WEDNESDAY AFTERNOON

Section A

Colorado Convention Center
Room 113

Agricultural & Food Chemistry General Papers

K. Deibler, *Organizer*
B. Park, *Presiding*

1:00 AGFD **153.** Accurate experimental design for the characterization and quantitation of *Antrodia cinnamomea* triterpenoids with RSM, qNMR, and HPLC-tandem MS: A tough case to crack. **T. Wu**, Y. Du, M. El-Shazly, M. Lu, Y. Hsu, K. Lai, C. Chiu, F. Chang, Y. Wu

1:20 AGFD **154.** Anti-inflammatory constituents of *Cordyceps militaris*. **C. Chiu**, T. Wu, C. Lee, Y. Du, M. El-Shazly, Y. Chan, C. Tang, F. Chang, Y. Wu

1:40 AGFD **155.** Isolation and structural characterization of five constituents from *Eucommia ulmoides* Oliv. by multistep process. **M. Zhu**, J. Wen, Y. Dong, Y. Su, Q. Wei, R. Sun

2:00 Intermission.

2:10 AGFD **156.** Improved the emulsion stability of phosvitin from hen egg yolk against different pH by the covalent attachment with dextran. **H. Chen**

2:30 AGFD **157.** Protein level determination in foods: A comparison of analytical methods. **M.C. Azih**

2:50 Intermission.

3:00 AGFD **158.** Influence of branched limit dextrin on wheat starch gels retrogradation. **J. Xu**, X. Fan, X. Xu

3:20 AGFD **159.** Modified fermentation method of producing virgin coconut oil. **N.D. Flores**, **J. Cuya**

Section B

Colorado Convention Center
Room 112

Water Our Most Critical Resource

Cosponsored by MPPG

J. Finley, *Organizer*
S. Ahuja, J. N. Seiber, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 AGFD **160.** Water is indeed a crucial resource. **S. Ahuja**

1:35 AGFD **161.** Water and wine. **J.N. Seiber**, V. Tianco, J. Real

2:05 AGFD **162.** Foundations of water quality monitoring and assessment in the United States. **D.N. Myers**

2:35 Intermission.

2:45 AGFD **163.** Chemical characterization of brackish groundwater resources of the United States. **P. McMahon**, J. Böhlke, K. Dahm, J. Stanton, D. Parkhurst

3:15 AGFD **164.** Water challenges in unconventional in situ energy resource extraction technologies. **T.J. Gallegos**, C. Bern, J.E. Birdwell, S.S. Haines, M. Engle

3:45 AGFD **165.** Energy and water nexus in urban environments. **T. Younos**

4:05 Intermission.

4:15 AGFD **166.** Effect of upflow velocity on nutrient recovery from swine wastewater by fluidized bed struvite crystallization. **R.M. Abarca**, R.S. Pusta, R.B. Labad, J.A. Andit, C.M. Rejas, **M.G. de Luna**, M. Lu

4:35 AGFD **167.** Contaminated irrigation water and the associated human health risks. **T. Tongesayi**

THURSDAY MORNING

Section B

Colorado Convention Center
Room 112

Water Our Most Critical Resource

Cosponsored by MPPG

S. Ahuja, *Organizer*
J. Finley, J. N. Seiber, *Organizers, Presiding*

8:00 AGFD **168.** Optimizing water resources: An Israeli approach. **H.L. Taft**

8:30 AGFD **169.** Impacts of EPA's Clean Power Plan on electricity generation and water use in Texas. **P. Faeth**

9:00 Intermission.

9:10 AGFD **170.** Desalination for expanding water supplies. **J.H. Lienhard**

9:40 AGFD **171.** Improving water use estimates for the United States. **N.L. Barber**

10:10 AGFD **172.** Water security in a warming world. **D. Michel**

10:40 Intermission.

10:50 AGFD **173.** Decreasing the severity of chemical pretreatment processes of switchgrass through storage. **D. Carrier**, M. Wilkins, M. Buser, N. Frederick

11:20 AGFD **174.** Coupling surface water remediation to sustainable energy: Toward off-grid production of algae for biofuels. **J.B. Miller**

11:50 AGFD **175.** Water for food production: Will we have enough? **J.W. Finley**

12:20 AGFD **176.** Sustaining groundwater resources for global food security. **T. Harter**

AGRO

Division of Agrochemicals

P. Rice, *Program Chair*

SUNDAY MORNING

Assessing Toxicity of Environmental Contaminants

Sponsored by ENVR, Cosponsored by AGRO, CEI and MPPG‡

Environmental Reactivity of Organic Micropollutants and Their Transformation Products in Receiving Waters

Sponsored by ENVR, Cosponsored by AGRO and MPPG‡

SUNDAY AFTERNOON

Assessing Toxicity of Environmental Contaminants

Sponsored by ENVR, Cosponsored by AGRO, CEI and MPPG‡

Environmental Reactivity of Organic Micropollutants and Their Transformation Products in Receiving Waters

Sponsored by ENVR, Cosponsored by AGRO and MPPG‡

Nanotechnology: Delivering on the Promise Research & Development

Sponsored by PRES, Cosponsored by AGFD, AGRO, ANYL, CARB, CCPA, CCS, CHAS, COLL, COMSCI, CORP, ENFL, HIST, I&EC, IAC, MPPG, PMSE, POLY, SCHB and SOCED

MONDAY MORNING

Medicinal & Aromatic Crops: Production, Phytochemistry, & Utilization

Sponsored by AGFD, Cosponsored by AGRO and MEDI

Nanotechnology: Delivering on the Promise

Opportunities and Challenges for Health, Safety and the Environment

Sponsored by PRES, Cosponsored by AGFD, AGRO, ANYL, CARB, CCPA, CCS, CHAS, COLL, COMSCI, CORP, ENFL, HIST, I&EC, IAC, MPPG, PMSE, POLY, SCHB and SOCED

MONDAY AFTERNOON

Medicinal & Aromatic Crops: Production, Phytochemistry, & Utilization

Sponsored by AGFD, Cosponsored by AGRO and MEDI

Nanotechnology: Delivering on the Promise

Bridging the Gap to a Thriving US Marketplace

Sponsored by PRES, Cosponsored by AGFD, AGRO, ANYL, CARB, CCPA, CCS, CHAS, COLL, COMSCI, CORP, ENFL, HIST, I&EC, IAC, MPPG, PMSE, POLY, SCHB and SOCED

TUESDAY MORNING

Advances in Analytical Chemistry for Discovering Emerging Contaminants in the Natural Environment

Sponsored by ENVR, Cosponsored by AGRO, ANYL and MPPG

Phenolic & Polyphenolic Chemistry in Food Processing

Reactions/Properties

Sponsored by AGFD, Cosponsored by AGRO, BIOT, COMP and MEDI

TUESDAY AFTERNOON

Advances in Analytical Chemistry for Discovering Emerging Contaminants in the Natural Environment

Sponsored by ENVR, Cosponsored by AGRO, ANYL and MPPG

Phenolic & Polyphenolic Chemistry in Food Processing Sources

Sponsored by AGFD, Cosponsored by AGRO, BIOT, COMP and MEDI

WEDNESDAY MORNING

Microalgae: A Renewable Energy Source and a Sustainable Solution for the Environment

Sponsored by ENVR, Cosponsored by AGRO

Surface Physicochemical Processes in Engineered and Natural Systems

Sponsored by ENVR, Cosponsored by AGRO and MPPG‡

WEDNESDAY AFTERNOON

Microalgae: A Renewable Energy Source and a Sustainable Solution for the Environment

Sponsored by ENVR, Cosponsored by AGRO

Surface Physicochemical Processes in Engineered and Natural Systems

Sponsored by ENVR, Cosponsored by AGRO and MPPG‡

WEDNESDAY EVENING

Environmental Reactivity of Organic Micropollutants and Their Transformation Products in Receiving Waters

Sponsored by ENVR, Cosponsored by AGRO and MPPG‡

Water Recycling in Domestic Use, Energy Extraction, and Agricultural Use

Sponsored by ENVR, Cosponsored by AGRO and MPPG‡

THURSDAY MORNING

Surface Physicochemical Processes in Engineered and Natural Systems

Sponsored by ENVR, Cosponsored by AGRO and MPPG‡

Water Recycling in Domestic Use, Energy Extraction, and Agricultural Use

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ANYL

Division of Analytical Chemistry

D. C. Duckworth, *Program Chair*

OTHER SYMPOSIA OF INTEREST:

DOE Nanoscience Research Centers National Resources for the Nanoscience Community *(see PRES, Tue)*

Modern Analytical Approaches for the Characterization of Natural Organic Matter in the Environment *(see ENVR, Mon, Tue, Wed)*

Advances in Analytical Chemistry for Discovering Emerging Contaminants in the Natural Environment *(see ENVR, Tue, Wed)*

Macromolecular and Nanoparticle Separation Science *(see POLY, Sun, Mon, Tue)*

SUNDAY AFTERNOON

Section A

Embassy Suites Denver–Downtown Convention Center
Aspen Room A

Environmental Analytical Chemistry: A Tool for Introducing Research

M. Crowe, J. C. Ingram, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 ANYL **1.** Environmental analytical chemistry summer research for high school students. **J.C. Ingram**

1:30 ANYL **2.** General Chemistry assignment analyzing environmental contamination for the DePue, IL, National Superfund site. **F.M. Geiger**

1:50 ANYL **3.** Environmental analytical chemistry research: An undergraduate's perspective. **J. Credo**, J.C. Ingram

2:10 ANYL **4.** Environmental analytical chemistry research with undergraduate students at Union College: Case studies and lessons learned. **L. MacManus-Spencer**

2:30 Intermission.

2:45 ANYL **5.** Environmental analytical chemistry at James Madison University. **R.D. Foust**, D.M. Downey, C.A. Hughey

3:05 ANYL **6.** Laboratory and field-based environmental analytical chemistry research experiences for undergraduates at Villanova University. **A.M. Grannas**

3:25 ANYL **7.** Novel scan method for differential ion mobility spectrometry separations. **R. Harris**, B. Santiago, S. Isenberg, G.L. Glish

3:45 ANYL **8.** Electrochemistry and "biofilms": Undergraduate research at the interface of chemistry and biology. **R.J. Lesuer**, A. Maselli

MONDAY MORNING

Section A

Embassy Suites Denver–Downtown Convention Center
Aspen Room A

Advances in Analytical Separations

J. L. Maclachlan, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 ANYL **9. Award Address** (ACS Award in Chromatography sponsored by Sigma-Aldrich/Supelco). Framework for the development of several new bioanalytical methods. **M.T. Hearn**

8:50 ANYL **10.** Profiling anionic polar metabolites in oral cancer using capillary ion chromatography and high resolution accurate mass spectrometry. **T. Christison**, J. Wang, Y. Huang, L. Lopez

9:15 ANYL **11.** Separation of guanidine derivatives in surface water with resorcinarene-based ion chromatography columns. T. Panahi

9:40 Intermission.

10:00 ANYL **12.** Critical experimental evaluation of key methods to detect, size, and quantify nanoparticolate silver. **L. Calzolai**, C. Cascio, D. Gilliland, F. Rossi, C. Contado

10:25 ANYL **13.** Evaluation of nanoparticle-ligand distributions to determine nanoparticle concentration. **U. Uddayasankar**, U.J. Krull

10:50 ANYL **14.** Hydrophobic surface modification of organo-silica hybrid monolithic columns using photografting and thiol-ene click chemistry. **Z. Zajickova**, D. Britsch, D.M. Gharbharan, T. Sabol, A.K. Weed

11:15 ANYL **15.** Separation of mercury from VOC's and selective detection using gold film amalgamation and photoionization detection. **J.L. Maclachlan**, J.N. Driscoll

11:35 Concluding Remarks.

Section B

Embassy Suites Denver–Downtown Convention Center

Aspen Room B

Advances in Bioanalytical Chemistry

Electrochemical and Dye Sensing

G. Patonay, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 ANYL **16.** Ca2+-controlled assembly for visualized detection of conformation changes of calmodulin. **C. Xing**

8:25 ANYL **17.** Probe-based nanopore biosensor for detection of copper ion. **X. Chen**, L. Wang, S. Zhou, G. Wang, X. Guan

8:45 ANYL **18.** Nanopore back titration analysis of dipicolinic acid. **S. Zhou**, Y. Han, L. Wang, X. Chen, X. Guan

9:05 ANYL **19.** Sensitive histidine sensors based on glucose derivatives. **R. Cheng**, **R. Guo**, **Y. Bu**, **Y. Liu**

9:25 ANYL **20.** Chiral microchip electrophoresis-mass spectrometric platform for studying cellular uptake and release of D-/L-serine. **Y. Liu**, X. Li

9:45 Intermission.

10:00 ANYL **21.** Ratiometric electrochemical biosensors for in vivo analysis. **Y. Tian**

10:20 ANYL **22.** Intercalating dyes for enhanced contrast in second harmonic generation imaging of protein crystals. **N. Scarborough**, J. Newman, N. Pogranichniy, G.J. Simpson

10:40 ANYL **23.** Amperometric disk-shaped microelectrode biosensor for in vivo detection of D-serine. **D. Polcari**, A. Kwan, M. Van Horn, L. Danis, L. Pollegioni, E. Ruthazer, J. Mauzeroll

11:00 ANYL **24.** Single-cell heterogeneity: Direct intracellular pH measurement with chitosan functionalized nanopipettes. **R.E. Ozel**, N. Pourmand

11:20 ANYL **25.** Development of new tools for characterization of the metabolomic effects of diabetes on serum proteins. **R. Matsuda**, V. Kolli, Z. Li, M. Woods, K. Hoy, J. Anguizola, O. Barnaby, E.D. Dodds, D.S. Hage

Technical program information known at press time.
The official technical program for the 249th ACS National Meeting is available at:
www.acs.org/denver2015

Modern Analytical Approaches for the Characterization of Natural Organic Matter in the Environment

Use of Mass Spectrometry and Other Methods to Characterize NOM in Diverse Environments

Sponsored by ENVR, Cosponsored by ANYL and MPPG

MONDAY AFTERNOON

Section A

Embassy Suites Denver–Downtown Convention Center

Aspen Room A

Advances in Analytical Separations

J. L. Maclachlan, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 ANYL **26.** Development of a high-throughput method for determination of terpenoid content in pine. **A.E. Ware**, R. Sykes, G.F. Peter, M.F. Davis

1:30 ANYL **27.** Determination of allyl isothiocyanate and related compounds in horseradish by GC/MS. **C. Qiu**, D.E. Raynie

1:55 ANYL **28.** Trapping of volatile compounds after supercritical fluid extraction and application to supercritical carbon dioxide essential oil extraction of selected plants. **J. Kiratu**, D.E. Raynie

2:20 ANYL **29.** Designing and characterization of high throughput multilayer micro fluidic device for single cell analysis. **D.R. Ediriweera Weerarathna Patabdige**, T. Mickleburgh, C.T. Culbertson

2:45 Intermission.

3:05 ANYL **30.** Improved extraction chromatographic materials for the separation and preconcentration of metal ions. A. Momen

3:30 ANYL **31.** Factors influencing the mode(s) of metal ion partitioning into *N*-alkylpyridinium-based ionic liquids (ILs). **J. Wankowski**, M.L. Dietz

3:55 ANYL **32.** Analysis of interactions for testosterone with human serum albumin and sex hormone-binding globulin using ultrafast affinity extraction and high performance affinity chromatography. **X. Zheng**, M. Brooks, D.S. Hage

4:20 ANYL **33.** Synthesis and characterization of methacroloyl phenyl alanine-co-vinyl imidazole based CEC monolithic column for the separation of aromatic hydrocarbons. **H. Ishaque**

4:45 Concluding Remarks.

Section B

Embassy Suites Denver–Downtown Convention Center

Aspen Room B

Advances in Bioanalytical Chemistry

Natural Product and Tumor Detection

G. Patonay, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 ANYL **34.** Mass spectrometry-based discovery of novel tylosin analogs from *Streptomyces fradia*. **K. Hensal**, A. Johnson, E.E. Carlson

1:25 ANYL **35.** Modified Folin-Ciocalteu colorimetry method for the determination of total phenolics in biomass samples. **K.P. Bastola**, V. Bhadriraju, Y.N. Guragain, P.V. Vadlani

1:45 ANYL **36.** High resolution MALDI imaging mass spectrometry: A molecular imaging of natural products *in planta*. **D.S. Dalisay**, L.B. Davin, O. Rübel, B.P. Bowen, N.G. Lewis

2:25 ANYL **37.** Hybrid nanoparticles for multiplexed isolation and detection of circulating tumor cells in whole blood. **X. Huang**

2:45 Intermission.

3:00 ANYL **38.** Hydroxl-graphene/Fe_3O_4 hybrids for selective inhibition of tumor metastasis. **W. Zhang**, X. Li, M. Lin, Y. Liu

3:20 ANYL **39.** Genotyping of COX-2 and BCL-2 polymorphisms associated with gastric cancer susceptibility based on magnetic nanoparticles and dual-color fluorescence hybridization. **N. He**, Y. Deng, S. Li, Y. Zhang

3:40 ANYL **40.** Metabolic snapshots of triglyceride transport in human blood circulation: A diagnostic toolkit. **R. Chandra**, K. Huerta-Ruiz-Garza, S. Hameed, J.M. Jurica, C. Chidi

4:00 ANYL **41.** Quantitative serine protease assays based on formation of copper - oligopeptide complexes. **K. Yang**, X. Ding

4:20 ANYL **42.** Use of NIR fluorescent silica nanoparticles as labels. **G. Patonay**, G. Chapman, M. Henary, K. Emer, S. Crow

Modern Analytical Approaches for the Characterization of Natural Organic Matter in the Environment

Extraction Techniques to Isolate NOM and Characterization of Pyrogenic Organic Matter (Biomass Burning)

Sponsored by ENVR, Cosponsored by ANYL and MPPG

MONDAY EVENING

Section A

Colorado Convention Center

Halls C/D

Sci-Mix

D. C. Duckworth, *Organizer*

8:00 - 10:00

86, 89, 95-96, 102, 105, 107, 109, 112, 116-117, 125, 128, 137, 147-148, 151, 155, 156, 164. See subsequent listings.

TUESDAY MORNING

Section A

Embassy Suites Denver–Downtown Convention Center

Aspen Room A

Advances in Mass Spectrometry

G. L. Glish, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 ANYL **43.** Nanoscale 3D molecular imaging by extreme ultraviolet laser ablation mass spectrometry: a new analytical tool for the organic and inorganic solid state. **I. Kuznetsov**, J. Filevich, M. Woolston, T. Green, D. Carlton, W. Chao, E. Anderson, E.R. Bernstein, D. Crick, E. Bukovsky, D.L. Calkins, D.C. Crans, O. Boltalina, S.H. Strauss, J.J. Rocca, C. Menoni

8:25 ANYL **44.** Collision crossSectional areas by Fourier transform ion cyclotron resonance mass spectrometry: CRAFTI. **D.V. Dearden**, A. Anupriya, C.A. Jones, J. Shen, C. Harper

8:45 ANYL **45.** Using online chemistry databases to facilitate structure identification in mass spectral data. **A.J. Williams**, V. Tkachenko, A. Pshenichnov

9:05 ANYL **46.** Toward theoretical mass spectrometry: from organic molecules to polypeptides. **R. Spezia**, K. Song

9:25 ANYL **47.** Constrained fitting of overlapping peaks in high-resolution mass spectra: Which ions should we fit, what is the precision of the fitted intensities, can we derive bulk chemical parameters without fitting? **J.L. Jimenez**, H. Stark, M.J. Cubison

9:45 Intermission.

10:00 ANYL **48.** High-throughput method for determining the sugar content in biomass with pyrolysis molecular beam mass spectrometry. **R.W. Sykes**, E.L. Gjersing, C.L. Doeppke, M.F. Davis

10:20 ANYL **49.** Trapped ion mobility spectrometry. **M. Ridgeway**, M. Park, J. Meier, J. Silveira

10:40 ANYL **50.** Ion mobility for the investigation of electrospray variability and structural elucidation: Applied protomer analysis. **D. Stevens**, M. McCullagh, G. Cleland, L. Mullin, J. Burgess

11:00 ANYL **51.** Ion mobility: Mass spectrometry driven discovery of neuropeptide-inspired Alzheimer's disease therapeutics. **M.T. Soper**, B.T. Ruotolo

11:20 ANYL **52.** Resolving power in differential ion mobility spectrometry: What does it really mean. B.G. Santiago, **G.L. Glish**

Section B

Embassy Suites Denver–Downtown Convention Center

Aspen Room B

Advances in Bioanalytical Chemistry

Biosensing and Bioassays

A. G. Cavinato, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 ANYL **53.** Detecting single nucleotide polymorphisms in DNA duplexes using Backscattering Interferometry. **G. Haddad-Weiser**, D.J. Bornhop, R.A. Flowers

8:25 ANYL **54.** Immobilization and functional coating of gold nanoparticles in a polydimethylsiloxane microfluidic device. **K. Kounovsky-Shafer**, J. Blum, R. Svatora, S.A. Darveau, C.L. Exstrom

8:45 ANYL **55.** Highly sensitive electrical biosensing based on nanogap electrode. **T.M. Terse**, S. Herrera, D. Yan, D.J. Kisailus, A.K. Mulchandani

9:05 ANYL **56.** Cellulose based bioassay for colorimetric detection of pathogens. **D. Saikrishnan**, A. Kukol

9:25 Intermission.

9:40 ANYL **57.** Development of an impedance-based TLR4/MD-2 complex-modified Au biosensor for detection of endotoxins from Gram-negative bacteria. **K. Amini**, H. Kraatz

10:00 ANYL **58.** Real-time label-free nanopore sensor for the detection of anthrax. **L. Wang**, S. Zhou, X. Chen, X. Guan

10:20 ANYL **59.** Label-free pathogen detection using siderophore microarrays. **N. Arora**, A. Wei, Y. Kim, P. Low

DOE Nanoscience Research Centers

National Resources for the Nanoscience Community

Sponsored by PRES, Cosponsored by ANYL, CCPA, CEI, ENFL and MPPG

GSSPC: Designed by Nature, Developed by Science: Interdisciplinary Perspectives on Biocatalysis

Sponsored by CHED, Cosponsored by ANYL, BIOL, CATL, ENVR, I&EC, MEDI, ORGN and PRES

The Interface of Chemical and Biological Sciences International Disarmament Efforts

Sponsored by IAC, Cosponsored by ANYL, CHAL, CPRC and PRES

Modern Analytical Approaches for the Characterization of Natural Organic Matter in the Environment

NMR and Photochemical Analysis of NOM

Sponsored by ENVR, Cosponsored by ANYL and MPPG

TUESDAY AFTERNOON

Section A

Embassy Suites Denver–Downtown Convention Center

Aspen Room A

Active Learning in the Undergraduate Analytical Chemistry Curriculum

T. J. Wenzel, *Organizer*

J. K. Robinson, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 ANYL **60.** Replacing analytical chemistry lectures with more effective collaborative learning activities. **T.J. Wenzel**

1:25 ANYL **61.** Team-based learning in a large analytical chemistry course. **A. Lekhi**

1:45 ANYL **62.** Mix and- match: Tools to promote active student participation in instrumental analysis lecture. **K. Slowinska**

‡ *Cooperative Cosponsorship*

2:05 ANYL **63.** Using technology to facilitate discussion in an instrumental analysis course. **J.K. Robinson**

2:25 ANYL **64.** Enhancing outcomes in analytical chemistry via special projects and co-curricular experiences. **D.G. Sykes**, J. Bortiatynski

2:45 Intermission.

3:00 ANYL **65.** Using nanotechnology as a vehicle for teaching in the analytical sciences laboratory. **P. Doolittle**, S. Jin, R.J. Hamers

3:20 ANYL **66.** Development of online resources to promote active learning in analytical chemistry. **M.B. Jensen**

3:40 ANYL **68.** Determination of protein contents of selected food items by Kjeldhal method: A guided inquiry laboratory experiment in a Quantitative Analysis I Laboratory curriculum. **S.O. Fakayode**

4:00 ANYL **67.** Active learning in undergraduate instrumental analysis. **K.J. Ho**

Section B

Embassy Suites Denver–Downtown Convention Center

Aspen Room B

Advances in Bioanalytical Chemistry

Aptamers and DNA

A. G. Cavinato, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 ANYL **69.** Electrochemistry of DNA monolayers modified with a perylenediimide base surrogate. C. Wohlgamuth, M. McWilliams, **A. Mazaheripour**, A.M. Burke, K. Lin, L. Doan, J. Slinker, A.A. Gorodetsky

1:25 ANYL **70.** Sequence specific detection of restriction enzymes at DNA-modified carbon nanotube field effect transistors. **D.D. Ordinario**, A.M. Burke, L. Phan, J. Jocson, H. Wang, M. Dickson, A.A. Gorodetsky

1:45 ANYL **71.** Cellular metal ion sensing using DNAzymes. **K. Hwang**, Y. Lu

2:05 ANYL **72.** Highly sensitive multitarget aptasensors using engineered aptamers for the detection of small molecules. **M. Gu**, Y. Kwon, V. Nguyen, N. Ahmad Raston

2:25 Intermission.

2:40 ANYL **73.** Aptamer-conjugated Si-Mag-CCCCs microparticles for chemical capturing. **N. Ahmad Raston**, E. Hwang, M. Gu

3:00 ANYL **74.** Ultrasensitive sandwich-type SPR aptasensor using dual aptamers developed by target immobilization-free SELEX. **N. Ahmad Raston**, M. Gu

3:20 ANYL **75.** Development of highly sensitive aptamers to metabolite X for an aptamer-based diagnostic system. **B. Lee**, Y. Kwon, M. Gu

3:40 ANYL **76.** Applications of metal ions and liquid crystals for multiplex detection of DNA. **Y. Liu**, K. Yang

GSSPC: Designed by Nature, Developed by Science: Interdisciplinary Perspectives on Biocatalysis

Sponsored by CHED, Cosponsored by ANYL, BIOL, CATL, ENVR, I&EC, MEDI, ORGN and PRES

TUESDAY EVENING

Section A

Embassy Suites Denver–Downtown Convention Center

Aspen Room A

General Analytical Posters

D. C. Duckworth, *Organizer*

7:00 - 9:00

ANYL **77.** Making of hydrocarbon standard mixture $C_{20}H_{42}$ — $C_{40}H_{82}$ from combination of natural product and individual hydrocarbon standards $C_{20}H_{42}$, $C_{22}H_{46}$, $C_{24}H_{50}$, $C_{34}H_{70}$, $C_{36}H_{74}$, $C_{38}H_{78}$,-and-$C_{40}H_{82}$ for qualitative identification based on Kovats Retention Index by using GC/MS/FID. **E.D. Pusfitasari**

ANYL **78.** Vespucci: A novel software tool for hyperspectral data analysis and imaging. **D.P. Foose**, A.C. Stahler, I.E. Pavel Sizemore

ANYL **79.** Gold nanoparticles of different shapes for SERS based environmental sensing applications. **R. Narayanan**, B. Saute

ANYL **81.** Analysis of drug-protein interactions during diabetes by high-performance affinity chromatography. **Z. Li**, R.E. Matsuda, D.S. Hage

ANYL **82.** Analysis of fatty acids by HPLC using 9-chloromethyl-anthracene as a flourescent label. **R.M. Hyslop**, J.B. Tapia

ANYL **83.** Solid-phase extraction using new divalent metal ion-loaded cation exchange resins and application to the isolation of oleandrin from *Nerium oleander*. **A. Li**, L.M. Jablonski, D.B. Green

ANYL **84.** Analytical resolution of recombinant protein identity issues using LC-MS/MS. **N. Yang**, J. Fishpaugh, C.S. Ramsay

ANYL **85.** Metallomics analysis of Hg binding proteins in *Escherichia coli*. **L.R. Walker**, R. Moore, M. Newburn, T. Fillmore, L. Paša-Tolić, D.W. Koppenaal

ANYL **86.** Characterization of lignin and its thermal and biological degradation products using gel permeation or size exclusion chromatography in combination with evaporative light scattering detection and high resolution mass spectrometry. **A.A. Artemyeva**, A. Kubatova, E.I. Kozliak

ANYL **87.** Detection of volatile organic compounds in breath samples as a tool for detecting brucellosis *(Brucella abortus)* in seropositive bison (*Bison bison*). **R.S. Stahl**, P. Nol, J. Rhyan, M. McCollum

ANYL **88.** Identification of Serpin 2 complex binding partners in *Anopheles gambiae* by immunoaffinity chromatography and mass spectrometry. **K. Sellens**, E. Metto, X. Zhang, C.T. Culbertson, K. Michel

ANYL **89.** Differential remnant lipoprotein profiling via immunoseparation and dynamic light scattering analysis. **S. Hameed**, J.M. Jurica, R. Chandra

ANYL **90.** Influenza A virus detection upon the aggregation of monoclonal antibody – conjugated – gold nanoparticles. **Y. Lai**, J.D. Driskell

ANYL **91.** Development of a kinetic spectro-electrochemical assay for uric acid in body fluids. **P.A. Flowers**, M.R. MacDougall

ANYL **92.** Voltammetric determination of sulfur-containing biomolecules using screen-printed electrodes. **M. Chen**, K. Webb, K. Benitez, J. Huang

ANYL **93.** Molecularly imprinted polymer-based electrochemical sensor for peptides. **L. Huang**, K.W. Hunter

ANYL **94.** Spectroelectrochemical studies of reversible attachment of *Shewanella putrefaciens* to an indium tin oxide electrode via applied potential under anaerobic conditions. **J. Muscolino**

ANYL **95.** Extraction and verification of hepatitis B virus DNA from whole blood based on magnetic nanoparticles and whole genome amplification. **C. Ma**, N. Ma, X. Mou, N. He

ANYL **96.** Comparative atomic force microscopy (AFM) and field emission scanning electron microscopy (FE-SEM) studies of mixed phospholipid monolayers. **A. Sunda-Meya**, N. Phambu

ANYL **97.** MALDI-TOF-MS and Q-TOF-MS characterization of mouse, rabbit, and sheep monoclonal antibodies. **P. Ozaeta**, J. Fishpaugh, C.S. Ramsay

ANYL **98.** Enhancement of molecular-ion intensity by Ar_{2500}^{+} -O_2^{+} cosputtering for depth profiling of soft materials in secondary ion mass spectrometry. **Y. Chu**, H. Chang, W. Kao, K. Chu, J. Shyue

ANYL **99.** High-throughput parallel detection and quantification of peptides with paper-based microarray and molecular time-of-flight secondary ion mass spectrometry (ToF-SIMS). **K. Chu**, H. Chang, W. Kao, Y. Chu, J. Shyue

ANYL **100.** Calibrating a HIMAS linear detector on a matrix-assisted laser desorption/ionization reflectron time-of-flight mass spectrometer. **T.L. Wilson**, C.J. Van Leeuwen, K.A. Reyes, K.S. Molek

ANYL **101.** 3D molecular imaging of HEK293T cell with internalized gold nanoparticles using ToF-SIMS. **H. Chang**, J. Shyue

ANYL **102.** Differentiation of *Staphylococci* by CeO_2-facilitated fatty acid metal oxide laser ionization-mass spectrometry profiling. **N. Saichek**, S. Kim, P.D. Harrington, C. Cox, K.J. Voorhees

ANYL **103.** Investigation of the aggregation and amide proton exchange in monomeric amino-acid-based surfactants. **C. Lewis**, A. Wall, K.F. Morris, F.H. Billiot, E. Billiot

ANYL **104.** Preparation of biocompatible magnetic-fluorescent nanocomposites of Fe_3O_4 magnetic particles and perylene-based small organic molecules. **L. Huang**, S.A. Dupre, K.W. Hunter

ANYL **105.** Raman spectroscopy and imaging of a ternary lipid mixture containing sphingomyelin. **N. Phambu**, A. Sunda-Meya

ANYL **106.** Nucleobase-functionalized conjugated polymer for detection of copper(II). **C. Xing**, **H. Yuan**, **H. An**, **Y. Zhan**

ANYL **107.** Detection of a panel of neurotransmitters in human urine using HPLC with UV/Vis detection. **L. Lowe**, J. Petway, Z. Pitcher, A. Krinickas, D.J. Weiss

ANYL **108.** Characterization of native and PEGylated Fab-arms using various modes of analytical chromatography. **J. Steve**, A. Chakrabarti

ANYL **109.** Analysis of free drug fractions in serum by ultrafast affinity extraction and multi-dimensional high-performance affinity chromatography using immobilized alpha 1-acid glycoprotein. **C. Bi**, X. Zheng, S. Beeram, D.S. Hage

ANYL **110.** Internal standard to standard ratio in determining content of EPA and DHA for free fatty acid and ethyl ester drugs. **L. Roy**

ANYL **111.** Microfluidic flow cytometry for the rapid characterization of individual cells. **S.A. Stewart-James**, C.T. Culbertson

ANYL **112.** Preparative isolation and characterization of the triglyceride rich lipoprotein subclass via high-speed Centrifugal Flotation and Dynamic Light Scattering Analysis. **K. Huerta-Ruiz-Garza**, **C. Chidi**, R. Chandra

ANYL **113.** Phage-PEI disposable urine assay for the purpose of early cancer detection. **C.J. Eggers**, K. Mohan, L. Kindra, K.C. Donavan, R.M. Penner, G.A. Weiss

ANYL **114.** Temperature effects in voltammetric DNA hybridization detection of SNPs and genetically modified maize sequences. **K.M. Biala**, G. Flechsig

ANYL **115.** Protein-based biosensor for probing the iron/tau interaction. **S. Ahmadi**

ANYL **116.** Upconverting nanoparticles in solid-phase luminescence resonance energy transfer based assays for the high capacity multiplexed detection of biomolecules. **S. Doughan**, U.J. Krull

ANYL **117.** Towards solid-phase assays using intrinsically labeled oligonucleotide probes on quantum dots fordetermination of selective hybridization. **A. Shahmuradyan**, A. Tavares, U.J. Krull

ANYL **118.** Using live-cell nanomechanical imaging with fluorescence microscopy to track the response of lung cells following toxin exposure. **E. Lau**, **N. Narang**, O. Coury, J. Lymberopolous, D. Burden, L. Keranen Burden

ANYL **119.** Development of a fluorescent method for the analysis of the antineoplastic agent 6-thiopurine. **R.M. Hyslop**, S. Hoskins

ANYL **120.** Chemoresistant lung cancer stem cells display high DNA repair capability for removing cisplatin-DNA damage. **W. Yu**, C. Fong, Z. Wang, D. Liu, G. Zhu, M. Yang

ANYL **121.** Rate of carboxylic acids enolization. **H. Patel**

ANYL **122.** Polycyclic aromatic hydrocarbons in the mainstream smoke of popular U.S. cigarettes. **A.T. Vu**, **K.M. Taylor**, M.R. Holman, Y.S. Ding, C.H. Watson

ANYL **123.** Study of the ozonation kinetics for commonly found EDCs in water. **A. Blondy**, L. Li, W. Han, K. Yeung

ANYL **124.** Exploring versatility: Chiral compound separations by both normal phase and reversed phase HPLC. **T. Jiang**, L. Kott

ANYL **125.** Colorimetric sensor arrays: Interplay of geometry, substrate, and immobilization. **M. LaGasse**, J.M. Rankin, J. Askim, K.S. Suslick

ANYL **126.** Amperometric probes for investigating energy storage processes. **Z.J. Barton**, J. Rodríguez-López

ANYL **127.** Synthesis of metal ion adsorbent using banana fiber and its adsorption properties to rare metal ions. **T. Kajiyama**, S. Sakai, K. Arai, H. Kokusen

ANYL **128.** Significant parameters in APPI FT-ICR mass spectra of molecular distillate samples of vacuum residues. **D.C. Palacio**, J.P. Arenas, X. Ramírez, J.A. Orrego-Ruiz, A. Guzman, R. Cabanzo, E. Mejía-Ospino

ANYL **129.** Compositional changes in uncracked and hydrocracked vacuum residue and its molecular distillation cut and end-cut by (+)APPI FTICR MS. **J.P. Arenas**, D.C. Palacio, A.Y. Leon, J.A. Orrego-Ruiz, A. Guzman, R. Cabanzo, E. Mejía-Ospino

ANYL **130.** Transition metal oxides for use as surfaces in surface assisted laser desorption/ionization of adsorbed asphaltenes. **K.A. Reyes**, C.J. Van Leeuwen, T.L. Wilson, K.S. Molek

ANYL **131.** Method for quantifying release of imidacloprid into water from granular agricultural carriers. **A.C. Litin**, Y. Bernal, B. Oberlin

ANYL **132.** Automated dispersive liquid-liquid microextraction and on-column derivatization coupled to gas chromatography-mass spectrometric for the determination of carbamate pesticides. **L. Gou**, H. Lee

ANYL **133.** Analysis of polychlorinated biphenyls in deep water shark liver tissue. **R. Lynch**, H. Pham, F.D. Hileman, R. Snyder

ANYL **134.** Products formed during the heterogeneous oxidation of polycyclic aromatic hydrocarbons (PAHs) during the aging of diesel exhaust in an atmospheric chamber. **Z. Hoggarth**, R.E. Cochran, H. Jeong, K. Ondrusova, S.G. Minchala, A. Kubatova

ANYL **135.** Identification of pharmaceutics in Utah's Jordan River. **C. Peak**, **G. Guitierres**, **J. Thompson**, **K.L. Nuckles**, C. Carr, T. Schreyer, S. Moore, N. Butler, L.D. Giddings, M. Alvarez, P.J. Iles, N.R. Bastian, R.V. Valcarce

ANYL **136.** Identification and quantification of taralytic Toxins in Puget Sound marine organisms. **K.M. Pierce**, M. Strawn, R. Ferrer

ANYL **137.** Investigation of the use of transition metal ions to remove chloride interference from nitrate ISEs. **P.J. Iles**, **I. Eugenio**, **G. Smith**, L.D. Giddings, N.R. Bastian, M. Alvarez, R.V. Valcarce

ANYL **138.** Analysis of dental parameters, fluoride, and pH in Utah's waters and drinks. **P.J. Iles**, A. Gooch, A. Timmerman, S. Huffaker, L.D. Giddings, M. Alvarez, N.R. Bastian, R.V. Valcarce

ANYL **139.** Simplified fish tissue digestion method for trace metals analysis by ICP-MS. **M. Spedale**

ANYL **140.** Nanomachines for environmental sensing and remediation. **B. Jurado**, J. Wang

ANYL **141.** Prediction of metal remobilization from sediments under various physical/chemical conditions: Design of experiment for Cd, Co, Pb, and Zn. **E. Alkhatib**, **A. Akhdhar**, **F. Altirad**

ANYL **142.** Determination of organic impurities in D&C violet No. 2 by ultraperformance liquid chromatography. H.W. Yang, **J.N. Barrows**

ANYL **143.** Chemical analysis of the taste of craft beers at two different temperatures. **D.E. Jordan**, **C.D. Jeter**, M.J. Kendrick-Murphy

ANYL **144.** Forensic discrimination of lipstick. **B.A. Esterlen**, **B.J. Bellott**

ANYL **145.** Determination of cocaine concentration in creek water via solid-phase extraction. **D.E. Huff**, S.L. Crawford, **B.J. Bellott**

ANYL **146.** Investigation of pen inks, red sealing-inks, and laser toners on questioned documents by nondestructive analytical techniques. **Y. Lee**, J. Lee, M. Kim, Y. Cho, Y. Nam, K. Lee

ANYL **147.** Environmental variables influencing surfactant mobility and soiling on artist's acrylic dispersion paints. **A.F. Lagalante**, R.C. Wolbers, I. Ziraldo, K. Watts

ANYL **148.** Electrospun polymer nanofibers with entrained explosives as potential field calibration standards for explosives. **S. Robertson**, A. Heflin, **B. Bui**, J. Lamb, C. Kneapler, D.E. Riegner, R. Hoff

ANYL **149.** Comparison of MEKC-UV and GC-MS in the analysis of explosives in environmental samples. **A.M. Genzman**, **J.M. Rine**, K.A. Brensinger, C.M. Rollman, I.S. Lurie, M. Moini, C.L. Copper

ANYL **150.** Separation of transition and heavy metal ions using gradient thin layer chromatography. **S. Stegall**, M. Collinson

ANYL **151.** Development of standard reference materials (SRMs) for quantitative nuclear magnetic resonance (qNMR) spectroscopy. **J.A. Widegren**, T.J. Bruno, T.M. Lovestead, T.J. Fortin

ANYL **152.** Interactions of drugs with model membrane systems: Focusing on the interactions near the water interface. **C. Beuning**, C. Rithner, D.C. Crans

ANYL **153.** Characterization of aqueous choline chloride deep eutectic solvents. **S. Asare**

ANYL **154.** Inorganic thermogravimetric analysis of hydrates of first-row transition metal salts revisited. **D.A. Habboush**, **M.A. Arab**, **N.M. Alanazi**

ANYL **155.** Magnesium wire templated microfluidic construction. S. Toussaint, T. Torgersen, J. Wickes, C. Lamb, L.M. Miller, S.L. McKay, **C.F. Monson**

ANYL **156.** Probing the sensitivity and applicability of differential magnetic catch and release for magnetic nanoparticle purification. **J. Morse**, R.E. Schaak, M.E. Williams

ANYL **157.** Mathematical models for quantitative spectrophotometric spectral bandwidth measurements. **A. Reid**, M. Labrie, J. Messman

ANYL **158.** Metrological evaluation of a potential certification bias for potassium dichromate solution measurement standards. **M. Labrie**, A. Reid, J. Messman

ANYL **159.** Particle size paradox. **J.G. Saad**, P.A. Webb

ANYL **160.** Characterization of earth pigments and study of their influence on the drying properties of linseed oil. **E. Portero**, L. de Viguerie, P. Walter

ANYL **161.** Effect of linked gold nanoparticles on the oxidation of silver nanoparticles. **K. Elmer**, R. Masitas, F.P. Zamborini

ANYL **162.** Tailored to suit: Fabricating specialized DETECHIP arrays. **R.M. Burks**, J. Atwater, A.E. Holmes

ANYL **163.** Determination of pyrazole and pyrrole pesticides in environmental water samples by Magnetic Metal-Organic Framework (MOF) as a novel adsorbent coupled with high performance liquid chromatography. **J. Ma**, Z. Yao, Y. Xia

ANYL **164.** Integrated geochemical fingerprinting of uranium deposits for sustainable exploration and development. **L.L. Van Loon**, N.R. Banerjee, M. Fayek, D. Quirt

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WEDNESDAY MORNING

Section A

Embassy Suites Denver–Downtown Convention Center

Aspen Room A

Advances in Electrochemistry

S. H. Pratt, *Organizer*

D. Polcari, C. A. Rusinek, *Presiding*

8:00 Introductory Remarks.

8:05 ANYL **165.** High-efficiency generation-collection microelectrochemical platform for interrogating electroactive thin films. **M.J. Anderson**, R.M. Crooks

8:25 ANYL **166.** New insights into magnesium alloy corrosion using scanning electrochemical microscopy. **P. Dauphin Ducharme**, U.M. Tefashe, R.M. Asmussen, M. Danaie, W.J. Binns, P. Jakupi, G. Botton, D.W. Shoesmith, J. Mauzeroll

8:45 ANYL **167.** Anodic stripping voltammetry at platinum-mercury nanoelectrodes: Trapping of Mn^{2+} by crown ethers. **L. Danis**, S.M. Gateman, M.E. Snowden, I.C. Halalay, J.Y. Howe, J. Mauzeroll

9:05 ANYL **168.** Fabrication of carbon, gold, platinum, silver, and mercury ultramicroelectrodes with controlled geometry. **D. Polcari**, L. Danis, A. Kwan, S. Gateman, J. Mauzeroll

9:25 ANYL **169.** New electrochemical sensors for wearable applications: Sniffing environmental inhalation hazards with ultralow power devices. **M.T. Carter**, J. Stetter, M. Findlay, V. Patel

9:45 Intermission.

10:05 ANYL **170.** 1000-fold sensitivity increase on solid-contact ion-selective electrodes by controlling the ionophore/polymer interface. **S. Granados Focil**, L. Mendecki, K.A. Stockmal, A. Radu

10:25 ANYL **171.** Erbium (III) tetraphenylporphyrin-based ion selective electrodes. **A.J. Kane**, E.D. Steinle

10:45 ANYL **172.** Electrochemical studies into the possible formation of germanene. **M. Ledina**, Y. Kim, J. Jung, J.L. Stickney

11:05 ANYL **173.** Cloud point extraction for electroanalysis: Anodic stripping voltammetry of cadmium. **C.A. Rusinek**, A.F. Bange, I. Papautsky, W.R. Heineman

11:25 Concluding Remarks.

Section B

Embassy Suites Denver–Downtown Convention Center

Aspen Room B

Analytical Chemistry of Natural Resources

Environmental Analysis: Analytical Methods for Natural Resource Assessment and Protection

Cosponsored by MPPG‡

W. T. Cooper, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 ANYL **174.** Raman study of the adsorption behavior of silver nanoparticles at mineral- and natural organic matter-water interfaces. **K.A. O'Neil**, J. Fraley, S.W. Brittle, J. Purvis, S.R. Kanel, S.R. Higgins, I.E. Pavel Sizemore

8:25 ANYL **175.** SP-ICP-MS for nanoparticle detection and size distribution determinations: Current state of the art and future perspectives. **C. Stephan**

8:45 ANYL **176.** Efficient association of chiral HPLC, polarimetric detection and chemometrics: Discrimination of lavender and lavandin essential oils using chiroptical fingerprint. S. Lafhal Sakiou, **I. Bombarda**, N. Dupuy, M. Jean, J. Kister, C. Roussel, P. Vanloot, N. Vanthuyne

9:05 ANYL **177.** Comparative assessment of analytical methods for the determination of total sugar content of energy drinks consumed in Nigeria. **J. U. Okere**

9:45 Intermission.

10:05 ANYL **179.** Toward chemiluminescence detection of cytotoxics in surface waters. **T. Reeves**, R. Popelka-Filcoff, C. Lenehan

10:25 ANYL **180.** Preparation, characterization, and application of activated tassel for the remediation of eutrophic phosphorus in contaminated water. **A.M. Shofolahan**, J. Okonkwo, N. AgyeiA

10:45 ANYL **181.** Withdrawn.

11:05 ANYL **182.** Analysis of trace elements in fuel gas for the prediction of masking events. **T. Bruno**, J. Burger

11:25 ANYL **183.** Comprehensive analytical approach for characterizing the impacts of climate change on carbon sequestration in Arctic peatlands. **S.B. Hodgkins**, R. Wilson, J. Chanton, W.T. Cooper

WEDNESDAY AFTERNOON

Section A

Embassy Suites Denver–Downtown Convention Center

Aspen Room A

Frank H. Field and Joe L. Franklin Award for Outstanding Achievement in Mass Spectrometry: Symposium in Honor of Hilkka I. Kenttämaa

Cosponsored by WCC

L. Yang, *Organizer, Presiding*

V. M. Bierbaum, *Presiding*

1:00 Introductory Remarks.

1:05 ANYL **184.** Mass spectrometry as a synthetic method. **R.G. Cooks**

1:40 ANYL **185.** Peptide and protein aggregation: The latest news. **M.T. Bowers**

2:15 ANYL **186.** SID-IM-SID: A new tool for substructure characterization of protein complexes. **V.H. Wysocki**

2:50 Intermission.

3:05 ANYL **187.** Remote but not disinterested: Measuring influence of charge on radical energetics in distonic radical ions. **S. Blanksby**, D. Marshall

3:40 ANYL **188. Award Address** (Frank H. Field and Joe L. Franklin Award for Outstanding Achievement in Mass Spectrometry sponsored by Waters Corp.). Recent studies on distonic mono- and polyradical cations. **H. I. Kenttamaa**

4:15 Concluding Remarks.

Section B

Embassy Suites Denver–Downtown Convention Center

Aspen Room B

Analytical Chemistry of Natural Resources

Instrumentation and Methods

Cosponsored by MPPG‡

M. Fayek, A. Karamalidis, A. Koenig, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 ANYL **189.** Withdrawn.

1:25 ANYL **190.** Multicollector ICP-MS for isotope ratio analysis of uranium. **G.L. Hart**, S.H. Pratt

1:45 ANYL **191.** Variations in hydrogen isotopes of individual plant waxes from four plant species during the growing season. A. **Oakes**, M.T. Hren

2:05 ANYL **192.** Dual isotopic ($\delta^{13}C$, $\delta^{2}H$) evidence for long-range transport of mining-related PAHs in the Athabasca oil sands region. **J.J. Jautzy**, J.M. Ahad, C. Gobeil, A. Smirnoff, B.D. Barst, M.M. Savard

2:25 ANYL **193.** Isotopic variability of nitrogen oxides (NO_x) from biomass burning. **D.L. Fibiger**, M. Hastings

2:45 Intermission.

3:00 ANYL **194.** Design and implementation of quantitative carbon detector (QCD) for calibration-free gas chromatography. **C. Krumm**, S. Maduskar, A.R. Teixeira, A. Paulsen, T. Mountziaris, W. Fan, P.J. Dauenhauer

3:20 ANYL **195.** Vapor sampling by PLOT-cryoadsorption: Examples in forensic sample analysis. **T. Bruno**

3:40 ANYL **196.** HPTLC and clustering analysis for the classification of colored wheat varieties by anthocyanin patterns. **S. Böhmdorfer**, G. Genta-Jouve, H. Grausgruber, T. Rosenau

4:00 ANYL **197.** Multichannel high frame-rate beam-scanning microscopy based on Lissajous scanning trajectories and model based image reconstruction. **S. Sullivan**, J. Newman, R. Muir, S. Sreeharu, C.A. Bouman, G.J. Simpson

4:20 ANYL **198.** Polymer screen-printing for paper-based device fabrication. **Y. Sameenoi**, P. NaNongkai, S. Nouanthavong, C. Henry

THURSDAY MORNING

Section A

Embassy Suites Denver–Downtown Convention Center

Aspen Room A

Nakanishi Prize: Symposium in Honor of Fred W. McLafferty

N. L. Kelleher, *Organizer*

P. Compton, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 ANYL **199.** Native electron capture dissociation: A droplet dissociation process used to elucidate iron-binding motifs in biological macromolecules. **O. Skinner**, M. McAnally, R.P. Van Duyne, P.D. Compton, N.L. Kelleher

8:50 ANYL **200.** New approaches to multiplex newborn screening of lysosomal storage disorders by tandem mass spectrometry. **F. Turecek**, M.H. Gelb, C.R. Scott

9:35 ANYL **201.** Developing native top-down mass spectrometry as a tool for protein structural biology. **J.A. Loo**

10:20 Intermission.

10:35 ANYL **202.** Top-down mass spectrometry of modified ribonucleic acids. **K. Breuker**

11:20 ANYL **203. Award Address** (Nakanishi Prize sponsored by the Nakanishi Prize Endowment). Analytical chemistry of gaseous ubiquitin ions. **F.W. McLafferty**, S. Castro, O. Skinner, K. Breuker

THURSDAY AFTERNOON

Section A

Embassy Suites Denver–Downtown Convention Center

Aspen Room A

Advances in Analytical Spectroscopy

X. Yu, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 ANYL **204.** Finding the needle in the haystack: Characterization of trace crystallinity in a commercial formulation of paclitaxel protein-bound particles by Raman spectroscopy and synchrotron X-ray diffraction enabled by second harmonic generation microscopy. **P.D. Schmitt**, N.S. Trasi, F. Deng, S. Zhang, L.S. Taylor, G.J. Simpson

1:25 ANYL **205.** Four-wave mixing imaging of nanorod aggregates. **K.A. Antonio**, Z.D. Schultz

1:45 ANYL **206.** Spectroscopic analyses of chemical adaptation processes within microalgal biomass in response to changing environments. **F. Vogt**

2:05 ANYL **207.** Correlative imaging of cancer cell and drug interactions in the liquid microenvironment. **X. Hua**, C. Szymanski, Z. Wang, B. Liu, Z. Zhu, J. Evans, G. Orr, s. Liu, X. Yu

2:25 ANYL **208.** Biomarker VOC concentration and desorption coupled with a TIR-Raman system. **R. Dodson**, A.R. Mercer-Smith, K. Park, P. Koonath, H. Lu, V. Sapirstein, A. Niemz, C. Taylor

2:45 Intermission.

‡ *Cooperative Cosponsorship*

3:00 ANYL **209.** Optimizing uptake and identification of volatile organic compounds for clinical diagnoses. **A.R. Mercer-Smith**, R. Dodson, K. Park, P. Koonath, H. Lu, V. Sapirstein, A. Niemz, C. Taylor

3:20 ANYL **210.** Spectroscopic analysis of weakly turbid systems: A generally useful simple algorithm. **P. Dent**, R. McDonough, K. Rawlins, S. Ortiz, J. Goodisman, J. Chaiken

3:40 ANYL **211.** Rapid, broadband, precision spectroscopy of carbon dioxide near 5000 cm^{-1} using optical frequency combs. **A. Klose**, G. Truong, L. Sinclair, I. Coddington, N. Newbury, S. Diddams

4:00 ANYL **212.** Brightness-equalized quantum dots. **S. Lim**, M.U. Zahid, D. Entenberg, A.S. Harney, J. Condeelis, A. Smith

4:20 ANYL **213.** Trace chemical sensing by photoionization through Rydberg states followed by detection of the laser induced plasma via microwave radiation. **F. Rudakov**, P. Weber

BIOT

Division of Biochemical Technology

M. Lazzara and A. Kantardjieff, *Program Chairs*

OTHER SYMPOSIA OF INTEREST:

Phenolic & Polyphenolic Chemistry in Food Processing *(see AGFD, Tue)*

Undergraduate Research Posters *(see CHED, Mon)*

Rising Stars Awards Symposium *(see WCC, Mon)*

SOCIAL EVENTS:

Membership Desk, 8:00 AM: Sun, Mon, Tue, Wed, Thu

Reception, 6:30 PM: Sun

Poster Session, 6:00 PM: Tue

Program Chair's Lunch 6:00 PM: Tue

Company Seminars 12:30 PM: Sun, Mon, Wed

Networking/ Mentoring Session 6:00 PM: Wed

BUSINESS MEETINGS:

BIOT Executive Committee Meeting, 7:00 PM: Mon

Future Programming Meeting, 12:30 PM: Tue

SUNDAY MORNING

Section A

Grand Hyatt Denver
Mt. Elbert A

Upstream Processes

Advances in Systems Biology

M. R. Antoniewicz, B. Mulukutla, *Organizers, Presiding*

8:30 BIOT **1.** New insight of the CHO cell transgene production level using next-generation genomic tools. **H. Fu**, N. Vishwanathan, M. Xiong, A. Bandyopadhyay, Y. Yang, W. Hu

8:50 BIOT **2.** Automated RNA-Seq analysis pipeline to identify and visualize differentially expressed genes and pathways in CHO cells. **C. Chen**, H. Le, C. Goudar

9:10 BIOT **3.** Transcriptome, methylome, and genome analysis in clonal variability. **L. Zhao**, N. Vishwanathan, H. Fu, A. Bandyopadhyay, W. Hu

9:30 BIOT **4.** Updating the Chinese hamster reference genome and applications to CHO HCP studies. **K.H. Lee**

10:10 BIOT **5.** Development of a comprehensive *Escherichia coli* kinetic metabolic model consistent with multiple genetic and environmental perturbations. **A. Khodayari**, C. Maranas

10:30 BIOT **6.** Reconstructing anaerobic microbiomes from the "bottom-up": New techniques to decipher interwoven metabolism. **J.A. Sexton**, K. Solomon, J. Henske, M.K. Theodorou, D.L. Valentine, M.A. O'Malley

10:50 BIOT **7.** Genome scale metabolic network reconstruction of *Synechocystis sp.* PCC6803 taking into account molecular mechanisms under photoautotrophic conditions. **C. Joshi**, F.E. Estep, M. Tracey, C.A. Peebles, A. Prasad

11:10 BIOT **8.** Development of regulated metabolic models for anaerobic organisms. **S. Dash**, C.D. Maranas

Section A

Grand Hyatt Denver
Mt. Evans

David Perlman Memorial Lectureship and Van Lanen and Peterson Award Presentations

M. Lazzara, *Organizer, Presiding*

11:30 BIOT **9.** Overcoming obstacles to expression and characterization of difficult proteins. A.S. Robinson

Section B

Grand Hyatt Denver
Mt. Evans

Downstream Processes

Advances in Chromatographic Separations

A. Hewig, J. Hubbuch, A. R. Lajmi, S. Yamamoto, *Organizers, Presiding*

8:30 BIOT **10.** Scalability of mechanistic models for ion exchange chromatography. **T. Huuk**, T. Hahn, J. Griesbach, H. Stefan, J. Hubbuch

8:50 BIOT **11.** Competitive binding of antibody monomer-dimer mixtures on CEX resins: Equilibrium and kinetics. **J. Reck**, T. Pabst, A. Hunter, X. Wang, G. Carta

9:10 BIOT **12.** Development of robust orthogonal methods for impurity clearance using high throughput screening. **S. Chollangi**

9:30 BIOT **13.** Optimization of monomer separation processes by electrostatic-interaction chromatography. **S. Yamamoto**, N. Yoshimoto, Y. Isakari, A. Podgornik

9:50 Intermission.

10:10 BIOT **14.** Chromatographic retention prediction using quantitative structure property relations. **M.E. Klijn**, A. Hanke, M. Ottens

10:30 BIOT **15.** Insights into the nature of multimodal chromatographic selectivity using *in silico* designed Fab fragment variants. **H. Karkov**, H. Ahmadian, B. Olsen Krogh, A. Bogsnes, S.M. Cramer

10:50 BIOT **16.** Modelling of pH and dual gradient ion exchange and multi modal chromatography for the purification of mAbs. **S. Kluters**, Y. Lee, C. Frech

11:10 BIOT **17.** Systematic exploration of homologous ligand library leads to improved design principles and tools for the prediction of protein selectivity in mixed-mode chromatographic systems. **J. Woo**, H. Chen, M.A. Snyder, S.M. Cramer

Section C

Grand Hyatt Denver
Grays Peak A

Biomolecular & Biophysical Processes

Protein Characterization Technologies

J. Kaar, A. R. Lajmi, *Organizers, Presiding*

8:30 BIOT **18.** Rapid screening of monoclonal antibody stability in serum using affinity-capture self-interaction nanoparticle spectroscopy. **S. Geng**, X. Li, M. Chiu, D. Saro, P.M. Tessier

8:50 BIOT **19.** Time evolution of protein gel bead microstructure. **D. Greene**, A.M. Lenhoff, N.J. Wagner, S.I. Sandler

9:10 BIOT **20.** Fitness landscapes as comprehensive measures of adaptive tradeoffs in the engineering of protein function. **B. Steinberg**, M.A. Ostermeier

9:30 BIOT **21.** Asparagine-repeat peptides: Synthesis, characterization, and comparison to glutamine repeats. **X. Lu**, R.M. Murphy

9:50 Intermission.

10:10 BIOT **22.** Quantifying the surface hydrophobicity of human gamma-D crystallin and its cataract-associated P23T mutant using molecular dynamics simulations. **E. Wu**, S. Garde

10:30 BIOT **23.** Biophysical characterization of reflectin isoforms from squid and cuttlefish. **L. Phan**, W.G. Walkup IV, D. Ordinario, **A.A. Gorodetsky**

10:50 BIOT **24.** Azo-group based noval Naked eye DNA sensors for alcohalic media. **A. Altaf**, U. **Hashmat**, A. Badshah, **B. Lal**, S. Ullah

11:10 BIOT **25.** Comparison of real-time and post-mortem techniques for detection of protein fouling. **A. Greenberg**, E. Kujundzic, A. Lajmi, X. Wu

Section D

Grand Hyatt Denver
Grays Peak B

Emerging Technologies

Molecular Delivery

W. Porter, G. Thurber, *Organizers, Presiding*

8:30 BIOT **26.** Near infrared-degradable crosslinkers for on-demand delivery of hydrophilic molecules. C. de Gracia Lux, S. Lee, M. Chan, **A. Almutairi**

8:50 BIOT **27.** Novel light-triggered therapeutics for selective cell phenotypes. **S.M. Goodman**, C.M. Courtney, J. McDaniel, A. Chatterjee, P. Nagpal

9:10 BIOT **28.** Kinome-level screening identifies kinase targets for enhancing transient transgene expression. **M. Christensen**, J. Elmer, S. Eaton, L. Gonzalez-Malerva, J. LaBaer, K. Rege

9:30 BIOT **29.** Local sustained co-delivery of 25-hydroxyvitamin D3 and parathyroid hormone-related peptide for overcoming antimicrobial resistance. **J. Xie**, J. Jiang

9:50 Intermission.

10:10 BIOT **30.** Phosphoramidation-based bioorthogonal reactions for synthesis of nucleic acid conjugates potentially useful in target delivery of DNA/RNA therapeutics. Y. Su, **T. Wang**

10:30 BIOT **31.** Histone-targeted gene delivery scaffolds for bone regeneration. E.V. Munsell, **M.O. Sullivan**

10:50 BIOT **32.** CMP-based method for achieving tunable, cell-mediated gene delivery. **M. Urello**, K.L. Kiick, M. Sullivan

11:10 BIOT **33.** Biomimetic pH-responsive polymers for intracellular therapeutic delivery and theranostic applications. **R. Chen**

Section E

Grand Hyatt Denver
Mt. Elbert B

Colorado Biotechnology

Biomedical Research

N. Boyle, C. A. Eckert, *Organizers*
S. Khetani, M. Krebs, *Presiding*

8:30 BIOT **34.** Modified aptamers and their uses in biomedical research and development. **N. Janjic**

9:10 BIOT **35.** Biodegradable, micropatterned wound dressings for enhanced epithelialization. **C.M. Magin**, M.C. Drinker, E.E. Mann, S.T. Reddy, G.S. Schultz, A.B. Brennan

9:50 Intermission.

10:10 BIOT **36.** Induced ketosis in mild to moderate Alzheimer's disease. **S. Henderson**

10:50 BIOT **37.** Intervening in complex disease biology with microRNA-targeting therapeutics. **W. Marshall**

SUNDAY AFTERNOON

Section A

Grand Hyatt Denver
Grays Peak A

Upstream Processes

Engineering Natural Product Biosynthesis

V. Roy, M. Thomas, *Organizers, Presiding*

2:00 BIOT **38.** Structure and substrate specificity of AtxE2, a lasso peptide isopeptidase. **J.D. Koos**, M. Maksimov, A. Link

2:20 BIOT **39.** Peptide that neutralizes rattlesnake venom in mice can be expressed in *E. coli*. E.E. Sanchez, M. Suntravat, Z. Ahmad, A. Cifelli, A.S. Rathore, **C.F. Komives**

2:40 BIOT **40.** Synthetic biochemical production of medicinal protoberberine alkaloids in yeast. S. Galanie, C.D. Smolke

3:00 BIOT **41.** Reinventing central carbon metabolism in *Saccharomyces cerevisiae* for high-volume biofuel production. **A. Tsong**, Y. Tsegaye, A. Meadows, L. Pickens, A. Tai, E. Antipov, Q. Mitrovich, K.A. Curran

3:20 Intermission.

3:40 BIOT **42.** Combinatorial design and assembly for engineering multi-gene systems. **M. Smanski**

4:00 BIOT **43.** Diverse opportunities for engineered biosynthesis of complex natural products. **B.A. Pfeifer**

4:20 BIOT **44.** Protein interactions in type II fatty acid and polyketide biosynthesis. **M.D. Burkart**

4:40 BIOT **45.** Carbon-neutral chemicals from sunlight and CO. **S. Liu**

Section B

Grand Hyatt Denver
Mt. Evans

Downstream Processes

Advances in Chromatographic Separations

A. Hewig, J. Hubbuch, A. R. Lajmi, S. Yamamoto, *Organizers, Presiding*

2:00 BIOT **46.** Using powerful HT chromatography screenings to develop purification steps modulating charge-related isoform patterns. **F. Rudolph**, G. Anja, M. Pauers, D. Michael, J. Studts, M. Hampel

2:20 BIOT **47.** Right tool for the job? A critical look at the needs of a diverse product pipeline. **L.W. Pampel**, J. Aucamp, B. Guelat

2:40 BIOT **48.** Robo-characterization: Can HTS miniature columns predict a manufacturing future? **J. Pollard**, H. Bao, M. Petroff, S. Kandula, N. Tugcu, J. Welsh, T. Linden

3:00 BIOT **49.** Comparison of PAT based approaches for making real-time pooling decisions for process chromatography – use of feed forward control. **A.S. Rathore**

3:20 Intermission.

3:40 BIOT **50.** Optimal elution gradient preparative chromatography. A. Holmqvist, F. Magnusson, A. Sellberg, **B. Nilsson**, A. Staby

4:00 BIOT **51.** Molecular study on the MabSelect SuRe ligand after treatment under alkaline conditions. **T. Bjorkman**, F. Berqvist, M. Wetterhall

4:20 BIOT **52.** Understanding the effect of salt ions on protein adsorption in novel responsive hydrophobic interaction membrane chromatography. **Z. Liu**, S.R. Wickramasinghe, X. Qian

4:40 BIOT **53.** New generation sorbents for the purification of biomolecules. J. Champagne, **M. Schofield**, A. Uzel, G. Balluet, R. Gantier, M. Toueille

TECHNICAL PROGRAM

Section C

Grand Hyatt Denver

Mt Elbert A

Biomolecular & Biophysical Processes

High Concentration Therapeutics: Development, Production & Delivery

T. Randolph, N. Warne, *Organizers, Presiding*

2:00 BIOT **54.** Biopharmaceutical informatics: Understanding behavior of highly concentrated antibody solutions at molecular level via coarse-grained modeling and simulations. **D. Tomar**, P. Buck, S. Kumar, S.K. Singh

2:20 BIOT **55.** Relating protein – protein and protein – solute interactions to protein aggregation rates for low to high protein concentration solutions. **R. Ghosh**, A. Saluja, C.J. Roberts

2:40 BIOT **56.** Biochemical characterization of the low viscosity reversible protein nanocluster platform. **J. Laber**, B.J. Dear, A. Borwankar, J. Maynard, T. Truskett, K.P. Johnston

3:00 BIOT **57.** Computational modeling of bulk scale freezing to predict freeze duration and cryoconcentration of biologics in a liquid nitrogen blast freezer. **K. Greco**, R. Falk, J. Cape, T.R. Gervais

3:20 Intermission.

3:40 BIOT **58.** Role of spatial heterogeneity in protein adsorption on polymeric membrane materials at the single-molecule level. **B. Langdon**, R. Mirhossani, **J. Mabry**, I. Sriram, A.R. Lajmi, D.K. Schwartz

4:00 BIOT **59.** Probing protein denaturation at the solid-liquid interface with single-molecule fluorescent microscopy. **J. Weltz**, D.K. Schwartz, J. Kaar

4:20 BIOT **60.** High concentration abstract TBD. **H. Samra**

4:40 Panel Discussion.

Section D

Grand Hyatt Denver

Grays Peak B

Emerging Technologies

Disease & Biomedical Applications

K. Lampe, J. Zartman, *Organizers, Presiding*

2:00 BIOT **61.** Peptoids modulate Aβ aggregation and alter morphology of fibril species. **J.P. Turner**, M. Moss, S.L. Servoss

2:20 BIOT **62.** Using backscattering interferometry to characterize interactions of the cystic fibrosis transmembrane conductance regulator with small molecule modulators. **A. Lockwood**, D. Heidary, C.I. Richards, M. Baksh, M. Finn

2:40 BIOT **63.** Mobile phone based microscopy for imaging and sizing of single DNA molecules. **Q. Wei**, W. Luo, S. Chiang, T. Kappel, C. Mejia, D. Tseng, R. Chan, E. Yan, H. Qi, F. Shabbir, H. Ozkan, S. Feng, A. Ozcan

3:00 Intermission.

3:20 BIOT **64.** Multifunctional hydrogel assays for 3D culture of melanoma cells reveal increased matrix metalloproteinase activity and migration in response to BRAF/MEK inhibitors. **E.Y. Tokuda**, J. Leight, K.S. Anseth

3:40 BIOT **65.** Cross species meta-analysis of transcriptome data to unveil the road block of stem cell differentiation to hepatocytes. **R. Raju**, D. Chau, H. Pei, W. Hu

4:00 BIOT **66.** Design principles of a robust genetic switch using antisense transcription in naturally occurring systems. **A. Escalas Bordoy**, U.S. Varanasi, A. Chatterjee

4:20 BIOT **67.** Engineered Prussian blue nanoparticles as multimodal molecular imaging agents. **R. Fernandes**

Section E

Grand Hyatt Denver

Mt. Elbert B

Colorado Biotechnology

The Science of Colorado's Craft Beer, Wine & Spirits Industries

N. Boyle, *Organizer*

C. A. Eckert, *Organizer, Presiding*

R. Sclafani, *Presiding*

2:00 Introductory Remarks.

2:20 BIOT **68.** Reticulated regulatory network governing glucose fermentation by yeasts. **M. Johnston**

2:40 BIOT **69.** Utilization of next generation sequencing to develop a real-time qPCR assay for cross-contamination of house brewing yeasts. **D. Driscoll**

3:00 BIOT **70.** Rapid measurement of beer flavor stability: Application of UPLC-MS metabolomics to develop non-volatile markers of beer stability. **D.L. Sedin**, A. Heuberger, C. Broeckling, J. Prenni

3:20 Intermission.

3:40 BIOT **71.** Operation of a craft brewery within a major brewery: An overview of Blue Moon Brewing Company. **K. Villa**

4:00 Panel Discussion.

MONDAY MORNING

Section A

Grand Hyatt Denver

Mt. Elbert A

Upstream Processes

Mammalian Cell Culture Process Development

N. Jacob, S. T. Sharfstein, *Organizers, Presiding*

8:30 BIOT **72.** Understanding cell line bubble sensitivity and preparing for future challenges. **R. Ferguson**, W. Hu, H. Peng, K. Wiltberger, T.K. Ryll

8:50 BIOT **73.** Genome-wide analysis of transgene expression in Chinese hamster ovary cells. **K. Lee**, H. Fu, W. Hu

9:10 BIOT **74.** Shear contributions to cell culture performance and product recovery in ATF and TFF perfusion systems. **S. Wang**, H. Lin, S. Godfrey, R.W. Leighty, J. Ravikrishnan, A. Osborne, J.L. Coffman, J. Vogel

9:30 BIOT **75.** Evaluating the impact of copper on CHO cell metabolism and antibody Fc glycan galactosylation using enzymatic assays. **J. Huang**, H. Zhang, M. Trentalange, B. Shah, Z. Zhang, C. Goudar

9:50 Intermission.

10:10 BIOT **76.** Developing a perfusion process for a novel protein. **S.G. Vajrala**, B. Holman, J.H. Lee, A.E. Schmelzer

10:30 BIOT **77.** Understanding the transcriptome responses of Chinese hamster ovary (CHO) cells using RNA-seq. **Y. Gowtham**, C. Saski, S.W. Harcum

10:50 BIOT **78.** Concentrated fed-batch cell culture increases manufacturing capacity without additional volumetric capacity. **W. Yang**, D. Minkler, R.R. Kshirsagar, T.K. Ryll, Y. Huang

11:10 BIOT **79.** Challenges associated when moving from a peptone-containing early stage cell culture process to a chemically-defined late stage cell culture process. **L. Brown**

Section A

Grand Hyatt Denver

Mt. Evans

Marvin J. Johnson Award in Microbial and Biochemical Technology

M. Lazzara, *Organizer, Presiding*

11:30 BIOT **80.** Mammalian cell factories: Taking small steps forward to keep from drowning in big data. **M.J. Betenbaugh**

Section B

Grand Hyatt Denver

Mt. Evans

Downstream Processes

Non-Chromatographic Separations & Process Integration

R. Aires-Barros, J. Cyganowski, *Organizers, Presiding*

8:30 BIOT **81.** High pressure refolding as an alternative technology in protein manufacturing. **L. Gombos**

8:50 BIOT **82.** Exploring options for continuous diafiltration. **M. Westoby**, A. Brinkmann

9:10 BIOT **83.** Integrated flocculation and depth filtration high-throughput process development for CHO supernatants. **G. Espuny Garcia del Real**, J.L. Davies, D.G. Bracewell

9:30 BIOT **84.** Smaller is better: Depth filtration at the 0.2 cm2 scale. **A. Noyes**, J. Basha, S. Cook, B. Huffman, D.P. LaCasse, R.S. Wright, R. Fahrner, R. Godavarti, N. Titchener-Hooker, J. Mullin, D. Millard, J. Frostad, K. Sunasara, T. Mukhopadhyay

9:50 Intermission.

10:10 BIOT **85.** Evaluation of precipitation driven processes for monoclonal antibody downstream processing. **U. Bhaskar**, K. Wei, P. Jorjorian, S. Shrivastava

10:30 BIOT **86.** Parvovirus filter robustness investigation: The characterization of higher order aggregates and membrane fouling. **B.V. Bhut**, M. Jin, J. Savard, D. Brody, N. De Mas, I. Pla, Z. Li

10:50 BIOT **87.** Understanding and modeling retention of mammalian cells in a fluidized bed centrifuge. **W.J. Kelly**, J. Scully, J. Rubin, V. Kamaraju, P. Wnukowski, R. Bhatia

11:10 BIOT **88.** Modelling high concentration tangential flow filtration unit operations. **Y. Lam**, M. Westoby, A. Brinkmann

Section C

Grand Hyatt Denver

Mt. Sopris A

Biomolecular & Biophysical Processes

Engineering Protein Function & Stability

E. Boder, D. Colby, A. Link, *Organizers, Presiding*

8:30 BIOT **89.** NMR-guided rational engineering of an ionic liquid tolerant lipase. **E. Nordwald**, G. Armstrong, J. Kaar

8:50 BIOT **90.** Sense codon reassignment in E. coli: Toward 22 amino acid genetic codes (and beyond). **J.D. Fisk**

9:10 BIOT **91.** Highly soluble and active human paraoxase variants for quorum quenching. C. Li, **X. Ge**

9:30 BIOT **92.** Rational design of protein switches based on the ensemble model of allostery. **J.H. Choi**, A.H. Laurent, V.J. Hilser, M. Ostermeier

9:50 Intermission.

10:10 BIOT **93.** Laser extraction from micropore arrays enables high-throughput enzyme engineering. **A. Kannan**, B. Chen, F. Sunden, S. Alford, S. Lim, I. Dimov, D. Herschlag, T. Baer, J. Cochran

10:30 BIOT **94.** Directed evolution of self-cleaving intein purification tags using yeast surface display. **S.D. Stimple**, M.J. Coolbaugh, M. Shakalli Tang, D.W. Wood

10:50 BIOT **95.** Library-scale evaluation of a computational design and thermostable cellulase. **L. Johnson**, L. Gintner, S. Park, C. Snow

11:10 BIOT **96.** Ultrahigh throughput method for the identification of orthogonal aminoacyl tRNA synthetase/tRNA pairs. **A. Hohl**, X. Liu, J. Eppinger

Section D

Grand Hyatt Denver

Grays Peak

Emerging Technologies

Stem Cells & Regenerative Medicine

Y. Kim, C. Kirschner, *Organizers, Presiding*

8:30 BIOT **97.** Emerging technologies for biomaterials at the biological interface. **K. Anseth**

9:10 BIOT **98.** Photopatterning of site-specifically modified proteins within hydrogel biomaterials. J.A. Shadish, C.K. Arakawa, **C.A. DeForest**

9:30 BIOT **99.** Hydrogels for controlling stem cell fate through intracellular redox state. **K. Lampe**, L. Russell

9:50 Intermission.

10:10 BIOT **100.** *Ex vivo* platelet production from hematopoietic stem cells: Understanding the environment and signaling pathways directing proplatelet formation. **T. DeLuca**, L. Helfrich, P. Weingarden, A. Schlinker, L. Shea, W.M. Miller

10:30 BIOT **101.** Scalable hepatic differentiation of human pluripotent stem cells. **H. Pei**, R. Raju, D. Chau, W. Hu

10:50 BIOT **102.** Chemical biology technologies to identify small-molecule regulators of cancer stem cells. **J. Lee**

11:10 BIOT **103.** Thiol-ene Photoclick chemistry as an approach for user directed covalent tethering of bioactive proteins to synthetic hydrogel scaffolds. **I. Marozas**, D. Alge, K.S. Anseth

Section E

Grand Hyatt Denver

Mt. Sopris B

Biosimilars & Follow-on Biologics

Process Development & Manufacturing Considerations for Biosimilars

F. He, S. Vunnum, *Organizers, Presiding*

8:30 Introductory Remarks.

8:50 BIOT **104.** Development and commercialization of biosimilar Products: challenges and opportunities. **A.S. Rathore**

9:30 BIOT **105.** High-throughput multi-parametric clone screening approach for the generation of biosimilar production cell lines. **K. Le**, H. Le, H. Victor, S. Fodor, C. Rollins, T. Munro

9:50 Intermission.

10:10 BIOT **106.** Overcoming challenges in biosimilar process development: Innovative purification tools to fine-tune biosimilarity. **O.A. Jaquez**, R.S. Gronke

10:30 BIOT **107.** Purification of a fusion protein containing high HMWs and LMWs. **B. Wang**, D. Wu, J. Shou, S. Liao, J. Fan

10:50 BIOT **108.** Development of biosimilar drug product in prefilled syringe presentations: Considerations and challenges. **M. Jayaraman**, K. Sampathkumar

11:10 Panel Discussion.

MONDAY AFTERNOON

Section A

Grand Hyatt Denver

Mt. Elbert A

Upstream Processes

Mammalian Cell Culture Process Development

V. Janakiraman, I. H. Yuk, *Organizers, Presiding*

2:00 BIOT **109.** Achieving glycosylation comparability and similarity through cell culture medium optimization. **L. Zhang**, I. Liu, M. Ambhaikar, V. Dandekar, C. Jung, C. Goudar

2:20 BIOT **110.** Epigenetic studies of antibody-producing CHO cells for therapeutic applications. **S. Nicoletti**, H. Dahodwala, Z. Keresztessy, S.T. Sharfstein

‡ *Cooperative Cosponsorship*

2:40 BIOT **111.** Matching dissolved carbon dioxide profiles to achieve comparable cell culture performance across scales. **J.J. Wuu**, A. Meier, S. Bhardwaj, L. Zheng, K. Tschudi, S.J. Meier

3:00 BIOT **112.** Control of antibody glycosylation: Application of statistical analysis of manufacturing data coupled with DOE in scale down models to significantly reduce variation in antibody glycosylation. **R.G. Beri**, V. Canning, B. Hadley, A. Maxwell, J. Kauten, J. Heimbach, R. Gerber

3:20 Intermission.

3:40 BIOT **113.** Inhibition of intracellular histone deacetylase (HDAC) enzymes for enhancement of transient transgene expression. J. Elmer, **M. Christensen**, S. Barua, J. Lehrman, K. Haynes, K. Rege

4:00 BIOT **114.** Application of metabolomic analysis to systematically design fed-batch media for process improvement. **Y. Li**, N. Aranibar, B.M. Warrack, J. Yee, M.C. Borys, Z. Li

4:20 BIOT **115.** Production of highly gamma carboxylated recombinant human factor II with consistent sialylation level in a fed-batch process. **J.H. Lee**, J. Reier, K. Heffner, C. Barton, D. Spencer, A. Schmelzer

4:40 BIOT **116.** Impact of pH control strategies on CO_2 accumulation in bioreactors at different scales. **S. Xu**, H. Chen

Section B

Grand Hyatt Denver
Mt. Evans

Downstream Processes

Non-Chromatographic Separations & Process Integration

R. Aires-Barros, J. Cyganowski, *Organizers, Presiding*

2:00 BIOT **117.** Aqueous two-phase systems from natural products to large biomolecules. **R.M. Aires-Barros**, A. Azevedo, D. Silva, R. Soares, V. Chu, J. Conde

2:20 BIOT **118.** Practical experiences in the development of a lab-scale process for the production and recovery of fucoxanthin from *Isochrysis galbana*. **A. Gómez-Loredo**, J. González-Valdez, J. Benavides, M.A. Rito-Palomares

2:40 BIOT **119.** Strategy for primary recovery of a mAb employing harvest treatment and depth filtration. **Z. Tan**, R. Martel, N. Singh, M. Jin, A.T. Lewandowski, Z. Li

3:00 BIOT **120.** Optimizing clarification of feed streams when nanoparticles are the product. **M. Collins**, A. Onraedt, R. Leibnitz

3:20 Intermission.

3:40 BIOT **121.** Constrained by the membrane: A case study of harvest process streams fouling single pass tangential flow filters. **K. Petty**, E. Gefroh, N. Soice, A. Hewig

4:00 BIOT **122.** Novel system design and cleaning strategies for single pass tangential flow filtration systems. **J. Parrella**, S. Lau, K. Chan, J. Steen, H. Lutz

4:20 BIOT **123.** Effect of operating parameters on parvovirus retention by membranes during flow interruption. **D.M. Bohonak**, A. Leahy, P. Greenhalgh

4:40 BIOT **124.** Avoiding the pitfalls of viral clearance experimental design: utilizing representative spiking conditions. **D. Strauss**, A. Schwartz, N. Hirotomi

Section C

Grand Hyatt Denver
Grays Peak

Biomolecular & Biophysical Processes

Engineering Protein Function & Stability

E. Boder, D. Colby, A. Link, *Organizers, Presiding*

2:00 BIOT **125.** Human therapeutic enzyme specifically sabotages tumor metabolism by an engineered cystine/cysteine degrading activity. **S. Cramer**, A. Saha, S. Tiziani, J. Digiovanni, E. Stone, G. Georgiou

2:20 BIOT **126.** Toward rational design of viscosity reducing mutants of monoclonal antibody therapeutics. **S. Kumar**, D. Tomar, P.E. Nichols, L. Li, S.K. Singh

2:40 BIOT **127.** Biophysical properties of antibody drugs: Predicting and engineering developability. **K. Wittrup**

3:20 Intermission.

3:40 BIOT **128.** Structure-based design of CDR mutations that increase the solubility of multi-domain antibody fragments. **L. Zhang**, S. Kumar, K. Sunasara, M. Allen, P.M. Tessier

4:00 BIOT **129.** Genetically encoded unstrained olefins for live cell labelling with tetrazine dyes. **Y. Lee**, W. Liu

4:20 BIOT **130.** Rational identification of scaffolds for combinatorial discovery of ligands. M. Kruziki, P. Holec, D. Woldring, H. Zhou, **B. Hackel**

4:40 BIOT **131.** Withdrawn.

Section D

Grand Hyatt Denver
Mt. Sopris A

Emerging Technologies

New Tools and Approaches

Y. Kim, J. Zartman, *Organizers, Presiding*

2:00 BIOT **132.** Sequence-specific synthetic RNA silencing overcomes antibiotic resistance. **C. Courtney**, A. Chatterjee

2:18 BIOT **133.** Endogenous CRISPR-Cas systems as convenient platforms for genetic screens and pathway engineering. M. Luo, **C. Beisel**

2:36 BIOT **134.** Zeolitic imidazolate framework nanoparticles for imaging and biomedical applications. **C.G. Jones**, V. Stavila, C. Ashley, M. Allendorf

2:54 BIOT **135.** Cell penetrating peptides for stem cell applications. G. Jin, F. Ghasemi Tahrir, W. Ma, **W.H. Suh**

3:12 Intermission.

3:30 BIOT **136.** Dynamic stiffening of poly(ethylene glycol)-based hydrogels to direct valvular interstitial cell phenotype in a 3D environment. **K. Mabry**, K.S. Anseth

3:48 BIOT **137.** Layered hydrogels to study development of iPSC-derived neural progenitor cells in 3D. Z. Zhang, J. Karpiak, A. Muotri, **A. Almutairi**

4:06 BIOT **138.** "Sandwich-type" nanofiber skin grafts for skin regeneration. J. Jiang, **J. Xie**

4:24 BIOT **139.** Development of a cellularly degradable PEG hydrogel to promote articular cartilage extracellular matrix deposition. **B.V. Sridhar**, J.L. Brock, J.S. Silver, M.A. Randolph, J. Leight, K.S. Anseth

4:42 BIOT **140.** Photonic crystal platform for biomoleculer sensing. **K. MacConaghy**, J. Kaar, M.P. Stoykovich

Section E

Grand Hyatt Denver
Mt. Elbert B

Colorado Biotechnology

Biofuels

C. A. Eckert, *Organizer*
N. Boyle, *Organizer, Presiding*
K. A. Brown, *Presiding*

2:00 BIOT **141.** Research in biofuels and bioproducts in Colorado. **R.M. Baldwin**

2:40 BIOT **142.** Biobased chemical and fuel development at OPXBIO. **D. Hogsett**

3:20 Intermission.

3:40 BIOT **143.** Novel sensors for continuous monitoring of fermentations for biofuels and bioproducts. **K.F. Reardon**

4:20 BIOT **144.** Development and commercialization of fermentative isobutanol production. **A. Hawkins**

MONDAY EVENING

Section A

Colorado Convention Center
Halls C/D

Sci-Mix

M. Lazzara, A. Kantardjieff *Organizers*

8:00 - 10:00

223-224, 234-235, 252, 257, 266, 269, 271-272, 274, 301, 320-321, 323, 332, 374, 377. See subsequent listings.

TUESDAY MORNING

Section A

Grand Hyatt Denver
Mt. Elbert A

Upstream Processes

Control of Protein Quality Attributes

B. Hackel, P. M. Hossler, *Organizers, Presiding*

8:30 BIOT **145.** Process development to lower tryptophan oxidation of a biopharmaceutical produced in chemically defined medium. **L.B. Hazeltine**, K.M. Knueven, Y. Zhang, A. Ouyang, Z. Lian, D.J. Olson

8:50 BIOT **146.** Controlling the glycosylation profile in MAbs by amino acid supplementation. **D. Radhakrishnan**, A.S. Robinson, B. Ogunnaike

9:10 BIOT **147.** Framework for real-time peptide-mapping (RT-PM) in bioreactor cultures of recombinant protein producing CHO cells. **T. Tharmalingam**, C. Wu, R. Hong, S. Benchaar, C. Goudar

9:30 BIOT **148.** Controlling fucose content of glycoproteins expressed in different CHO cell lines. **A. Zhang**, V.L. Tsang, L. Markely, G. Kennedy, S. Prajapati, Y. Huang

9:50 Intermission.

10:10 BIOT **149.** Unraveling the effect of energy metabolism on *N*-glycosylation of recombinant protein produced in mammalian cells. **T. Le**, A. Yongky, S. Grimm, W. Hu

10:30 BIOT **150.** Ways to improve process performance and product quality in high performing fed-batch and perfusion CHO cultures. **T. Falkman**, E. Fäldt, **O. Larsson**, A. Vitina, C. Kaisermayer, A. Castan

10:50 BIOT **151.** Engineering secretion machinery for high-throughput protein production. A. Azam, K.J. Metcalf, **D.T. Ercek**

Section A

Grand Hyatt Denver
Mt. Evans

BIOT Young Investigator Award

M. Lazzara, *Organizer, Presiding*

11:30 BIOT **152.** Toward antibodies by design. **P.M. Tessier**

Section B

Grand Hyatt Denver
Mt. Evans

Downstream Processes

Vaccines, Non-Antibody & Non-Protein Biological Products

A. Noyes, T. M. Przybycien, *Organizers, Presiding*

8:30 BIOT **153.** Virus flocculation and recovery with osmolytes. M. Gencoglu, **C. Heldt**

8:50 BIOT **154.** Purification of viruses and virus-like particles by ion-exchange and hydrophobic interaction monoliths. **A. Jungbauer**, P. Steppert

9:10 BIOT **155.** Downstream processing of a large live virus: Challenges in developing a sterile purification process. **A. Kristopeit**, M. Wenger, M. Woodling, J. Konietzko, T. Nguyen, S. Wang, K. Phillips, A. Swartz

9:30 BIOT **156.** Aminoglycoside antibiotic derived anion-exchange microbeads and monoliths for plasmid DNA binding and in-situ DNA capture. **T. Grandhi**, A. Mallik, N. Lin, B. Miryala, T. Potta, Y. Tian, K. Rege

9:50 Intermission.

10:10 BIOT **157.** Accelerated process development for the purification and conjugation of a novel protein carrier for a polysaccharide conjugate vaccine candidate. **M.A. Winters**, T.J. Svab, S. Wang, J.G. Joyce

10:30 BIOT **158.** Integrated bioprocess development based on microscale cultivations and feed stock characterization by chromatography modeling. **P. Baumann**, T. Hahn, J. Hubbuch

10:50 BIOT **159.** Design and optimization of peptide affinity resins for downstream processing. **S. Timmick**, D. Chandra, D. Shastry, C. Goodwine, S. Ruppel, P. Karande, S.M. Cramer

11:10 BIOT **160.** Protecting target glycoenzyme from proteolysis during purification. **X. He**, M.A. Snyder

Section C

Grand Hyatt Denver
Mt. Sopris A

Biomolecular & Biophysical Processes

Biomolecular Sensing & Actuation in Membranes

A. Brown, J. Rucker, *Organizers, Presiding*

8:30 BIOT **161.** Manipulation of vesicle formation and characteristics using photo-initiated chemistry. **D. Konetski**, T. Gong, W. Xi, A.D. Baranek, C. Bowman

8:50 BIOT **162.** Developing a chemically specific stimulus-response nanopore. A. Geiger, L. Keranen Burden, **D. Burden**

9:10 BIOT **163.** Exosome capture technology based on peptide-lipid interactions. **J.P. Saludes**

9:30 Intermission.

9:50 BIOT **164.** Aggregation of alpha-synuclein in functional model membrane systems. S. Corvaglia, D. Scaini, **L. Casalis**

10:10 BIOT **165.** Understanding the significance of fibroblast activation protein (FAP) homo- and heterodimerization in relation to proteolytic activity. B. Berger, **B. Wonganu**

10:30 BIOT **166.** Nanodiscs for purification and functional studies of family B G protein-coupled receptors (GPCRs). Y. Liu, Y. Cai, K. Culhane, R. Sunahara, **E.C. Yan**

10:50 BIOT **167.** Discovery and characterization of antibodies against membrane proteins using virus-like particles. **J. Rucker**

Section D

Grand Hyatt Denver
Grays Peak

Emerging Technologies

Cellular & Molecular Engineering

A. Chatterjee, D. Colby, *Organizers, Presiding*

8:30 BIOT **168.** Transition between multipotent stem cells and embryonic stem cells by chemical factors. **D. Cho**, B. Kuang, H. Pei, C.M. Verfaillie, W. Hu

8:50 BIOT **169.** High-throughput single-cell imaging reveals that $CD4^+$ CAR^+ T-cell can participate in multikilling through simultaneous conjugation with multiple tumor cells. **I. Liadi**, H. Singh, G. Romain, N. Rey-Villamizar, A. Merouane, P. Kebriaei, H. Huls, P. Qiu, B. Roysam, L. Cooper, N. Varadarajan

9:10 BIOT **170.** DNA strand displacement induced prodrug activation for cancer treatment. **R.P. Chen**, W. Chen

Technical program information known at press time.
The official technical program for the 249th ACS National Meeting is available at: www.acs.org/denver2015

TECHNICAL PROGRAM

9:30 BIOT **171.** *Bacillus subtilis* spore display of laccase for evolution under extreme conditions of high concentrations of organic solvent. **E.T. Farinas**

9:50 Intermission.

10:10 BIOT **172.** Co-evolution of affinity and stability for domain antibodies that recognize hydrophobic antigens. M. Julian, **L. Rabia**, K. Tiller, F. Meng, P.M. Tessier

10:30 BIOT **173.** Development of a ligand-regulated adhesive protein molecular switch. J.V. Price, C. Barnes, **E. Boder**

10:50 BIOT **174.** Autonomous 'bacterial vacuums' that control communication and enable tunable gene expression. **A. Zargar**, C. Tsao, D. Quan, M. Emamian, W.E. Bentley

11:10 BIOT **175.** Perturbing bacterial adaptive resistance using CRISPR-Cas9 mediated gene targeting: Emerging applications in synthetic biology. **P.B. Otoupal**, K.E. Erickson, A. Chatterjee

Section E

Grand Hyatt Denver

Mt. Elbert B

Biosimilars & Follow-on Biologics

Similarity Assessment: Regulatory Expectations, Proposed Strategies & Challenges

B. Bernat, S. Ramanan, *Organizers, Presiding*

8:30 Introductory Remarks.

8:50 BIOT **176.** Biosimilar Keynote: Marjorie Shapiro. **M. Shapiro**

9:30 BIOT **177.** Challenges and approaches in demonstrating biosimilarity at the physicochemical and biological level. **J.L. Glajch**, J. Anderson

9:50 Intermission.

10:10 BIOT **178.** Biosimilar mAb higher order structure characterization with protein conformational array. **X. Wang**

10:30 BIOT **179.** Characterization of monoclonal antibody drug products by 2D NMR techniques. **L.W. Arbogast**, R.G. Brinson, J.P. Marino

10:50 BIOT **180.** Optimized approach to the rapid assessment and detection of sequence variants in recombinant protein products: Application to biosimilars. **R. Scott**, L. Brady, A. Balland

11:10 BIOT **181.** Role for bioassays in biosimilarity assessment. K. Wilson-Landy, N. Hellman, L. Liu, Y. Wang, S. Ennis, P. Han, S. Lumayag, **J. TerWee**

Phenolic & Polyphenolic Chemistry in Food Processing

Reactions/Properties

Sponsored by AGFD, Cosponsored by AGRO, BIOT, COMP and MEDI

TUESDAY AFTERNOON

Section A

Grand Hyatt Denver

Mt. Elbert A

Upstream Processes

Metabolic Engineering & Synthetic Biology

F. Chaplen, N. Mouncey, *Organizers, Presiding*

2:00 BIOT **182.** ^{13}C metabolic flux analysis of *E. coli*/*E. coli* and *E. coli*/yeast co-culture. **M.R. Antoniewicz**

2:20 BIOT **183.** Dynamic knockdown of *E. coli* central metabolism for redirecting fluxes of primary metabolites. **I. Brockman**, K.L. Jones Prather

2:40 BIOT **184.** Constrictor: Flux balance analysis constraint modification provides insight for design of biochemical networks. **K.E. Erickson**, R.T. Gill, A. Chatterjee

3:00 BIOT **185.** 13C Metabolic flux analysis at the genome-scale. **S. Gopalakrishnan**, C. Maranas

3:20 Intermission.

3:40 BIOT **186.** Regulatory tools for applications in synthetic biology and metabolic engineering. **B. Pfleger**

4:00 BIOT **187.** Computational life cycle modeling of M13 bacteriophage: Toward rational engineering of a biotechnologically-important scaffold. **J.D. Fisk**

4:20 BIOT **188.** Electrochemical monitoring of synthetic biology constructs. **T. Gordonov**, X. Zhou, C. Tsao, H. Ueda, E. Kim, G.F. Payne, W.E. Bentley

4:40 BIOT **189.** Aptazyme-based suicide circuit for screening of metabolite overproducer in yeast. S. Lee, **M. Oh**

Section A

Grand Hyatt Denver

Mt. Evans

Alan S. Michaels Award in the Recovery of Biological Products

M. Lazzara, *Organizer, Presiding*

5:00 BIOT **190.** Transforming basic science into innovations in bioproduct recovery. **M.T. Hearn**

Section B

Grand Hyatt Denver

Mt. Evans

Downstream Processes

Technology Transfer and Scale-Up

V. Natarajan, N. Tugcu, *Organizers, Presiding*

2:00 BIOT **191.** Driving value through innovation in biologics manufacturing. **J.P. Thommes**

2:40 BIOT **192.** E. coli purification technology transfer: Challenges and novel processing strategies. **J. Bill**, A. Mehta, A. Goerke

3:00 BIOT **193.** Direct scale-up of a mAb production process developed in high throughput format. S. Siva, **A. Henry**, E.K. Koepf, A. Zhang, L. Conley, D. Cecchini

3:20 Intermission.

3:40 BIOT **194.** Understanding minicolumn system operational differences and their impact on process performance and scale-up using column simulations. **W. Keller**, S.T. Evans, G. Ferreira, D. Robbins, S.M. Cramer

4:00 BIOT **195.** Verification of small-scale models to understand commercial-scale process and predict performance and capability. **T. Mammo**, G. Ferreira, G. Miro-Quesada, M. Zhu, D. Robbins

4:20 BIOT **196.** First intent gradient elution for the purification of biopharmaceuticals: Practical approach to accelerate process development and reduce cost of goods. **A.C. Dumetz**, Y. Feng, K.M. Jones, J.F. Kurdyla, A.R. Ubiera, G.J. Terfloth

4:40 BIOT **197.** Commercial scale single-pass TFF technology and hardware to achieve final pool concentrations >220 g/L with >95% recovery. **J. Griffin**

Section C

Grand Hyatt Denver

Grays Peak

Biomolecular & Biophysical Processes

Protein Conjugates: From Basic Principles to Clinically Active Drugs

R. W. Lee, S. L. Servoss, *Organizers, Presiding*

2:00 BIOT **198.** Development of a clickable spliceostatin antibody-drug conjugate (ADC) to probe ADC uptake and trafficking in cancer cells. **C. Kulkarni**, E.I. Graziani

2:20 BIOT **199.** Ligase-mediated bioorthogonal insertion of click reactive groups for site-specific protein modification. **J. Plaks**, J. Berberich, J. Kaar

2:40 BIOT **200.** Nanoparticle formulations linking pharmaceutical components by electrostatic and hydrophobic binding: A faster and more flexible alternative to ADC. **R.S. Becker**, D.N. Ringhoff, R.W. Lee, M.A. Mitchnick

3:00 BIOT **201.** Synthesis of polyvalent aptamer-toxin-polymer conjugates. **J.T. Martin**, M. Douaisi, C. Kratschmer, M. Levy, R.S. Kane

3:20 Intermission.

3:40 BIOT **202.** Hydrazinyl-Iso-Pictet-Spengler (HIPS) ligation as a novel method for the generation of highly stable, site-specifically modified antibody drug conjugates (ADCs). **A.E. Albers**

4:00 BIOT **203.** Effect of PEGylation on protein stability and release from melt-processed biodegradable poly(lactic-*co*-glycolic acid) implants. **P. Lee**, J. Maia, J.K. Pokorski

4:20 BIOT **204.** Structural characterization of nanoliposomes–polypeptides complexes by field flow fractionation and multidetector analysis. **L. Calzolai**, P. Iavicoli, M. Ryadnov, F. Rossi

4:20 BIOT **205.** Evaluating biophysical properties of fluorescent probes with a super-resolution in vitro assay. **E.E. Cacao**, S. Biswas, O. Golfetto, R. Jorand, T. Jovanovic-Talisman

Section D

Grand Hyatt Denver

Mt. Elbert B

Biofuels & Sustainable Energy

Engineering Microbes to Utilize Next Generation Feedstocks

L. Giver, C. T. Trinh, *Organizers, Presiding*

2:00 BIOT **206.** Stimulation of lipid and chitin production in the photosynthetic diatom *Cyclotella* by co-limitation of silicon and nitrate in batch and perfusion cultivation. **O. Chiriboga**, N. Chotyakul, S. Wu, A. Torres, G. Rorrer

2:20 BIOT **207.** Novel co-culture approach to compartmentalize biomass deconstruction and biofuel production. **J.K. Henske**, K. Solomon, M.A. OMalley

2:40 BIOT **208.** Role of novel, multi-domain, cell surface-associated, glycoside hydrolases during lignocellulose degradation by extremely thermophilic *Caldicellulosiruptor* species. **J.M. Conway**, W.S. Pierce, A.L. Tucker, J. Zurawski, L.L. Lee, S.E. Blumer-Schuette, R.M. Kelly

3:00 BIOT **209.** Optimization of photobiological production of ethylene in engineered *Synechocystis*. **B. Wang**, W. Xiong, J. Ungerer, C.A. Eckert, P. Maness, J. Yu

3:20 Intermission.

3:40 BIOT **210.** From lignin depolymerization to coproduct generation by using a single bacterial catalyst. **D. Salvachua**, E. Karp, D. Vardon, G. Beckham

4:00 BIOT **211.** Improve resistance of *Saccharomyces cerevisiae* to mixed fermentation inhibitors through inverse metabolic engineering for harnessing lignocellulosic biomass. Y. Chen, T. Jiang, X. Feng, **N. Wei**

4:20 BIOT **212.** Engineering a synthetic sugar sensing yeast strain. **K.M. Blocker**, A.S. Robinson

4:40 BIOT **213.** Improving solvent tolerance in *Saccharomyces cerevisiae* by reducing alcohol-induced inhibition of translation. **S. López**, D.T. Ercek

Section E

Grand Hyatt Denver

Mt. Sopris A

Emerging Technologies

General Topics

J. Oakey, B. F. Shaw, *Organizers, Presiding*

2:00 BIOT **214.** Factors impacting aluminum hydroxide lyophilization and stability. **N. Li**, A.P. Mehta, S.S. Ganser, K. Muthurania, A.L. Young, S.K. Singh

2:20 BIOT **215.** Discovery of novel neutralizing antibodies against Bordetella adenylate cyclase toxin and its implication for vaccine design. **X. Wang**, J. Maynard

2:40 BIOT **216.** Scalable biosynthesis of quantum dots: evolution of size selectivity, solubility, and extracellular production. Z. Yang, L. Lu, V. Berard, Q. He, C.J. Kiely, S. McIntosh, **B. Berger**

3:00 BIOT **217.** Photothermal response of protein-gold nanorod plasmonic solders for laser tissue welding. R. Urie, **K. Rege**

3:20 Intermission.

3:40 BIOT **218.** DNA methylation for programming biochemical flux. **J. Terrell**, H. Wu, C. Tsao, A. Dunn, G.F. Payne, W.E. Bentley

4:00 BIOT **219.** Study of cell communications by barcode microchips. **J. Wang**

4:20 BIOT **220.** Carbohydrate chip for multiplex bacterial toxin detection. **H. Shin**, J. Seo, C. Kim, B. Hwang, H. Cha

4:40 BIOT **221.** Deposition of a metal organic framework on a flexible polymer surface for biomedical applications. **M. Neufeld**, M.M. Reynolds, J. Harding

Phenolic & Polyphenolic Chemistry in Food Processing

Sources

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TUESDAY EVENING

Section A

Grand Hyatt Denver

Imperial Ballroom

Poster Session

C. F. Komives, *Organizer*

6:00 - 9:00

BIOT **222.** Exploration of gold nanoparticle functionalized peptide based nanocarriers for encapsulation of chemotherapeutic drugs. **S.M. Romanelli**, K.R. Fath, A.P. Phekoo, I.A. Banerjee

BIOT **223.** Simulating the capture dynamics of molecules within proximity to the alpha-hemolysin nanopore. **E. Pederson**, B. Drown, J. Barbalas, L. Keranen Burden, D. Burden

BIOT **224.** Engineering silica forming peptides on ferritin cage for dual drug delivery system. **S. Pack**, K. Nguyen, K. Park, M. Ki

BIOT **225.** Development of adhesive hydrogel based on mussel-mimetic protein. **E. Jeon**, B. Kim, D. Oh, J. Seo, D. Hwang, A. Masic, D. Han, H.J. Cha

BIOT **226.** Biointerfaces augmented with nitric oxide generating metal-organic frameworks. **E. Lauzon**

BIOT **227.** Engineering proteins capable of inducing silica deposition. **M. Ki**, K. Yeo, E. Jang, S. Pack

BIOT **228.** BMP-2 immobilization using mussel-inspired complex coacervate for tissue engineering. **H. Kim**, B. Choi, B. Hwang, H.J. Cha

BIOT **229.** Silanized oxides and nanoparticles for use in biosensor and energy applications. **R.A. Shircliff**, I.T. Martin, I. Anderson, P. Stradins, M. Ghirardi, S. Cowley, R. Collins, H. Branz

BIOT **230.** New way of producing fully covered microsized particles using chemical vapor deposition method. **Y. Liang**, J. Lahann, X. Deng

BIOT **231.** One-step flotation immunoassay using position-dependent screening of luminescence. **H. Chen**, A. Hagstrom, J. Kim, G. Garvey, A. Paterson, F.R. Ruiz, B. Raja, A. Gasic, J. Conrad, U. Strych, K. Kourentzi, R. Atmar, R.C. Willson

BIOT **232.** Material considerations in the design of sensitive and rapid biosensors based on optically diffracting hydrogels. **K. MacConaghy**, J. Kaar, M.P. Stoykovich

BIOT **233.** Electrochemical biosensor development for detection of botulinum toxin A (BoNT/A). **J. Richards**, A.J. Bonham

BIOT **234.** Optimization of electrochemical biosensors of the transcription factor c-Myc for point-of-care cancer diagnosis. **L. Roon**, J. Sowick, A.J. Bonham

BIOT **235.** Gradient-induced migration of cancer stem cells in a microfluidic network revealed chemotactic acceleration and the involvement of Wnt/β-catenin pathway. **H. Zou**, W. Yue, W. Yu, D. Liu, C. Fong, M. Yang

‡ *Cooperative Cosponsorship*

BIOT **236.** Developing optimal MWCNT-modified electrodes for studying the electrochemistry of key redox cofactors and their complexes with aptamers. **I. Emahi**, M.P. Mitchell, P.R. Gruenke, D.A. Baum

BIOT **237.** Expanding electrochemical DNA biosensors to detect ricin. **L. Fetter**, A.J. Bonham

BIOT **238.** Diagnostic application of molecular recognition element. **K.L. Hong**, K. Imlay, L. Battistella, R.M. Williams, K.M. Hickey, C.D. Bostick, P.M. Gannett, L.J. Sooter

BIOT **239.** Peptide internalization triggered by temperature. **M. Oh**, C. Hu, M. Arostegui, K. Slowinska

BIOT **240.** Recombinant Pif80 protein for nacre-mimicking calcium carbonate biomineralization. **S. Bahn**, Y. Choi, H.J. Cha

BIOT **241.** Developing microscale themophoresis techniques for analysis of proteins. **J. Devriendt**

BIOT **242.** Rapid identification of *Listeria monocytogenes* using bacteriophage A511 amplification and enhanced lateral flow immunochromatography. **N. Stambach**, S. Carr, C. Cox, K.J. Voorhees

BIOT **243.** "Sequence-specific" and "pathogen-specific" antimicrobials using phage-delivered CRISPR-Cas9 gene targeting. **P.B. Otoupal**, K.E. Erickson, A. Chatterjee

BIOT **244.** Comparison of serotonin-expressing mammalian and yeast responses to selected ligands. **K.M. Blocker**, A.S. Robinson

BIOT **245.** Detection of toxin producing Vibrio *cholerae* and *Escherichia coli* using double biomolecular marker microarray. **H. Shin**, C. Kim, B. Hwang, J. Seo, H. Cha

BIOT **246.** Directed evolution of haptocorrin into an oral zinc supplement. **Y. Nie**

BIOT **247.** Investigation of the evolutionary relationship between Rio2 kinases and the canonical eukaryotic protein kinases using X-ray crystallography. **S. Bahmanjah**, N.O. Laronde

BIOT **248.** Mechanistic study of unusual enzyme activation caused by addition of inert betaine-type metabolite and the analogs. **Y. Nakagawa**, K. Koumoto

BIOT **249.** Direct observation of single-molecule adsorption/desorption kinetics on ion-exchange adsorbents. S**. Dhamane**, M. Poongavanam, W. Chen, U. Patil, L. Kisley, J. Chen, A.P. Mansur, B. Shuang, S. Dominguez Medina, E. Kulla, M. Kang, K. Kourentzi, C.F. Landes, R.C. Willson

BIOT **250.** Bacterial adhesion to complex surfaces: Pair-additive model and pattern-matching. **S. Yoon**, L. Edens, J.A. Brozik, D. Keller

BIOT **251.** Enzyme-based approaches to kill *Bacillus* spores and other resistant pathogens. **R.V. Mundra**, K. Mehta, X. Wu, E. Paskaleva, R.S. Kane, J.S. Dordick

BIOT **252.** Identification of the amidase activity and in vitro characterization of the cortex lytic enzyme CwlJ1 of Bacillus anthracis spores. **X. Wu**, N. Grover, E.E. Paskaleva, R.V. Mundra, M.A. Page, J.S. Dordick, R.S. Kane

BIOT **253.** Neuronal differentiation of human stem cells via electrostimulation. F. Ghasemi Tahrir, G. Jin, W. Ma, **W.H. Suh**

BIOT **254.** Effects of cross-sequence interaction between β-amyloid and human islet amyloid polypeptide on the structure and aggregation of amyloids. **R. Hu**, M. Zhang, H. Chen, J. Zheng

BIOT **255.** Analysis of monoclonal antibodies using capillary zone electrophoresis: Application to formulation screening. A. Brousseau, P. Casaz, **S. Ozturk**

BIOT **256.** Feasibility of targeting cells without unique molecular targets. **K. Slowinska**, M. Oh, C. Hu, M. Arostegui

BIOT **257.** Deimmunization of lectins using computational prediction and membrane-anchored display of correctly folded proteins. **X. Zheng**, Y. Choi, C. Bailey-Kellogg, K.E. Griswold, M.P. DeLisa

BIOT **258.** Bending lasso peptide structure. **C. Allen**, A. Link

BIOT **259.** Selective C(sp^3)—H bond functionalization with engineered P450 catalysts. **R. Fasan**

BIOT **260.** Probing the binding interactions of peptide-polymer coated gold nanoparticle encapsulated drugs with tumor cells by SPR. **A. Brown**, Y. Miranda, G. Knoll, I.A. Banerjee

BIOT **261.** Improved stability of a model, difficult to formulate IgG3 by DoE-based evaluation of buffer formulations. **B. Chavez**, C. Agarabi, E. Read, M. Khan, K.A. Brorson

BIOT **262.** Measurement of charge: An important molecular property for predicting high concentration behavior. **B. Balthazor**, S. Goswami, Y. He, R. Walters, S. Kumar, D. Boardman, D. Luisi

BIOT **263.** Evaluation of different commercially available Protein A resins on the DBC to Nanobodies. W. Van De Velde, W. Martens, B. Van Der Jeugt, R. Lievrouw, **A. Naresh**

BIOT **264.** Evaluation of various wash and elution buffers across a panel of four monoclonal antibodies for host cell protein reduction during Amsphere Protein A chromatography. **A. Naresh**, R. Lievrouw, M. Siwak

BIOT **265.** Systematic approach for evaluation of the different DOE designs for biotech applications. **V. Kumar**, A.S. Rathore

BIOT **266.** Binding mechanisms of viral clearance utilizing multimodal anion exchange chromatography. **M. Brown**, K.A. Brorson, S. Lute, B. Chavez, D.J. Roush, T. Linden

BIOT **267.** Charge-tunable polyampholytes for the enhanced flocculation of cellular biomass. **K.L. Morrissey**, Y. Inaba, M.I. Keirn, A.J. Denham, G.J. Henry, M.P. Stoykovich

BIOT **268.** Characterization of CaPure-HA, a new hydroxyapatite resin for the purification of monoclonal antibodies (mAbs) and other biomolecules. **W. Evans**, **K. Motter**, A. Chakrabarti

BIOT **269.** Purification of a bispecific antibody using hydrophobic interaction chromatography. **N. Gupta**, P.J. Alfonso, D. Bezila, R. Bertrand, M. Capaldi, M. Chiu, P. Haytko, T. Seagreaves

BIOT **270.** Development and characterization of a protein A capture step for improved impurity clearance. **N.E. Levy**, J.R. Molek, K.E. Goklen

BIOT **271.** Engineering of novel staphylococcal Protein A ligands to enablemilder elution pH and high dynamic binding capacity. R. Palmgren, J. Vasic, **B. Noren**, A. Forss

BIOT **272.** Affinity purification of Fab feedstreams. **M. Holstein**, N. Bian, M. Jung, M. Bruce, J. Orlando

BIOT **273.** HCP clearance strategies for protein A chromatography. **M. Holstein**, K.A. Cotoni, N. Bian

BIOT **274.** Investigation of variability in the throughput of a platform viral filter. B. Olson, R. Tedstone, **S. Rajendran**

BIOT **275.** Automated scale-down model for characterization of an affinity chromatography step. **A. Mohanty**, R. Tedstone, S. Rajendran

BIOT **276.** Ensuring long term robustness of a CIEX chromatographic step for separation of charge variants with optimized yield. **K. Haeringer**, E. Rosenberg, S. Hepbildikler, K. Lacki, E. Brekkan, M. Ahnfelt

BIOT **277.** Model-based biopurification process development. **S. Pirrung**, A. Hanke, L. van der Wielen, P. Verhaert, E. van de Sandt, M. Eppink, M. Ottens

BIOT **278.** Model-based comparison of protein aggregation in integrated and batch-wise downstream processing. **A. Sellberg**, F. Ojala, B. Nilsson

BIOT **279.** Subtractive panning in phage display for identification of chromatographic affinity peptide ligands. **C. Goodwine**, D. Shastry, S.M. Cramer, P. Karande

BIOT **280.** Use of multimodal chromatography and protein-protein interaction studies to create separation between antibodies and associated host cell proteins. **S. Ranjan**, W.K. Chung, M. Zhu, D. Robbins, S.M. Cramer

BIOT **281.** Comparison of binding capacity of TOYOPEARL AF-rProtein A HC-650F affinity resin at varying bed heights. **K. Motter**, A. Chakrabarti

BIOT **282.** Improvements in downstream processing: minimization in chromatographic steps for early milestones. **D. Shah**, H. Li, T. Linden, M. Iammarino

BIOT **283.** Feasibility study of Raman probe for online measurement of protein concentration during UFDF. J. Wylie, Y. Xie, **H. Cui**

BIOT **284.** Virus detection using restricted-access adsorbents. **S. Dhamane**, M. Adhikari, U. Patil, A. Hagström, K. Kourentzi, U. Strych, R.C. Willson

BIOT **285.** Purification of a non-enveloped virus using an aqueous two-phase system. **K. Vijayaragavan**, A. Zahid, J. Young, C. Heldt

BIOT **286.** Chromabolt® prepacked and pre-validated columns: A three-resin validation approach. **S. Rahane**, M. Turiano, S. Josephson, N. Bian

BIOT **287.** Adsorption characteristics of newly developed protein A and ion exchange media for affinity chromatography. **M. Kiyono**

BIOT **288.** Method comparison for determining steric mass action isotherm parameters for a multicomponent chromatography model. **K. Tolley**, T. Larsen, S. Hunt, R.J. Todd, W. Heymann

BIOT **289.** Metal-catalyzed fragmentation of a mAb: A case study. M. Grooms, E. Wilson, T.B. Vickroy, R.G. Collier, M. Monck, J. Dally, R. Luo, **K.E. Goklen**

BIOT **290.** Development of a novel affinity chromatography medium for platform purification of lambda Fabs. **L. Laurin**, P. Hermans, N. Eifler

BIOT **291.** Avoiding antibody aggregation in downstream processing: Establishing hold time. **V. Yadav**, A.S. Rathore

BIOT **292.** Circular dichroism spectroscopy as a tool for rapid screening of monoclonal antibody stability. **V. Yadav**, A.S. Rathore

BIOT **293.** Neutron reflectivity for characterization of chromatographic interfaces in bioprocessing. **A. Mazzer**, L. Clifton, C.J. Roberts, D.G. Bracewell

BIOT **294.** Process analytical technologies using a multipath length UV/VIS spectroscopy Flow cell. **R. Orozco**, J. Miller, S. Godfrey, W. Chang, J. Vogel, J.L. Coffman

BIOT **295.** Connecting molecular adsorption processes to liquid chromatography. **J. Mabry**, M. Skaug, D.K. Schwartz

BIOT **296.** High throughput tools and methods for faster protein purification process development. **M. Toueille**, J. Champagne, G. Balluet, R. Gantier

BIOT **297.** Rapid characterization of HCP removal on adsorptive membranes using protein surrogate markers. **M. Siwak**

BIOT **298.** Design of a novel agarose-based resin platform. **H.J. Johansson**

BIOT **299.** High-throughput screening and analytics as tools for efficient purification process design. **J. Spitz**, J. Studts

BIOT **300.** Toward high-throughput protein refolding and purification: Model-based process development. **P. Saremirad**, Y. Zhang, A. Ray

BIOT **301.** Investigation and mitigation of high molecular weight species formation on cation exchange chromatography for a monoclonal antibody. **A. White**

BIOT **302.** Facility fit prediction and debottlenecking of antibody purification facilities. **Y. Yang**, S. Farid, N. Thornhill

BIOT **303.** Optimization of tangential flow filtration: Control and characterization of aggregates and particles. **E. Schutsky**, D. Yu, A.T. Lewandowski, Z. Li

BIOT **304.** Automated scale-down model of a commercial chromatography process. **A. Mohanty**, R. Tedstone, S. Rajendran

BIOT **305.** Effective synthesis of cadaverine from L-lysine using recombinant decarboxylase under CO_2 purging condition. **S. Jeong**, E. Choi, S. Byun, D. Cho, Y. Kim

BIOT **306.** Influenza vaccine titre determination using Biolayer Interferometry (BLI). **D. Wheatley**

BIOT **307.** On-column low pH viral inactivation of a pH sensitive protein. **J. Armando**, J.P. Pieracci, M. Bakhshayeshi, D. Houde

BIOT **308.** Pulse gradient experiments for fast chromatography model development. **K. Westerberg**, K. Tolley, S. Hunt, O. Kaltenbrunner

BIOT **309.** Process fit modeling to aid in contract manufacturer selection. **S. Hohwald**, M. Gallup, A. Goerke

BIOT **310.** Biopharmaceutical process monitoring using statistical stability metrics. **T. Mistretta**

BIOT **311.** Reverse phase high performance liquid chromatography (RP-HPLC) as an in-process analytics core competency for upstream and downstream process development. **K. McLaughlin**, D. Shah, E. Wu, S.D. Schussler, B. Kilgore, H. Li, T. Linden

BIOT **312.** Production planning, scheduling, and debottlenecking practices in the biopharmaceutical industries. **D. Carmichael**, C.A. Siletti, D. Petrides

BIOT **313.** Biomaterial production process intensification, analysis, and optimization with process simulation tools. **D. Carmichael**, C.A. Siletti, D. Petrides

BIOT **314.** Engineering synthetic fungal cellulose-degrading complexes. **S.P. Gilmore**, C.H. Haitjema, M.A. OMalley

BIOT **315.** Process analytical technology solutions for robust measurement and control of upstream bioprocesses. **E.R. Gibson**, K. Lanz, E. Koerperick, D. Cooley, J. Olesberg, C. Evans, G. Small, M. Arnold

BIOT **316.** Translating unnatural amino acids with phenotypically-diverse, computationally-engineered EF-Tu variants. **V. Cox**, E. Gaucher

BIOT **317.** Effect of plant and microbe associated compounds on bacterial cellulose production. **J.L. Strap**, A.J. Varley

BIOT **318.** Understanding the effect of glycosylation on the stability and biochemical characteristics of cutinases. **A. Shirke**, A. Su, D. Basore, M. Ullo, C. Bystroff, R.A. Gross

BIOT **319.** In vitro transcription/translation in emulsion produced by a simple flow-focusing device. **M. Murzabaev**, T. Mizoguchi, T. Kojima, I. Kobayashi, H. Nakano

BIOT **320.** Rapid and high throughput fluorescent protein engineering performed in micro-pore arrays. **S.C. Alford**, B. Chen, T. Baer, J. Cochran

BIOT **321.** Toward engineering bacterial transcriptional regulators through continuous directed evolution. **T. Cook**, A. Yaguchi, M.A. Blenner

BIOT **322.** Engineering transcriptional and post-transcriptional repression for synthetic cellular circuits. **T.J. Mansell**, A.D. Corts, A. Choudhury, R.T. Gill

BIOT **323.** Direct production of propene from the thermolysis of poly(β-hydroxybutyrate). **A. Mittal**, H.M. Pilath, D.K. Johnson

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BIOT **324.** Chaperone overexpression to enhance domain antibody secretion in *E. coli*. **J. Brady**, D.B. Ritz, Y. Zhu

BIOT **325.** Engineered bacterium with periplasmic carbonic anhydrase as a biocatalyst for CO_2 sequestration. **B. Jo**, J. Seo, H. Cha

BIOT **326.** Molecular toolkit development for a model cyanobacterium. **H.R. Aucoin**, W.E. Sinclair, C. Witherell, N.R. Boyle

BIOT **327.** Grafted cellulose with ferulic acid from the residual liquid of corn processing. **E. Torres**, R. Manriquez Gonzalez, J. Meza-Contreras, J. Andrade-Hernández, A. Méndez-Albores

BIOT **328.** Process parameter screening utilizing a Plackett-Burman design for a model monoclonal antibody and exploring the linkage between cell culture and downstream processing. C. Agarabi, E. Read, **S. Lute**, M. Boyne, J. Schiel, B. Chavez, K.A. Brorson

BIOT **329.** Media components for reducing waste accumulation in mammalian cell culture. **C. Caffalette**, W. Yang, A. Ray, V. Shen, R.R. Kshirsagar, T.K. Ryll, Y. Huang

BIOT **330.** Microbial production of a hydrocarbon fuel intermediate polyhydroxybutyrate (PHB) from a process relevant lignocellulosic derived sugar stream. **W. Wang**, A. Mittal, A. Mohagheghi, D.K. Johnson

BIOT **331.** Dosing considerations and impacts on the clarification of mammalian cell culture feed streams using polydiallyldimethylammonium chloride flocculant in conjunction with Clarisolve depth filters. **M. Peck**

BIOT **332.** High-throughput screening metabolic assay to improve media design for mammalian fed-batch culture. **Y. Li**, J. Yee, M.C. Borys, Z. Li

BIOT **333.** Methods for quantitative analysis in plant synthetic biology. **K. Schaumberg**, W. Xu, C. Zalewski, T. Kassaw, M. Antunes, J. Medford, A. Prasad

BIOT **334.** Characterization and modeling of metabolic changes in cyanobacteria during photosynthesis. **F.E. Estep**, A. Zimont, G. Peers, A. Prasad, C.A. Peebles

BIOT **335.** Analyzing the degradation capacity within *Pseudomonas* sp. strain ADP biofilm. **V. Henry**, J.L. Jessop, T.L. Peeples

BIOT **336.** Uniaxially aligned, porous collagen-GAG scaffolds for in vitro modeling of human trabecular meshwork. **S. Bernier**, M. Pantcheva, M. Krebs

BIOT **337.** Using backscattering interferometry to observe label-free observations of molecular interactions of membrane-associated species. **M. Baksh**, A. Lockwood, C.I. Richards, M. Finn, D. Heidary

BIOT **338.** Ultrathin coatings on polymer substrates for chemically defined culture of human mesenchymal stem cells. **S. Schmitt**, A. Xie, W.L. Murphy, P. Gopalan

BIOT **340.** Characterization of the alginate lyases from *Vibrio splendidus* 12B01. **A. Badur**, G. Yalamanchali, C.V. Rao

BIOT **341.** Bioinspired silica nanoparticle with auto-encapsulated carbonic anhydrase as a robust biocatalyst for biomimetic CO_2 sequestration. **B. Jo**, J. Seo, K. Baek, Y. Choi, S. Pack, S. Oh, H.J. Cha

BIOT **342.** Characterizing technical and biological variance in CHO cell time-series metabolomics data. **H. Le**, C. Goudar

Technical program information known at press time.
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www.acs.org/denver2015

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BIOT **343.** Differential gene expression variability underlies adaptive resistance in heterogeneous populations. **K.E. Erickson**, A. Chatterjee

BIOT **344.** Effects of key cell culture process parameters on the quality attributes of a therapeutic protein produced by an NS0 cell line. **T. Bui**, M. Berge

BIOT **345.** Efficient approach to perfusion medium development using design of experiments (DoE). **A. Castan**, E. Fäldt, T. Persson, H. Bergling

BIOT **346.** Process development to increase productivity with minimal impact to product quality. **L. Cella**, Y. Yang, M. Dowling, P. Russo, G.A. Tulloch

BIOT **347.** Constraints-based modeling to elucidate the impacts of environmental dynamics on nitrogen gases production by the soil nitrifying bacteria *Nitrosomonas europaea* and *Nitrobacter winogradskyi*. **F. Chaplen**, C. Ta, C. Higgins, P. Bottomley, L. Sayavedra-Soto

BIOT **348.** *Nitrobacter winogradskyi* responses to Fe limitation. **C. Ta**, R. Ferrell, L. Sayavedra-Soto, F. Chaplen

BIOT **349.** Transcriptional activation of yeast by split intein-mediated reconstitution of synthetic peptide signals. **K. Siu**, W. Chen

BIOT **350.** Modulation of gene expression via directed electrical signaling: Electrically sensitive promoters. **Y. Okasheh**, R.M. McBee, N.M. Marshall, A.D. Ellington

BIOT **351.** Utilization of the separatome of E. coli for the development of a protein expression and purification platform. **E. Brune**, M.S. Fruchtl

BIOT **352.** Large scale algal oil production for biofuel use: Techno-economic analysis and evaluation. **D. Carmichael**, C.A. Siletti, D. Petrides

BIOT **353.** Specifically tuned light activated nano-therapeutics for selective cell phenotypes. **C. Courtney**, S.M. Goodman, P. Nagpal, A. Chatterjee

BIOT **354.** Combinatorial synthesis and cheminformatics modeling of aminoglycoside lipopolymers for transgene expression. B. Miryala, Z. Zhen, T. Potta, C.M. Breneman, **K. Rege**

BIOT **355.** Aqueous ionic liquid (IL) enzyme mixtures for single-step dissolution and hydrolysis of cellulosic materials. **T. Schutt**, C.M. Maupin

BIOT **356.** Single cell capture and biochemical analysis using self-folding biocompatible devices. **Q. Jin**, M. Li, I. Barman, D.H. Gracias

BIOT **357.** Silver nanoparticle-generating mussel adhesive fusion protein as a novel bioinspired surface-independent antibacterial coating material. **B. Hwang**, Y. JO, J. Seo, B. Choi, B. Kim, H. Shin, H.J. Cha

BIOT **358.** Cellulose hydrolysis in acidified molten salt hydrate reaction media: Insights from kinetic and spectroscopic studies. W. Deng, G. Tsilomelekis, J. Kennedy, **V. Nikolakis**

BIOT **359.** Response surface methodology for efficient production of biomass and lipids by *Rhodotorula glutinis* grown in pulp and paper wastewater. **M. AmirSadeghi**, W.T. French, R. Hernandez, S. Shields-Menard, B. Sukhbaatar

BIOT **360.** Fabrication of a nanoconjugate for synergistic antibiotic and photothermal treatment of resistant bacteria. **S.V. Jenkins**, D. Meeker, K.E. Beenken, M.S. Smeltzer, J. Chen

BIOT **361.** Comprehensive utilization of waste hemicelluloses during ethanol production to increase lactic acid yield: from pretreatment to fermentation. **L. Zhang**, T. You, L. Zhang, F. Xu

BIOT **362.** Understanding population fluctuations in marine environment. **J. Gardner**, N. Boyle, B. Hodge

BIOT **363.** Isotope tracer and mass spectrometry reveal engineered xylose metabolism in cyanobacteria. **W. Xiong**, J. Yu

BIOT **364.** Integration of the alpha-amylase gene into single and high-copy number loci within the *Saccharomyces diastaticus* genome to elicit a high degradation efficiency on a unique starch source. **M.P. Pinto**, W. Haggren, S.B. Braun-Sand

BIOT **365.** What makes phosphatidylserine a novel regulator of ceramide-1-phosphate transfer proteins? **X. Zhai**, D.K. Simanshu, H. Pike, J. Mundy, J.G. Molotkovsky, D.J. Patel, L. Malinina, R.E. Brown

BIOT **366.** High throughput process development: Utilization of high-throughput bioreactors and high-throughput analytics for rapid and robust cell culture process development. **S. Rameez**, S. Gopalakrishnan, J.S. Notey, S.S. Mostafa, A.A. Shukla

BIOT **367.** Evaluation of bicarbonate free medium for improved mammalian cell growth and monitoring in controlled bioreactors. **D. Odenwelder**, S.W. Harcum

BIOT **368.** Development of a NS0 monoclonal antibody producing scale-down model for support of a technical transfer. **E. Hodgman**

BIOT **369.** Improving scale-up of medium filtration for cell culture processes through understanding of iron effect during large-scale preparation. **J. Tressel**, A. Khetan, H. Lin

BIOT **370.** Identifying cell signaling regulators of epithelial-mesenchymal transition in carcinoma. **J.M. Buonato**, S.S. Yee, E.L. Carpenter, M. Lazzara

BIOT **371.** Strategies and considerations for the development of perfusion process for continuous processing based on existing fed-batch platform. **H. Lin**, S. Wang, R. Leighty, S. Godfrey, S. Yildirim, A. Osborne, R. Orozco, G. Setiabudi, J. Coby, J.H. Vogel, J.L. Coffman

BIOT **372.** Clarification platform evaluation and optimization. **K. Humbard**, B. Wang, M. Wagner, K. Chefer, K. Dhanasekharan

BIOT **373.** Assessment of down-hole membrane-diffused hydrogen for stimulating uranium reduction and immobilization. **L. Haynes**

BIOT **374.** Remote activation of TRPV1 for therapeutic effect. **J. Sauer**, S. Stanley, R.S. Kane, J. Friedman, J.S. Dordick

BIOT **375.** Toward a unified process development strategy for batch and continuous chromatography. **A. Forss**, H. Blom, K. Lacki

BIOT **376.** Unamic control in periodic counter current chromatography. **H. Blom**, H. Skoglar, A. Åkerblom, L. Mathiasson, K. Lacki, A. Forss

BIOT **377.** Use of multivariate techniques to develop a predictive model for viral vaccine potency based on raw material components. **A. Purdy**, C. Cameron, N. Afanador, H. Fahmy, J. ONeill

WEDNESDAY MORNING

Section A

Grand Hyatt Denver
Mt. Elbert A

Upstream Processes

Advances in Biocatalysis

M. A. Blenner, I. R. Wheeldon, *Organizers, Presiding*

8:30 BIOT **378.** Metabolic channeling and spatial effects of bifunctional enzymes. **W. Xu**, A. Prasad

8:50 BIOT **379.** Controlling local substrate concentrations and enzyme kinetics through rationally designed intermolecular interactions. Y. Gao, J. Zhu, J. Lin, **I. Wheeldon**

9:10 BIOT **380.** Microscale tools for rapid evaluation of the two-phase whole-cell bio-oxidation of highly volatile substrates. **J.F. Kolmar**, F. Baganz, P. Engel

9:30 BIOT **381.** Engineering recombinant *Escherichia coli* for improved triacetic acid lactone production by screening transposon insertion libraries. **Y. Li**, P. Cirino

9:50 Intermission.

10:10 BIOT **382.** Methods to increase substrate conversion in the fungus, *Beauveria bassiana*. **F. Nicolau** Manterola, T.L. Peeples

10:30 BIOT **383.** De novo biosynthesis of 1,2-propanediol from renewable feedstock through lactic acid. **W. Niu**, J. Guo

10:50 BIOT **384.** Engineering of *Saccharomyces cerevisiae* for the production of long and short chain fatty acids. **C. Leber**, B. Polson, R. Fernandez-Moya, N.A. Da Silva

11:10 BIOT **385.** Biosynthesis of key gasoline-range alkanes using engineered *E. coli*. **A.M. Kunjapur**, M. Sheppard, K.L. Jones Prather

Section A

Grand Hyatt Denver
Mt. Evans

Biotechnology & Bioengineering Awards Presentation and Gaden Award

M. Lazzara, *Organizer, Presiding*

11:30 BIOT **386.** Sex and the better biocatalyst. **F.H. Arnold**

Section B

Grand Hyatt Denver
Mt. Evans

Downstream Processes

Advances and Case Studies in the Use of Disposables, Continuous Processing & Flexible Manufacturing

S. M. Cramer, J. Salm, *Organizers, Presiding*

8:30 BIOT **387.** Continuous precipitation-based capture step for recombinant antibodies. **N. Hammerschmidt**, S. Hobiger, A. Jungbauer

8:50 BIOT **388.** Control and optimization of a twin-column counter-current chromatography process for affinity capture of biopharmaceuticals. **T. Muller-Spath**, N. Ulmer, L. Aumann, M. Bavand

9:10 BIOT **389.** Design and characterization of an incubation chamber for continuous viral inactivation. **R. Orozco**, N. Guillen, S. Godfrey, J. Vogel, J.L. Coffman

9:30 BIOT **390.** Development of a continuous MAb purification process. **A. Forss**, H. Blom, T. Bjorkman, A. Ljunglöf, B. Westerlund

9:50 Intermission.

10:10 BIOT **391.** Continuous downstream processing for monoclonal antibodies: Are we there yet? **J.Y. Zhang**, L. Conley, D. Cecchini, V. Natarajan, S. Ghose

10:30 BIOT **392.** Process economics of continuous mAb processing with single-pass tangential flow filtration. **E. Ayturk**, R. Gantier

10:50 BIOT **393.** PAT tool for chromatography supporting batch and continuous processing. **N. Brestrich**, A. Sanden, T. Briskot, J. Hubbuch

11:10 BIOT **394.** Feasibility of pH measurement by spectroscopy during continuous low pH virus inactivation in monoclonal antibody production. **J. Goby**, J.L. Coffman, E. Zimmermann, M. Strawn, M. Noguchi, J.A. Beller, M. Cortese, J.F. Breit, J. Vogel

Section C

Grand Hyatt Denver
Grays Peak

Biomolecular & Biophysical Processes

Bionanotechnology

P. Millili, K. Schultz, *Organizers, Presiding*

8:30 BIOT **395.** Biofabrication and engineering of ZnS:Mn nanocrystals. **B. Swift**, W. Zhou, F. Baneyx

8:50 BIOT **396.** Photoresponsive on/off dormancy in polyplexes for patterned control of cell behavior. **C.T. Greco**, T.H. Epps, III, M.O. Sullivan

9:10 BIOT **397.** Functionalization of hydrogels with matrix metalloproteinase-sensitive fluorogenic biosensors to measure cancer cell response to drug treatment. **J.L. Leight**, E.Y. Tokuda, K.S. Anseth

9:30 BIOT **398.** Synthesis and characterization of a micelle-templated, sub-100 nm PLGA nanoparticle for targeted drug delivery. B.L. Miller, G. Nabar, M.C. Calhoun, J. Xu, M.N. Gurcan, V.K. Puduvalli, **J.O. Winter**

9:50 Intermission.

10:10 BIOT **399.** Quantum molecular-sequencing (QM-Seq): Single molecule DNA and RNA sequencing. **J. Casamada-Ribot**, A. Chatterjee, P. Nagpal

10:30 BIOT **400.** Therapeutic nucleic acid complex micelles. **L. Leon Gibbons**, E. Chung, Y. Fang, M.V. Tirrell

10:50 BIOT **401.** Hemocompatibility of colloidally stable glycopolymer-DNA complexes for gene therapy. **H.R. Phillips**

11:10 BIOT **402.** Tunable composite nanocarriers for magnetic resonance imaging, multimodal imaging, and theranostic applications. **R.K. Prudhomme**

Section D

Grand Hyatt Denver
Mt. Sopris A

Biofuels & Sustainable Energy

Biological Fuel & Energy Production Using Photons & Electrons

C. A. Peebles, A. Singh, *Organizers, Presiding*

8:30 BIOT **403.** Prospective bioethylene production process from photosynthetically-fixed CO_2 in recombinant cyanobacteria. **J. Markham**, J. Yu, **L. Tao**

8:50 BIOT **404.** Understanding and optimizing free fatty acid production in *Synechocystis* sp. PCC 6803. **Y. Cheah**, C.A. Peebles

9:10 BIOT **405.** Metabolic flux analysis of the micro-algae *Chlorella vulgaris* at different CO_2 concentrations under autotrophic, heterotrophic, and mixotrophic growth. **M.R. Antoniewicz**

9:30 BIOT **406.** Role of PII in the nitrogen-stress response of *Chlamydomonas reinhardtii*. **J. Sweeley**

9:50 Intermission.

10:10 BIOT **407.** Impact of salinity on the kinetics of CO_2 fixation by Spirulina platensis cultivated in semicontinuous photobioreactors. **J. Ramirez-Perez**, H. Janes

10:30 BIOT **408.** Understanding the performance of sugar-yeast-ethanol biohybrid fuel cells. **J. Jahnke**, D. Mackie, M. Benyamin, S. Liu, R. Ganguli, J. Sumner

10:50 BIOT **409.** Engineering the chemolithoautotroph *Acidithiobacillus ferrooxidans* for chemical and fuel production. **S. Banta**, X. Li, T. Kernan, S. Majumdar, A. West

11:10 BIOT **410.** High performance nanocomposites produced with cross-linked glucose oxidase aggregates and graphitized mesoporous carbon. **T. Garcia-Perez**, J. Kim, S. Ha

Section E

Grand Hyatt Denver
Mt. Elbert B

Quality-by-Design for Biopharmaceuticals

Case Studies in QbD Implementation

B. Junker, A. S. Rathore, *Organizers, Presiding*

8:30 BIOT **411.** Is QbD more difficult for less defined biopharmaceuticals? A comparison of 3 case studies. **M. Streefland**, S. Mercier, R. Wijffels

9:10 BIOT **412.** Multivariate data analysis methods for qualifying scale-down models. **A. Meier**, S. Meier

9:30 BIOT **413.** QbD as basis for effective development of biopharmaceuticals. **J. Panek**, J. Gampfer

9:50 Intermission.

10:10 BIOT **414.** Implementation of QbD for development of a downstream process for a therapeutic biosimilar. **A.S. Rathore**

10:30 BIOT **415.** Virus filtration QbD knowledge base. **H. Lutz**

10:50 BIOT **416.** Effective strategy for a comprehensive QbD characterization of Viresolve® filter: A collaboration between medImmune and EMD millipore. **G. Ferreira**, J. Prentice, S. Rajarajan, M. Zhu, M.L. Dickson, H. Lutz, D. Robbins

11:10 BIOT **417.** Design space assessment focused on value and probability of success. **M. Trexler Schmidt**, M. Mun, S. Khoo, N.L. McKnight, A. Mehta, S.J. Meier, R. St. John, B.D. Kelley

WEDNESDAY AFTERNOON

Section A

Grand Hyatt Denver
Mt. Elbert A

Upstream Processes

Microbial Process Development

M. Lipscomb, D. B. Ritz, *Organizers, Presiding*

2:00 BIOT **418.** Standarized two-stage bioprocess development using synthetic metabolic valves and dynamic metabolic control. **M.D. Lynch**, A. Trahan, Z. Ye

2:20 BIOT **422.** Optimization of valuable intermediates synthesis by 11 alpha-hydroxylation of steroid DHEA by solvent-enhanced biocatalyst. **R. Gonzalez**

2:40 BIOT **419.** Optimization of microbes for industrial bioprocesses using high throughput genome engineering. **Z. Serber**

3:00 BIOT **424.** Increasing soluble expression of an intact Fab (fragmented antibody) in *E. coli* by smart plasmid design and chaperone co-expression. **V. Roy,** K. Bhere, P. Navarathna, S. Machhi, M. Berge, L. Qu

3:20 Intermission.

3:40 BIOT **420.** Engineering a modular network of nonnatural pathways for aromatic chemicals and muconic acid. **B. Thompson**, S. Pugh, R. McKenna, D.R. Nielsen

4:00 BIOT **421.** Development of an enzyme-free process for converting lignocellulosic biomass to fuels and chemicals. **B. Pfleger**, J.A. Dumesic, C. Maravelias

4:20 BIOT **339.** Regulation of photosynthetic carbon partitioning in a cyanobacterium. **M.A. Cano**, W. Xiong, D.J. Carrieri, T. Paddock, P. Maness, M.L. Ghirardi, J. Yu

4:40 BIOT **423.** New method for peptide production: Modular secretion from *Bacillus megaterium*. **N. Marchand**, C.H. Collins

Section A

Grand Hyatt Denver
Mt. Evans

Biotechnology & Bioengineering Daniel I. C. Wang Award

M. Lazzara, *Organizer, Presiding*

5:00 BIOT **425.** Toward a holistic understanding of cellular metabolism. **M.R. Antoniewicz**

Section B

Grand Hyatt Denver
Mt. Evans

Downstream Processes

Advances and Case Studies in the Use of Disposables, Continuous Processing & Flexible Manufacturing

S. M. Cramer, J. Salm, *Organizers, Presiding*

2:00 BIOT **426.** Single-use nonchromatographic purification method for antibodies. **P. Jorjorian**

2:20 BIOT **427.** Development and GMP production of novel antibody immuno-PET conjugates using single use/disposable technologies. **T. Peram**, D. Olson, J. Keba

2:40 BIOT **428.** Antibody sieving analysis of multiple microfiltration membranes during a single perfusion cell culture. **N. Pinto**, W. Napoli, C. Kistler, M. Brower

3:00 BIOT **429.** PALL single-use strategy to increase flexibility in manufacturing. **J. Griffin**

3:20 Intermission.

3:40 BIOT **430.** Implementation and characterization of solvent detergent viral inactivation in single use bags. **M.A. Cunningham**, V. Raman, N. Sood, J. Shea, L. Mullin, E. Youssef, P. Almeida, E.M. Goodrich

4:00 BIOT **431.** Considerations when building a single use technology ADC manufacturing. **D. Lok**, E. Mahajan

4:20 Panel Discussion.

Section C

Grand Hyatt Denver
Mt. Sorpis A

Biomolecular & Biophysical Processes

General Topics

C. J. Roberts, H. Samra, *Organizers, Presiding*

2:00 BIOT **432.** Understanding the mechanism of in surfo crystallization of membrane proteins. **A. Samadzoda**, A. Vaish, A.S. Robinson, A.M. Lenhoff

2:20 BIOT **433.** Specific-ion effects on the aggregation mechanisms and protein-protein interactions for antistreptavidin immunoglobulin Gamma-1. **G.V. Barnett**, V. Razinkov, B.A. Kerwin, T. Laue, A. Woodka, P. Butler, T. Perevozchikova, C.J. Roberts

2:40 BIOT **434.** High-throughput passive microrheology of therapeutic protein solutions. **L. Josephson**, W.J. Galush, E.M. Furst

3:00 BIOT **435.** Can aggregation prone states of an antibody fragment be predicted through biophysical analysis? **D. Hilton**

3:20 Intermission.

3:40 BIOT **436.** Cell-material interactions in synthetic hydrogel scaffolds. **K. Schultz**, F. Escobar, K. Kyburz, D. McKinnon, K.S. Anseth

4:00 BIOT **437.** Impact of asymmetric flow field-flow fractionation on antistreptavidin IgG1 protein aggregation. **C. Bria**, K.R. Williams

4:20 BIOT **438.** Parameters Influencing cavitation within therapeutic vials subjected to drop shock. **C. Lengsfeld**, D. Sederstrom, M. Puryear, R. Rodrigues

4:40 BIOT **439.** Silicone oil microdroplets can act as an adjuvant in protein formulations containing foreign antigen or self antigen. **C.F. Chisholm**, J. Carpenter, T. Randolph

Section D

Grand Hyatt Denver
Grays Peak

Biofuels & Sustainable Energy

Synthetic Biology Approaches to Engineer Production of Fuels & Energy Molecules

J. Carothers, A. Froehlich, *Organizers, Presiding*

2:00 BIOT **440.** Utilization of modular cell and pathway design for combinatorial synthesis of designer bioesters. D.S. Layton, **C.T. Trinh**

2:20 BIOT **441.** 2-Keto acids based biosynthesis pathways for renewable fuels and chemicals. **Y. Tashiro**, S.H. Desai, G.M. Rodriguez, S. Atsumi

2:40 BIOT **442.** Advanced pathways for microbial production of branched C_5 alcohols in *E. coli*. **T. Lee**, A. Kang, K. George

3:00 BIOT **443.** Strain engineering, high-throughput screening, and systems biology analysis for the successful production of renewable chemicals and fuels. **M. Leavell**

3:20 Intermission.

3:40 BIOT **444.** Genome-scale strategies for designing, building, and testing biological systems. **R.T. Gill**

4:20 BIOT **445.** Synthetic biology-enabled strategies for improving ethylene production from engineered *E. coli*. **S. Lynch**, C.A. Eckert, J. Yu, P. Maness, R.T. Gill

4:40 BIOT **446.** Building important molecules from methanol. **I.W. Bogorad**, C. Chen, M. Theisen, T. Wu, J.C. Liao

Section E

Grand Hyatt Denver
Elbert B

Quality-by-Design for Biopharmaceuticals

Approaches to Process Characterization & Design Space Definition

S. Ahuja, S. Tobler, *Organizers, Presiding*

2:00 BIOT **447.** Characterization of a CHO-based monoclonal antibody production process using a quality by design approach. **J.C. Goodrick**

2:20 BIOT **448.** Modeling the preparation of a concentrated nutrient feed solution for a large scale cell culture process. **B. Russell**, S. Ahuja, G. Miro-Quesada, L. Qu

2:40 BIOT **449.** Addressing solution composition variability for process buffers and product intermediates in PC studies and control strategy definition. **S.A. Tobler**

3:00 BIOT **450.** Process characterization: A quality by design approach to scale-down studies across multiple HTPD formats. **A. Berrill**, J.S. Feliciano, A. Mattias, K. Nilsson Välimaa, Z. Fung, E. Brekkan, B. Evans, J. Salm, R. Godavarti, K. Lacki

3:20 Intermission.

3:40 BIOT **451.** Development and characterization challenges of an ion exchange chromatography step. **J.F. Hsii**, A. Mehta, L. Gao, B. Thayer, R. St. John

4:00 BIOT **452.** Employment of QbD principles to control charge variants with anion exchange chromatography. **B.F. Marques**, T. Wiley, S. Weisser, P.R. Smith, K.E. Goklen

4:20 BIOT **453.** QbD approach to aggregate control in affinity chromatography. **L. Leone**, A.T. Lewandowski, Z. Li

4:40 BIOT **454.** Quantitative process parameter classification approach for biopharmaceutical development in QbD paradigm. **S. Singh**, G. Miro-Quesada, L. Qu, R.V. Venkat

THURSDAY MORNING

Section A

Grand Hyatt Denver
Mt. Evans

Upstream Processes

General Topics

N. Agarwal, C. F. Komives, *Organizers, Presiding*

8:30 BIOT **455.** Evaluation of extended passaging during inoculum expansion of a CHO cell line: a case-study of improving manufacturing flexibility. **P. Apostolidis**, L. Zhou, P. Thompson, H. Graham

8:50 BIOT **456.** Can we predict production instability? Detection of karyotypic changes related to phenotypic changes in CHO cells. **J. Baik**, K.H. Lee

9:10 BIOT **457.** Achieving comparable product quality profiles through cell culture process and media optimization. **N.M. Jacob**, V. Marczewski, R. Li, S.B. Rianna, E. Kraus, K. Camberg

9:30 BIOT **458.** Real-time, continuous monitoring of cellular nutrients and metabolites for optimization of upstream bioprocesses. **M.A. Arnold**, E.R. Gibson, K. Lanz, E. Koerperick, D. Cooley, J. Olesberg, C. Evans, G.W. Small

9:50 Intermission.

10:10 BIOT **459.** UNICAN: Dual capability in single use bioreactors. **E. Mahajan**, E. Chan, T. Hudson

10:30 BIOT **460.** Efficient, high-titer monoclonal antibody production in a fed-batch process using single-use stirred-tank and rocking bioreactor systems. **T. Falkman**, E. Fäldt, O. Larsson

10:50 BIOT **461.** Sparger design for improved bubble-liquid hydrodynamics in bioreactors. Y. Liu, R. Ferguson, W. Hu, **K. Wiltberger,** S. Hourn, F. Li

11:10 BIOT **462.** Improved monitoring in upstream clean-in-place (CIP) operations. **V. Saucedo**, Z. Li, D. Schimizzi, M. Su, A. Phillips, T.W. Hudson, B. Gan

Section B

Grand Hyatt Denver

Mt. Sopris B

Downstream Processes

Antibodies, Drug Conjugates & Related Molecules

G. Carta, S. Kandula, *Organizers, Presiding*

8:30 BIOT **463.** Development of a manufacturable process to control IgG4 half antibody. **K. Brower**, R. Koduri, M. Yu, K. Karaveg, V. Dhawan, P. Finn, C. Hwang, V. Warikoo, K.B. Konstantinov

8:50 BIOT **464.** Approaches to platforming antibody drug conjugate development. **J. Liddell**

9:10 BIOT **465.** Downstream process solution to mAb occupancy in glycoengineered p*ichia*. **S. Rios**

9:30 BIOT **466.** Development of a downstream purification process for an early phase bispecific antibody: A case study. **A. Ladiwala**, J. Lee, M. Bhaumik, M. Lee, S. Woon, M. Fedesco, C.A. Teske, M. Butler, P. Lester

9:50 Intermission.

10:10 BIOT **467.** Antibody drug conjugates: A new platform of protein therapeutic molecules with duocarmycins as cytotoxic agents. **M. Eppink**, G. De Roo, P. Beusker, R. Coumans, R. Verstegen, B. Kamps, H. Spijker

10:30 BIOT **468.** Protein A affinity chromatography for efficient purification of recombinant antibody fragments. **A. Stein**, A. Heinen-Kreuzig, A. Kiesewetter, M. Jung, M. Holstein, M. Bruce, J. Orlando, N. Bian

10:50 BIOT **469.** Capacity assessment: DBC is not the whole story – implications for resin lifetime and sequential multicolumn chromatography. E. Trilisky, **J. Ladwig**, S. Trimble, J.S. Moscariello

11:10 BIOT **470.** Thorough investigation of the effect of novel sanitization agents on affinity chromatography media. **E. Monie**, A. Grönberg, A. Ljunglöf, M. Wetterhall, T. Bjorkman

Section C

Grand Hyatt Denver

Grays Peak A

Biomolecular & Biophysical Processes

General Topics

C. J. Roberts, H. Samra, *Organizers, Presiding*

8:30 BIOT **471.** Mechanism of cholesterol binding by an RTX leukotoxin. E. Koufos, **A.C. Brown**

8:50 BIOT **472.** Photocrosslinking with p-azidophenylalanine used to identify the location of Cic binding on ERK. **A. Futran**, S.Y. Shvartsman, A. Link

9:10 BIOT **473.** Rare example of a protein where an isolated domain is more stable than the full-length. S. Bandi, S. Singh, **K. Mallela**

9:30 BIOT **474.** Mechanistic details of pH dependent non-photochemical quenching mediated by CP29. **C.A. Lopez**, B. Gennady, R.T. Sayre, S. Gnanakaran

9:50 Intermission.

10:10 BIOT **475.** Engineering cellulose-degrading complexes from anaerobic gut fungi. **C. Haitjema**, S. Gilmore, K. Solomon, M.A. O'Malley

10:30 BIOT **476.** Promoting binding of protein-targeting substrates by regulating interdomain dynamics within a signal recognition particle: Implications for biotechnology. F. Gao, A. Kight, S. Jayanthi, P. Patel, R.L. Goforth, S.K. Thallapuranam, R. Henry, R. Henderson, **C.D. Heyes**

10:50 BIOT **477.** Effect of DNA base orientation on charge transfer reaction. **A. Khan**

11:10 BIOT **478.** Conformational study of Δ°<-tetrahydrocannabinol (Δ<°-THC) linear and nonlinear circular dichroism. **J. Donnelly**, F.E. Hernández

Section D

Grand Hyatt Denver

Grays Peak B

Biofuels & Sustainable Energy

Development and Deconstruction of Sustainable and Low-cost Feedstocks for Biofuels and Bioproducts

H. Scheller, G. Sriram, *Organizers, Presiding*

8:30 BIOT **479.** Dynamics of CO_2 consumption, and biomass and lipid production during photobioreactor cultivation of the diatom *Cyclotella* under constant incident and constant mean light modes. **A. Ozkan**, G. Rorrer

8:50 BIOT **480.** Use of synthetic biology to improve bioenergy crops. A. Eudes, Y. Liang, **D. Loque**

9:10 BIOT **481.** Base-catalyzed depolymerization of residual solid biomass from a biochemical conversion process. **R. Katahira**, A. Mittal, K.A. McKinney, G.T. Beckham

9:30 BIOT **482.** Innovative pretreatment strategies to generate high-quality sugars from a broad spectrum of biomass resources. **Y.N. Guragain**, K.P. Bastola, R. Barrios, A.R. Kingsly, P.V. Vadlani

9:50 Intermission.

10:10 BIOT **483.** Amberlyst 35DRY enhanced 1-butyl-3-methylimidazolium chloride pretreatment of *Arundo donax* Linn. T. You, L. Zhang, **F. Xu**

10:30 BIOT **484.** Charge engineering of cellulases improves ionic liquid tolerance and reduces lignin inhibition. E. Nordwald

10:50 BIOT **485.** Increased lipid production via genetically engineered oleaginous yeast *Rhodosporidium toruloides*. **S. Zhang**, C.V. Rao

11:10 BIOT **486.** Over-expression and characterization of four alginate lyases from *Vibrio splendidus* 12B01. **A.H. Badur**, G. Yalamanchali, C.V. Rao

Section E

Grand Hyatt Denver

Mt. Sopris A

Downstream Processes

Mini Topics: Biobased Industry Challenges and a Focus on Impurities

J. J. Stickel, S. A. Tobler, L. A. van der Wielen, R. C. Willson, *Organizers, Presiding*

8:30 BIOT **487.** Continuous enzymatic hydrolysis: Membrane fractionation. **B. Adhikari**, D. Sievers, J.J. Stickel, J. Pellegrino

8:50 BIOT **488.** On fractionation of organic fuel precursors from electrolytes with RO and NF membranes. M. Rickman, R.H. Davis, **J. Pellegrino**

9:10 BIOT **489.** Flocculant-aided solid-liquid separation of algal and lignocellulosic biomass slurries. **N.C. Crawford**, M. Minot, J.J. Lischeske, D. Sievers, N. Nagle, J.J. Stickel

9:30 BIOT **490.** Comparing In situ removal strategies for improving styrene biosynthesis. R. McKenna, **B. Thompson**, L. Moya, M. McDaniel, D.R. Nielsen

9:50 Intermission.

10:10 BIOT **491.** Impact of elution pH on product and process related impurities in Protein A chromatography. **D. Yu**, E. Schutsky, L. Leone, Z. Tan, A. Lewandoski, M.C. Borys, Z. Li

10:30 BIOT **492.** Two-stage chromatographic separation of aggregates for monoclonal antibody therapeutics. **V. Kumar**, A.S. Rathore

10:50 BIOT **493.** Heterogeneous high molecular weight species in purification platform. **Y. Li**

11:10 BIOT **494.** Development of platform host cell protein enrichment strategies for use in impurity spike challenge studies. **R.G. Soderquist**, R. Hart

THURSDAY AFTERNOON

Section A

Grand Hyatt Denver

Mt. Evans

Upstream Processes

Engineering Non-model Hosts for Biological Production

S. Atsumi, Y. Huo, A. Sato, *Organizers, Presiding*

2:00 BIOT **495.** Production of bispecific antibodies in "Knobs-into-Holes" using a cell-free expression system. **Y. Xu**

2:20 BIOT **496.** Robustness and productivity: Lessons from metabolic engineering and RNA-Seq studies in *Zymomonas mobilis*. **S. Yang**, M. Zhang, Y. Chou, T. Vander Wall, W. Michener, P. Pienkos

2:40 BIOT **497.** Anaerobic advanced biofuel production in *Zymomonas mobilis*. **M. Zhang**, Y. Chou, M. Franden, S. Yang

3:00 BIOT **498.** Engineering *Clostridium thermocellum* for hydrogen production. **K.J. Chou**, L. Magnusson, P. Maness

3:20 Intermission.

3:40 BIOT **499.** Photosynthetic limonene and bisabolene production in wild type and a glycogen-deficient mutant of *Synechococcus* sp. PCC 7002. **F.K. Davies**, S.A. Jackson, J.J. Eaton-Rye, M. Posewitz

4:00 BIOT **500.** Synthetic biology approach to improving cyanobacterial chemical production. **N. Nozzi**, S. Atsumi

4:20 BIOT **501.** Transferring nitrogen fixing capabilities to an oxygenic photosynthetic organism. A. Balassy, M. Bhattacharyya, A. Hoynes-O'Connor, C. Immethun, M. Liberton, D. Liu, **T. Mueller**, Y. Xiao, J. Yu, T. Moon, F. Zhang, C. Maranas, H. Pakrasi

4:40 BIOT **502.** Engineering ORCA3 and SGD in *Catharanthus roseus* hairy roots increase alkaloid production. **J. Sun**

Section B

Grand Hyatt Denver

Mt. Sopris B

Downstream Processes

Antibodies, Drug Conjugates & Related Molecules

G. Carta, S. Kandula, *Organizers, Presiding*

2:00 BIOT **503.** Toward improving selectivity in Protein A chromatography with PEGylated ligands: High throughput characterization of PEGylation strategies. **J.B. Weinberg**, T.M. Przybycien

2:20 BIOT **504.** Alternative multimodal process for the capture of monoclonal antibodies based on phenylboronic acid chromatography. **A.M. Azevedo**, S. Rosa, R. Santos, R.M. Aires-Barros

2:40 BIOT **505.** Antibody aggregation in the mobile phase. **F. Ojala**, A. Sellberg, T. Budde Hansen, E. Broberg Hansen, A. Staby, B. Nilsson

3:00 BIOT **506.** Rapid ranking of high-concentration monoclonal antibody formulations using manufacturability indices. **Y. Yang**, A. Velayudhan, S. Farid, N. Thornhill

3:20 Intermission.

3:40 BIOT **507.** Withdrawn.

4:00 BIOT **508.** High capacity salt tolerant weak cation exchange media for mAb purification: Improved process performance through efficient pH transition and control. **D.M. Kanani**, N. Sidhu, N. Paghdal, J. Stout

4:20 BIOT **509.** Eliminate downstream facility constraints for high titer cell culture processes. **M. Zhu**, J. Savery, J. Bender, G. Miro-Quesada, D. Robbins

4:40 BIOT **510.** Understanding HCP binding to depth filters: Can we qualify depth filters for purification? **N. Soice**, E. Zinn, K. Petty, R. Alvarado, J. Espinoza, A. Hewig

Section C

Grand Hyatt Denver

Grays Peak A

Biomolecular & Biophysical Processes

High-Throughput Biomolecular Engineering and Characterization

I. V. Korendovych, I. R. Wheeldon, *Organizers, Presiding*

2:00 BIOT **511.** Engineering a lasso peptide display system for directed evolution applications. **C. Zong**, A. Link

2:20 BIOT **512.** Characterization and directed evolution of aminoacyl tRNA synthetases. **J. Tullman**, L. Wu, S. Li, J.P. Marino

2:40 BIOT **513.** Physiological assay designed to quantify the efficacy and potency of antimalarials. **M.A. Ketchum**, J.D. Rimer, P.G. Vekilov

3:00 BIOT **514.** Application of automated micro-UF/DF system for high-throughput formulation development. **C. Ren**, K. Westland, R. Rajan, S. Lambert, R. Burge

3:20 Intermission.

3:40 BIOT **515.** Design and selection of peptides with specific recognition properties for protein purification and analysis. **D. Chandra**, S. Timmick, C. Goodwine, D. Shastry, S.M. Cramer, P. Karande

4:00 BIOT **516.** Computational design and directed evolution of allosterically regulated enzymes. **I.V. Korendovych**

4:20 BIOT **517.** Design and discovery of short peptides for biocatalysis and self-assembly. **R. Ulijn**

4:40 Panel Discussion.

Section D

Grand Hyatt Denver

Grays Peak B

Biofuels & Sustainable Energy

Biomass Pretreatment & Hydrolysis

K. Brandon Sutton, M. A. OMalley, *Organizers, Presiding*

2:00 BIOT **518.** RAPT (reversible acid pretreatment) for cellulosic ethanol production. **P.R. Weider**, R. Blackbourn

2:20 BIOT **519.** Identification of topochemical features associated with cell wall recalcitrance to dilute acid pretreatment in *Miscanthus x giganteus*. **Z. Ji**, X. Zhang, Z. Ling, B. Wu, F. Xu

2:40 BIOT **520.** Alkaline pretreatment of corn stover: Optimal pretreatment conditions and development of new analytical methods for quantification of chemical compounds within lignin rich liquors. **E.M. Karp**, P. Ciesielski, B. Donohoe, S. Deutch, M.J. Biddy, G.T. Beckham

3:00 BIOT **521.** Comparative analysis of extremely thermophilic *Caldicellulosiruptor* species provides insights into cellular strategies for plant biomass deconstruction. **J. Zurawski**, H. Simpson, J.A. Izquierdo, J.M. Conway, L.L. Lee, S.E. Blumer-Schuette, R.M. Kelly

3:20 Intermission.

3:40 BIOT **522.** Combination of enzyme paradigms and biomass pretreatment reveal novel saccharification mechanisms. **M. Resch**, B. Donohoe, C.H. Haitjema, A. Mittal, P. Ciesielski, G. Beckham, M. Himmel, M.A. OMalley, S. Decker

4:00 BIOT **523.** Differential binding of biomass hydrolyzing enzymes to lignin: Conversion yields suggest a paradigm shift. **J. Yarbrough**, A. Mittal, L.E. Taylor, S.E. Hobdey, E. Mansfield, D. Sammond, S. Decker, M.E. Himmel, T.B. Vinzant

4:20 BIOT **524.** SPORL for robust bioconversion of Douglas-fir forest residue: Pilot scale-up design, lignin co-product, and high solids fermentation without detoxification. **J. Zhu**

4:40 BIOT **525.** SSF-IL: Enabling simultaneous saccharification and fermentation in ionic liquid for high-yield conversion of cellulose into alpha-ketoglutaric acid. S. Ryu, N. Labbe, **C.T. Trinh**

‡ *Cooperative Cosponsorship*

Section E

Grand Hyatt Denver

Mt. Sopris A

Downstream Processes

Leveraging Fundamentals for Accelerated Downstream Process Development

A. C. Dumetz, M. Ottens, E. von Lieres, *Organizers, Presiding*

2:00 BIOT **526.** Robust characterization of the chromatographic behaviour of complex biological feedstocks. **A.T. Hanke**, P.D. Verhaert, L.A. van der Wielen, E.J. van de Sandt, M.H. Eppink, M. Ottens

2:20 BIOT **527.** Efficient and reliable model calibration in column chromatography with Optimal Experimental Design (OED). **T. Hahn**, G. Wang, T. Huuk, J. Hubbuch

2:40 BIOT **528.** Computational investigation into mAb adsorption behavior under high loading conditions for cation exchange chromatography. **S. Hunt**, K. Tolley, T. Larsen, B. Smith, E. von Lieres, R.J. Todd

3:00 BIOT **529.** Model-based optimization and control of process scale ion exchange chromatography for therapeutic proteins. **V. Kumar**, E. von Lieres, A.S. Rathore

3:20 Intermission.

3:40 BIOT **530.** Rationale purification development: Leveraging molecular biophysics to target purification modalities. **D.J. Roush**, F. Insaidoo, J. Welsh, T. Linden

4:00 BIOT **531.** Binding of proteins to multimodal chromatographic surfaces: A molecular modeling perspective. **S. Banerjee**, S. Parimal, S. Garde, S.M. Cramer

4:20 BIOT **532.** Mass transfer resistance as evidence of resin fouling: Accelerated experimental techniques. **P. Smith**, A. Pike, B.F. Marques, A.R. Ubiera, K.E. Goklen

4:40 BIOT **533.** Multi-addition batch uptake: A novel high-throughput approach for measuring intra-particle mass transfer. **S.J. Traylor**, X. Xu, Y. Li, M. Jin, Z. Li

BIOL

Division of Biological Chemistry

C. M. Crews and V. Bandarian, *Program Chairs*

OTHER SYMPOSIA OF INTEREST:

Interfacial and Biomolecular Recognition *(see COLL, Sun, Tue, Wed, Thu)*

Undergraduate Research Posters *(see CHED, Sun, Mon)*

GSSPC: Designed by Nature, Developed by Science: Interdisciplinary Perspectives on Biocatalysis *(see CHED, Tue)*

SUNDAY MORNING

Section A

Hyatt Regency Denver at Colorado Convention Center

Capitol Ballroom 4

Young Investigators in Biological Chemistry

C. M. Crews, *Organizer, Presiding*

8:30 BIOL **1. Award Address** (Nobel Laureate Signature Award for Graduate Education in Chemistry Sponsored by Avantor Performance Materials). Expansion of the genetic alphabet in vitro and in vivo. **D. Malyshev**, K. Dhami, T. Lavergne, T. Chen, N. Dai, J. Foster, I. Correa, F.E. Romesberg

8:50 BIOL **2.** Chemical probes to explore histidine kinase signaling. **K. Wilke**, R. Godsey, **E.E. Carlson**

9:10 BIOL **3.** Novel base-modified nucleotides terminating DNA synthesis and their applications in chemistry of life processes. **V.A. Litosh**

9:30 BIOL **4.** Small-molecule modulation of apoptosis via direct targeting of pro-apoptotic BAX. D. Reyna, T. Garner, F. Kopp, Y. Wu, N. Biris, U. Steidl, R. Kitsis, **E. Gavathiotis**

9:50 BIOL **5.** Chemoproteomic profiling of lysine acetyltransferases highlights an expanded landscape of catalytic acetylation. **J.L. Meier**, D. Montgomery, A. Sorum

10:10 Intermission.

10:30 BIOL **6.** Tabtoxinine-β-lactam inhibits glutamine synthetase by an ammonia capture mechanism. **T.A. Wencewicz**, U. Wanninayake, G.J. Patrick

10:50 BIOL **7.** Evolution of Src homology 2 domain. T. Ju, W. Niu, **J. Guo**

11:10 BIOL **8.** Quadruplet codon decoding. N. Wang, W. Niu, E.D. Hankore, **J. Guo**

11:30 BIOL **9.** Substoichiometric hydroxynonenylation of a single protein recapitulates whole-cell-stimulated antioxidant response. **Y. Aye**, S. Parvez

SUNDAY AFTERNOON

Section A

Hyatt Regency Denver at Colorado Convention Center

Capitol Ballroom 4

Complex Enzymatic Transformations

V. Bandarian, *Organizer, Presiding*

2:30 BIOL **10.** Gut reactions: Understanding radical enzymes from the human microbiota. **E.P. Balskus**

3:15 BIOL **11.** Mechanism of the C5 stereoinversion reaction catalyzed by the Fe(II)- and 2-oxoglutarate-dependent enzyme, CarC, in the biosynthesis of carbapenem antibiotics. W. Chang, Y. Guo, C. Wang, S.E. Butch, A.C. Rosenzweig, A.K. Boal, **C. Krebs**, J.M. Bollinger

4:00 BIOL **12.** Experimental strategies for functional annotation and metabolism discovery: Targeted screening of solute binding proteins and unbiased panning of metabolomes. **S. Almo**

4:45 BIOL **13.** Mechanistic studies of tRNA hypermodification. **V. Bandarian**

SUNDAY EVENING

Section A

Hyatt Regency Denver at Colorado Convention Center

Capitol Ballroom 4

Alfred Bader Award in Bioinorganic or Bioorganic Chemistry: Symposium in Honor of Michael A. Marletta

C. M. Crews, *Organizer, Presiding*

7:00 BIOL **14. Award Address** (Alfred Bader Award in Bioinorganic or Bioorganic Chemistry sponsored by the Alfred R. Bader Fund). At the interface between chemistry and biology: Two examples. **M.A. Marletta**

Section A

Hyatt Regency Denver at Colorado Convention Center

Capitol Ballroom 4

Current Topics in Biological Chemistry

V. Bandarian, C. M. Crews, *Organizers*

8:15 - 9:45

BIOL **15.** Quantifying vGlut2 terminals in the rat medial geniculate body. **Z.J. Diaz-Reguero**

BIOL **16.** Identification of unique cell surface receptors on breast cancer stem cells by using combinatorial chemical library. **C. Long**, J. Lee

BIOL **17.** Biophysical parameters that determine RNA-metal complex formation. **R. Whitaker**

BIOL **18.** Characterization of the pyruvyltransferase WcfO from the CPSA biosynthetic pathway. **S. Sharma**, J.M. Troutman

BIOL **19.** Advancing tetrazine ligations to develop fluorogenic probes for cellular imaging. **N.K. Devaraj**

BIOL **20.** Design and biological screening of steroidal analogs as selective estrogen receptor modulators. **F.T. Halaweish**, A. Alsayari, L. Kopel, M. Ahmed

BIOL **21.** Thermostabilization of 3-dehydroshikimate dehydratase: A pivotal enzyme in commodity chemical biosynthesis. L. Harrington, R. Jha, T. Kern, C. Strauss, G. Canales, K. Hotta, A.T. Koppisch, **D.T. Fox**

BIOL **22.** Helicase recruitment to sub-cellular granules during viral infection. **M. Corby**, A. Mahim, G. Biener, V. Raicu, D.N. Frick

BIOL **23.** Exploiting molten salts for concerted pathogen neutralization and transdermal drug delivery. T. Kern, K.S. Lovejoy, M. Zakrewsky, M. Janicke, A. Newsham, M. Jones, S. Mitragotri, A.T. Koppisch, R.E. Del Sesto, **D.T. Fox**

BIOL **24.** Characterization and manipulation of acylase enzymatic activity of calreticulin using redesigned ligands. **A. Akinyemi**, **L. Larkin**, **W. Marsh**, L. Maynard

BIOL **25.** Structural biochemistry of a fungal LOV domain photoreceptor reveals an evolutionarily conserved pathway integrating blue-light and oxidative stress. **B.D. Zoltowski**, J. Lokhandwala

BIOL **26.** Identification of novel inhibitors of 6-phosphogluconate dehydrogenase (6PGDH) in *Trypanosoma brucei* through virtual drug screening. **V. Gomez**, K. Kolavasi

BIOL **27.** Detection of heavy metal ions using green fluorescent protein biosensors by quenching FRET from endogenous aromatic amino acids. **A. Beranek**, B. Hicks

BIOL **28.** Alternative ELISA using a RNA aptamer against calf intestinal alkaline phosphatase. **V.D. Huynh**, E. Wei, G.M. Stovall

BIOL **29.** Insights into the biochemical characterization of [FeFe]-hydrogenase Maturase HydF. **A. Byer**, J.B. Broderick

BIOL **30.** Benefits of being contained: The protection of nucleic acids inside prebiotic cell models. M. Joseph, D. Gifeisman, **S.E. Maurer**

BIOL **31.** Peptidomimetics as dual function antimicrobial and anti-inflammatory agents. **C. Smith**, J. Cai, H.H. Yin

BIOL **32.** Withdrawn.

BIOL **33.** Selective G-quadruplex DNA photocleavage agents: *N*-methyl-mesoporphyrin IX. **D. McBrayer**, M.L. Schoonover, S.M. Kerwin

BIOL **34.** mRNA expression of amino acid transporters in Eimeria tenella infected broilers. K. Miska, **J. Santiago-Feliciano**

BIOL **35.** H-loop and E-loop of human glutathione synthetase. **M.E. Anderson**, T.R. Cundari, B.L. Ingle

BIOL **36.** Chemical tools to study E3 ubiqutin ligases. **A. Statsyuk**, S. Park, D.T. Krist, S.G. Kathman, Z. Xu

BIOL **37.** Structural and functional studies of TSPO. **C.T. Nordyke**, N. Susanti, J. Sharpe, K. Varga

BIOL **38.** Engineering virus-like particles toward directing protective immunologic responses. **D. Patterson**, A. Rynda-Apple, A. Harmsen, T. Douglas

BIOL **39.** Biosynthetic studies on the antitumor antibiotic pactamycin. **C.J. Brumsted**, T. Mahmud, M.E. Abugreen

BIOL **40.** Withdrawn.

BIOL **41.** Studies toward the total synthesis of chrolactomycin and the development of novel small molecule telomerase inhibitors. **E.J. Lee**, K. Scheidt

BIOL **42.** Thermal stability and functional implications of short RNA strands containing 7,8-dihydro-8-hydroxyadenosine. **M.J. Resendiz**

BIOL **43.** Cellular response to sertraline, paroxetine, and fluoxetine of IMR-32 neuroblastoma cells in vitro. **M. Feuerstein**, M.L. Pajski

BIOL **44.** Development of new BF_2 azadipyrromethene near-infrared fluorochromes. **D. Wu**

BIOL **45.** Interaction of the antimicrobial peptide aurein 1.2 with lipid raft model membranes. **A. Alhewaitey**, A. Sunda-Meya, N. Phambu

BIOL **46.** Selectivity, cooperativity, and competition in the binding of heterocyclic diamidines to DNA. **S.A. Winkle**, A. Hassan, d. rodriguez, C. Vega, C. Winkle

BIOL **47.** Sequence and topological specificity in the binding of tetra(N-methylpyridyl) porphines to DNAs. S.A. Winkle, **A. Llodra**, J. Barretta, M. Ballester, R. Castillo, D. Edgar

BIOL **48.** Investigating the structural dynamics transitions of human adipocyte fatty acid binding protein by NMR spectroscopy. K. Ha, Y. Xia, Y. Tran, **A. Ojoawo**, G. Veglia, D. Bernlohr

BIOL **49.** Use of site-directed mutagenesis and cyanide binding studies to understand the oxygen sensing mechanism of the SmFixL protein, a member of the heme-PAS and histidine kinase families. **M.F. Reynolds**

BIOL **50.** What makes Lyme disease tick? Impact on DNA-protein interactions by mutations to regulator BosR. **S.E. Evans**, L. Evans

BIOL **51.** Structure and inhibition of acyl protein thioesterases. **K.J. Labby**, B.R. Martin

BIOL **52.** Characterization of the colanic acid biosynthesis pathway with a novel isoprenoid analog. **P. Scott**

BIOL **53.** Mutant firefly luciferases catalyze light emission with complementary synthetically modified luciferins. **M.A. Paley**, W.B. Porterfield, D.C. McCutcheon, R.C. Steinhardt, C.M. Rathbun, J.A. Prescher

BIOL **54.** Structural and functional characterization of the antifreeze protein ApAFP752. **K.W. Elliott**, S. Follett, P. Jevtic, D. Levy, K. Varga

BIOL **55.** Probing phagocytosis of Janus particles. **L. Sanchez**, Y. Yu

BIOL **56.** Synthesis and evaluation of substituted coumarin derivatives as inhibitors of monoamine oxidase B. **I. Kieffer**, E. Oduaran

BIOL **57.** Oxidation of α-crystallin Len protein resulting from xanthurenic acid radical. **C.N. Folluo**, C. Knuston, J.E. Roberts, B.E. Sturgeon

BIOL **58.** Lipoic acid organic nanoparticles (ONPs) for bacterial inhibition: Synthesis, characterization, and antibacterial studies of doped and undoped ONPs with Ag/Au NPs. **T. Pandiyan**, A. Pérez Jiménez, C. Huerta Aguilar, A. Romero Silva, J. Vázquez Ramos, J. Narayanan

BIOL **59.** Biochemical analyses of ATP binding and hydrolysis in DEAD-box proteins. **H. Englert**, I. Garcia

BIOL **60.** Blinking of quantum dot probes in measurements of molecular rotation on cell surfaces. **D. Zhang**, P. Winter, D. Roess, B. Barisas

BIOL **61.** Molecular dynamics studies of the role of protein flexibility in immunological molecular recognition. **C. Ayres**, D. Scott, B. Baker, S. Corcelli

BIOL **62.** Antimicrobial peptide and anisotropy. **S. Jocelin**, E.R. Middleton

BIOL **63.** Effect of cell treatment conditions on glutathione levels and cell viability. A.M. Khobeir, J. Shultz, J. Cali, **J. Kelts**

BIOL **64.** 2D Spectral-spatial rapid scan electron paramagnetic resonance imaging of spin trapped adducts at 250 MHz. **D.G. Mitchell**, J.R. Biller, S. Eaton, G.R. Eaton, G.M. Rosen, J.P. Kao

BIOL **65.** Structural and kinetic characterization of E. coli oxidoreductase YqhD. **J.M. Ellis**, R. Verma, J. Bann, K.R. Mitchell-Koch

BIOL **66.** Study and characterization of the sugar-modifying enzymes of the capsule biosynthesis pathway of *Vibrio vulnificus*. **J.M. Hazel**, K.M. Erickson, M.A. Chahoud, J.M. Troutman

BIOL **67.** Characterization of the C-terminal domain of CGI-112, a protein involved in the ER-associated degradation pathway. **K.R. Gallagher**, N. Bachman, S. Bolde, A. Rothfuss

BIOL **68.** Riboregulators as tunable gene switches for post-transcriptional control of gene expression. **M. Krishnamurthy**, S.P. Hennelly, K.Y. Sanbonmatsu, C.J. Unkefer

BIOL **69.** Ribosome-associated complex antagonizes prion formation in yeast. **A. van Ooy**, D. Cameron, A. Amor, D. Selechnik, S. Delaney, D. Castanzo

BIOL **70.** Magnetic field effects on charge transport through DNA. **T.J. Zwang**, S. Hurlimann, M.G. Hill, J.K. Barton

BIOL **71.** Identifying the direct effects of Mn^{2+}, Fe^{2+} and small molecule drugs on the iron responsive element in the human FTH1 IRE/IRP complex. **E.T. Mendenhall**, B. Wang, M.L. Norton, W.L. Patterson, M. Rahman, B.S. Day

BIOL **72.** Kinetic investigation of the active site base of recombinant F_{420}-dependent glucose-6-phosphate dehydrogenase from *Mycobacteria tuberculosis*. **M. Oyugi**, E. Joseph, K.L. Johnson-Winters

BIOL **73.** Design, synthesis, and protein crystallography of novel potent inhibitors of macrophage migration inhibitory factor. **J. Cisneros Trigo**, P. Dziedzic, M.J. Robertson, W.L. Jorgensen

BIOL **74.** Chemical modifications of catalytically important residues of enzyme lysyl oxidase. **E.J. Ste.Marie**, C. Gomes, C.D. Palmer, M. Zinter

BIOL **75.** Excess iron and copper induced alterations in microRNA expression as a new role for metals in neurodegeneration. **N.L. Iyer**, C. Hung, S.K. Szwed, K. Khanuja, **M.J. Sever**

BIOL **76.** Cytoskeletal protein analysis from *Tetrahymena thermophila* utilizing solution NMR studies and confocal microscopy. **R. Sterner**, J. Honts, A. Kilpatrick

BIOL **77.** Progress toward the synthesis and evaluation of luciferin derivatives for bioluminescene imaging. **I. Fields**, K.S. Huang, C. Miller

BIOL **78.** Profiling the role of galectin-9 in modulating the HA/CD44 interaction. **S.V. Durbin**, **R.G. Barkley**, **L.N. Jude**, A.M. Campbell, N.L. Snyder

BIOL **79.** Menaquinone biosynthesis: An antibacterial target? **J. Matarlo**, C. Evans, D.S. Tan, P.J. Tonge

BIOL **80.** Recycling histidine tagged thermophilic enzymes with magnetic beads. D. Finocchietti, J. Howland, **P. Woodruff**

BIOL **81.** KinExA-based immunosensor for measuring the salivary level of CA15-3: An efficient technology for diagnosis and management of breast cancer. **I. Darwish**, T. Wani

BIOL **82.** Nanoluciferase fragments as sensitive probes for protein solubility in living cells. **J. Zhao**, Q. Vu, T. Truong, T. Nelson, C. Stains

BIOL **83.** 2-Iminohydantoin, a mutagenic lesion, is a major oxidation product of 2'-deoxyguanosine with hydroxyl radical. **O. Alshykhly**, A.M. Fleming, C.J. Burrows

BIOL **84.** Fluorogenic chemical inducers of protein oligomerization. **B. Xu**, X. Zhou, C. Stains

BIOL **85.** Isolation and purification of *Entamoeba histolytica* alcohol dehydrogenase 2 (EhADH2) enzymatic activities and inhibition by pyrazoline derivatives. **J.A. Leitao**, **H. Kumar**, L. Rossi, D. Oduaran, A. Espinosa

BIOL **86.** Withdrawn.

BIOL **87.** Controlling the phosphoproteome: Ligand activated split-kinases. **M. M.E. Ghaffari**, K. Camacho-Soto, J. Castillo-Montoya, I. Ghosh

BIOL **88.** Disruption of insect isoprenoid biosynthesis with pyridinium bisphosphonates. S.E. Sen, **A. Jones**, T. Horsfield

BIOL **89.** Unique features of isoprenoid forming enzymes in moths: implications for the biosynthesis of homologous juvenile hormones. S.E. Sen, M. Grasso, J. Macor, L.M. Wood, R. Jacob, **A. Jones**, T. Horsfield, A. Tomasello, J. Hitchcock, M. Cusson

BIOL **90.** C-reactive protein conformational states alter biological reactivity. **C.L. Moon**, A.A. Alnaas, I. Roche, M.K. Knowles

BIOL **91.** Novel azo-stilbenes as photoresponsive chemical tools. C.N. Streu, M. Paterson, **Y. Yen**, K. Jensen, J. Jespersen, A.J. Engdahl, T. Scheckelhoff, T.S. Crum, A.D. Mesecar

BIOL **92.** Increasing thermo- and pH stability in carbonic anhydrase II for bioremediation purposes: A novel approach to industrial CO_2 sequestration. **V. Rasi**, B.P. Mahon, A.M. Hendon, C.D. Boone, R. McKenna

BIOL **93.** Cloning, expression, and characterization of bacterial enzymes with predicted structural similarity to mammalian cyclooxygenases. **B.S. Selinsky**, M. Butchy, S. Neumann, C. Nichols

BIOL **94.** Predicting membrane binding interface of peripheral proteins and beyond. **L. Zhang**, M. Rajendram, A. Yethiraj, D.B. Weibel, Q. Cui

BIOL **95.** Unraveling the slow onset inhibition of InhA, the enoyl ACP reductase from mycobacterium tuberbulosis: Mechanism and inhibitor design. **W. Yu**, H. Li, S. Eltschkner, L.A. Spagnuolo, A. Perryman, A. Chang, C. Kisker, P.J. Tonge

BIOL **96.** SialoPen: A new class of protease resistant membrane permeable peptides for intracellular biomolecule delivery. **E.M. Contreras**, A. Monreal, J.P. Saludes

BIOL **97.** Re(I) polypyridyl complexes in chemotherapy. **P. Ahuja**, F.M. MacDonnell

BIOL **98.** Connecting the global protein folding free energy and the heme affinity using the formal reduction potential of heme. **B.R. Gibney**

BIOL **99.** Hemostats that target hidden injuries. **M. Gkikas**, T. Mesar, R.K. Avery, G. Velmachos, B.D. Olsen

BIOL **100.** PLP proteomics: Probing and identifying of PLP-dependent proteins in bacteria. **Y. Liu, B. Shome**, D. Fedoseyenko, T.P. Begley

BIOL **101.** Hapalindole-linked welwitindolinone and ambiguine gene clusters from Stigonematalean cyanobacteria are delivering interesting chemistry via an unprecedented stereoselective halogenation of an sp^3-carbon by a freestanding enzyme encoded within *wel*. **M.L. Hillwig**, X. Liu

BIOL **102.** Compensatory kinetic effects of viscogen and crowding agent PEG8000 on the reaction of human uracil DNA glycosylase (hUNG). **A. Rodriguez**, S.L. Cravens, J.T. Stivers

BIOL **103.** Withdrawn.

BIOL **104.** Combination therapeutic nanoparticles for chemoresistant prostate cancer. **R. Pathak**, S. Dhar

BIOL **105.** Kinetic characterization and optimization of mechanism-based inhibitors of BioA. **C. Eiden**, C.C. Aldrich, J.D. Lipscomb

BIOL **106.** Differences in protein unfolding mechanisms revealed characterized in aqueous ionic liquid solutions. M.C. Miller, O.C. Fiebig, S.L. Hanna, M. Enriquez, G.A. Caputo, **T.D. Vaden**

BIOL **107.** Zinc fluxes in control of gamete maturation, cell cycle, and fertilization. **A.R. Bayer**, E.L. Que, F.E. Duncan, T.K. Woodruff, T.V. O'Halloran

BIOL **108.** SHH transcription factors Gli-1 and Gli-3R: Modulators of retina regeneration. **B.D. Center**, K. Barbosa, A. Luz-Madrigal, K. Del Rio-Tsonis

BIOL **109.** Mutation of yeast hexokinase I for structure-function analysis. G. Geibel, **J. Diaz**, E. Munk, W. Haggren, S.B. Braun-Sand

BIOL **110.** Structures of complexes of G-quadruplex DNA with drug like molecules. **H. Ranpura**, P.H. Bolton

BIOL **111.** Role of biochemical composition and extracellular polymeric substances on forward osmosis membrane fouling during algae separation. **W. Fang**

BIOL **112.** Identification of cellular targets in *Saccharomyces cerevisiae* of K20, an antifungal derived from kanamycin. **A. LeRoy**, J. Takemoto, C.T. Chang, D.N. Heaton

BIOL **113.** DNA-mediated redox signaling by UvrC. **M.A. Grodick**, R.M. Silva, A. Zhou, J.K. Barton

BIOL **114.** Structure of the periplasmic sensor domain of the histidine kinase CusS shows unusual metal ion coordination at the dimeric interface. **T. Affandi**, A.V. Issaian, S.A. Roberts, M.M. McEvoy

BIOL **115.** Synthesis of photoresponsive single stranded DNA aggregates via click chemistry. **S.K. Rastogi**, R. Gu, J. Lamas, X. Li, S. Zauscher, W.J. Brittain

BIOL **116.** Withdrawn.

BIOL **117.** Development of an electrochemical microRNA sensor. **J. Philippe**, S. MacArdle, M.C. Buzzeo

BIOL **118.** Electrochemical reactivity of selenocystine. **H. Wang**, E. Karnaukh, L.M. Walker, M.C. Buzzeo

BIOL **119.** Withdrawn.

BIOL **120.** Unraveling the dynamics of the EF1 hand upon Ca^{2+} binding in neurocalcin delta. **Y. Yang**, A. Krishnan, J. Viviano, V. Venkataraman

BIOL **121.** Alteration of the reaction profile of serine racemase via site-directed mutagenesis: Identification of an apparent "hotspot" with regard to reaction manifold. **D.L. Nelson**, G.A. Applegate, D.B. Berkowitz

BIOL **122.** Hydrogen-bonded Interaction of perfluorooctanoic acid with DNA. **D. Meng**, H. Zhang

BIOL **123.** Mechanistic investigation of hydrolytic decompositions of Roussin's black and Roussin's red salts in aqueous acidic and basic solutions. **T. Drummond**, P. Maragh, T. Dasgupta

BIOL **124.** Neuroprotective effect of Buyang Huanwu Decoction in ischemic stroke mice by proteomics study. H. Chen, Y. Shen, Y. Chen, **Y. Lin**

BIOL **125.** Seeing double: Evolution may utilize multiple parallel paths to optimize new protein folds. **T.N. Szyszka**, V. Kumirov, M. Cordes

BIOL **126.** Investigating the redox properties of human DNA primase. **E. O'Brien**, M. Holt, A. Ehlinger, W.J. Chazin, J.K. Barton

BIOL **127.** Peptide inhibitors of coagulation factor complex assembly. **N. Kastelowitz**, H.H. Yin

BIOL **128.** Functional characterization of a polyketide synthase (PKS) dehydratase domain using chemical probes. **Y. Li**, G. Dodge, R. Fecik, J. Smith, C.C. Aldrich

BIOL **129.** Electron transfer and DNA replication: Assessing the functional role of the yeast DNA polymerase δ $[4Fe\text{-}4S]^{2+}$ cluster. **P.L. Bartels**, J.L. Stodola, P.M. Burgers, J.K. Barton

BIOL **130.** Active site explorations of carotenoid oxygenases via integration of spectroscopy, crystallography, and enzymology. **E.R. Farquhar**, X. Sui, P. Kiser, M.P. Hendrich, K. Palczewski, M.R. Chance

BIOL **131.** Influence of the role of dehydroshikimate dehydrogenase in production of β-carboxymuconic acid from D-glucose using an *Escherichia coli* heterologous host. **G. Canales**, **K.B. Finney**, L. Harrington, R. Jha, K. Hotta, D. Fox, A.T. Koppisch

BIOL **132.** Ionic liquids as a matrix for delivery of chemically diverse antibiotics to bacterial biofilms. K.S. Lovejoy, **N.V. Warrington**, T. Kern, **K.L. Merrett**, P. Manchen, P. Phillips, K. Ong, N. Nieto, R.J. Vierling, C.L. Meyers, R.E. Del Sesto, D. Fox, A.T. Koppisch

BIOL **133.** Biological and mechanical properties of cartilage proteoglycans. **F. Horkay**, I. Horkayne Szakaly, E.K. Dimitriadis, I.L. Morgan, P.J. Basser

BIOL **134.** Highly selective RNA-based sensor for quick and easy detection of lead. **S. DasGupta**, J.A. Piccirilli

BIOL **135.** Fluorescence microspectroscopy assessment of the in vitro dimerization of BACE1-GFP fusion protein in cultured cells. **S. Gardeen**, J.L. Johnson, A.A. Heikal

BIOL **136.** Progress toward multisite incorporation of noncanonical amino acids into coat proteins of M13 bacteriophage. **D.G. Schwark**, M.A. Schmitt, **J.D. Fisk**

BIOL **137.** Posttranslational modification of tumor suppressor protein par-4. **W. Chen**, A.K. Swain, K. Ponniah, J. Ramchandani, M.M. Tomovic, M.S. Warden, S.M. Pascal

BIOL **138.** Protein photo-oxidation: The effects of singlet oxygen on protein function. **M.F. Eatwell**, J.D. Thoemke

BIOL **139.** Detection of enzyme activities with diamagnetic catalyCEST MRI contrast agents. **S. Sinharay**, J. Cardenas-Rodriguez, M. Pagel

BIOL **140.** Systematic engineering and synergistic binding of PEG-ylated ligands on phage for the detection of prostate cancer cells. **K. Mohan**, G.A. Weiss

BIOL **141.** Soybean lipoxygenase activity measured by lipid-coated gold nanoparticle biosensors. **Y. Cai**, S.M. Budy, S.M. Reed, M.K. Knowles

BIOL **142.** Novel biomarkers for HIV-1 disease progression. **T. Taylor**, A. Ghorpade, K. Borgmann, A. Pandya

BIOL **143.** Developing an enzymatic switch from HSV-thymidine kinase as a potential cancer therapeutic. **N. Shelat**, M.A. Ostermeier

BIOL **144.** Investigating the structural impact of the antimicrobial peptide combi-2 in model membranes. **B.M. Almarwani**, A. Sunda-Meya, N. Phambu

BIOL **145.** Optimal conditions for expression and purification of recombinant U-specific MC1 ribonuclease. **N.P. Lesner**, P.A. Limbach, B. Addepalli

BIOL **146.** Investigation into the energetic processes of peptide bond formation on prebiotic earth. **C.M. Nevin**, K. Cody, G. Hassell, T. Hughes, **D.F. Moriarty**, K.P. Rhoads, A. Weatherwax

BIOL **147.** Design of ionic liquid materials for transdermal delivery and pathogen neutralization. **R.E. Del Sesto**, D. Fox, A.T. Koppisch, A. Newsham, M. Jones, B. Hammontree, A. Palacios, K.S. Lovejoy, T. Kern, M. Zakrewsky, S. Mitragotri

BIOL **148.** Inhibiting β-ketoacyl acyl carrier protein synthases in *Staphylococcus aureus*. **C. Gu**, K. Kapilashrami, G.R. Bommineni, N. Nesbitt, P.J. Tonge

BIOL **149.** Reaction of Zn-proteome with diethylamine NONOate (DEA-NO): Measurement of labilized zinc by TSQ, Zinquin and FluoZin-3 is sensor dependent. **M. Karim**

BIOL **150.** Development and qualification of cell culture bioreactor scale-down models. **P. Yeung**, C. Okediadi, P. Lanter, B. Figueroa

BIOL **151.** Exploring the role of a distant domain dynamics on substrate binding of *Escherichia coli* prolyl-tRNA synthetase. **M.P. Mocol**, S. Bhattacharyay, S. Hati

BIOL **152.** Exploring the intrinsic dynamics of proteins involved in metabolic pathways using coarse-grained normal mode analysis. **R.D. McMunn**, S. Bhattacharyay, S. Hati

BIOL **153.** EGFR tyrosine kinase targeted compounds: Synthesis, in vitro antitumor activity, and molecular modeling studies of new series of benzothiazole and pyrimido[2,1-b]benzothiazole derivatives. **M. Gabr**, N. El Gohary, E. El Bendary, M. El Kerdawy

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‡ *Cooperative Cosponsorship*

BIOL **154.** Dynamic regulation of p97 ATPase activity by p37 and p47 is Impaired in pathogenic p97 IBMPFD/ALS mutants. **X. Zhang**, L. Gui, T. Chou, D. Wong, D. Moen

BIOL **155.** Calorimetric studies of therapeutic compounds binding to modified DNA. **R.E. McKnight**, L.T. Marr

BIOL **156.** Quantitative analysis of the cellular internalization of Engrailed-2 homeoprotein. **L. Molina**, L. Carlier, F. Burlina, O. Lequin, S. Sagan

BIOL **157.** Monitoring nanoparticle self-assembly using a bifurcated fluorescent aptamer. D. Marashi, T.A. Rogers, L. Jaeger, **W.W. Grabow**

BIOL **158.** Design, synthesis, and evaluation of small molecule probes for caspase-1. **C.E. Karver**, M. Kawarski, T. Hagerman

BIOL **159.** Structural and energetic determinants of adhesive binding specificity in type I cadherins. **H. Song**, J. Vendome, K. Felsovalyi, Z. Yang, W.L. Hubbell, L. Shapiro, B.H. Honig

BIOL **160.** Staphyloferrin B: Total synthesis, structure activity relationship studies, and bioactivity. **J. Lybaek Hoj Madsen**, E.M. Nolan

BIOL **161.** Building new protein mimics for siRNA delivery. **B.M. deRonde**, L.M. Minter, G.N. Tew

BIOL **162.** Small molecules as chemical biology probes of chlamydial effector molecules: Efforts toward the development of an antichlamydial therapeutic. **K. Alser**, D.G. McCafferty

BIOL **163.** Light harvesting DNA-protein biosensor. **M. Naganbabu**, M. Skwierczynski, M.P. Bruchez

BIOL **164.** Blue dyes: Blue-red tandem dyes as bright fluorogenic biosensors. **M. Naganbabu**, Y. Wang, J. Kurish, M.P. Bruchez

BIOL **165.** Interaction of pyrazinamide and structural analogs with reverse micelle membrane models. **B. Peters**, Z. Arhouma, F. Fontes, C. Morris, A. Pena, D. Crick, D.C. Crans

BIOL **166.** Sense codon reassignment: Toward multisite incorporation of multiple noncanonical amino acids. **W. Biddle**, M.A. Schmitt, J.D. Fisk

BIOL **167.** Thermodynamic determination of RNA duplex stability in magnesium solutions. **N. Meyer**, B. Znosko

BIOL **168.** Investigation of radiolabeled holo-intrinsic factor in the detection of the cubilin receptor. **J. Workinger**

BIOL **169.** Withdrawn.

BIOL **170.** Oxidation of p53 via DNA-mediated charge transport. **K.N. Schaefer**, W.M. Geil, J.K. Barton

BIOL **172.** Withdrawn.

BIOL **173.** New nucleoside antibiotics synthesis via an enzyme catalyzed amide-ester exchange reaction. **X. Liu**, S.G. Van Lanen, K.D. Green, S. Garneau-Tsodikova

BIOL **174.** Solution structure of a 2:1 complex of anticancer drug XR5944 with TFF1 estrogen response element: Insights into DNA recognition by a bis-intercalator. **C. Lin**, R.I. Mathad, N. Sidell, D. Yang

BIOL **175.** Understanding single-molecule protein dynamics with carbon nanocircuits. **M. Iftikhar**

BIOL **176.** Survival mechanism of blood typing IgM antibodies sorbed into paper. **L. Guan**, R. Cao, J. Tian, W. Shen

BIOL **177.** Determination of *trans*-resveratrol and its metabolites in rat serum and liver using liquid chromatography with high resolution time of flight-mass spectrometry. K. Kusler, **J. Rousova**, M. Leadbetter, D.S. Liyanage, N. Dongari, E. Sauter, A.V. Novikov, A. Kubatova

BIOL **178.** Buckminster fullerene effect on cytochrome P450 mediated metabolism. **C. Bostick**, T.S. Tracy, W.D. Tish, P.M. Gannett

BIOL **179.** Investigating the link between environmental exposure and dry eye syndrome. **A. Alhalwani**

BIOL **180.** Cr(VI) reduction by *Acinetobacter* sp. HK-1 with the assistance of a novel quinone/graphene oxide composite. **H. Zhang**, H. Lu

BIOL **181.** Examining the effect of 2-aminoanthracene exposure in Sprague Dawley dams from gestation through postnatal period. **S.L. Whitby**, D. Hunter, W. Yau, E.W. Howerth, W.E. Gato

BIOL **182.** DFT study elucidates proximal pocket hydrogen bond influence on mechanism of compound I formation in chloroperoxidase. **A.D. Pardillo**, O. Morozov, D.C. Chatfield

BIOL **183.** Concentration and time dependent accumulation of Creighton silver nanoparticles in Vero 76 cells. **S.A. Paluri**, N.H. Lam, I.E. Pavel Sizemore

BIOL **184.** O-GlcNAc modification blocks the aggregation and toxicity of the Parkinson's disease associated protein α-synuclein. **N.P. Marotta**, Y. Lin, B. Zaro, M.R. Pratt

BIOL **185.** Withdrawn.

BIOL **186.** Bioorthogonal approach to chemical virology. **S.M. Jensen**, J.C. Jewett

BIOL **187.** Highly potent and selective metalloinhibitors for SH3 domains based on rhodium(II) metallopeptides. **F. Vohidov**, Z.T. Ball

BIOL **188.** Streptomonomicin: An unusual lasso peptide antibiotic from the understudied halophilic actinomycete *Streptomonospora alba*. **J.I. Tietz**, M. Metelev, J.O. Melby, P.M. Blair, L. Zhu, I. Livnat, K. Severinov, D.A. Mitchell

BIOL **189.** Interaction between the antimicrobial peptide Leucrocin and model membranes. **A. Stone**, A. Sunda-Meya, N. Phambu

BIOL **190.** Characterization of the hexose-1-phosphate transferase from the *Vibrio vulnificus* capsular polysaccharide biosynthesis pathway. **K.M. Erickson**, M.A. Chahoud, J.M. Hazel, J. Troutman

BIOL **191.** Linking airborne biological particles and ice nuclei in a rural, marine environment near Ucluelet, British Columbia. **J. Li**, R. Mason

BIOL **192.** Site-specific protein-PEG-like/zwitterionic polymer conjugates by in situ atom transfer radical polymerization: A comparative study. S. Bhattacharjee, **X. Li**, W. Liu, A. Chilkoti

BIOL **193.** Structural characterization of the N-terminal domain of *Plasmodium falciparum* copper P-ATPase. **J. Kisaka**, D.L. Huffman

BIOL **194.** Promising thermostable alternative scaffold protein for M13 phage display. **N. Zhao**, M.A. Schmitt, J.D. Fisk

BIOL **195.** Withdrawn.

BIOL **196.** Improve blood typing performance within paper substrate through cellulosic network structure design. **L. Li**, X. Huang, W. Liu, W. Shen

BIOL **197.** In vitro model for measuring efficacy of GABAnergic medicines in the treatment of bipolar disorder by studying expression of the protein GAD_{67}. **S.N. Frank**, A. Jacoby

BIOL **198.** Novel G-quadruplex formed in the proximal P1 promoter of bcl-2 gene is a gene suppressor. **B. Onel**, M. Carver, D. Yang

BIOL **199.** Mechanistic Investigation of chelation-assisted copper-catalyzed click chemistry. **A. Tuley**, E. Vatansever, W. Liu

BIOL **200.** Role of proximal thiolate ligand in chloroperoxidase catalysis. **E. Shersher**, X. Wang, A. Bolhassani

BIOL **201.** Modified $p27^{KIP1}$ promoter-reporters in the context of cancer stem cells. **A.M. Cabreriza**, S.K. Szwed, L. Bouchez, M.J. Sever

BIOL **202.** How nature makes vitamin B_{12}; The last unsolved biosynthetic module. **D.J. Diaz**, S.H. Abdelwahed, T.P. Begley

BIOL **203.** Curacin biosynthesis: A model for unexpected dehydatase domain activity. **W. Fiers**, G. Dodge, R. Fecik, D.H. Sherman, J. Smith, C.C. Aldrich

BIOL **204.** Employing mass spectrometry: The proteomic discovery of chlamydomonas *reinhardtii's* nutritional metal metabolism. **D. Jarrett**, M. Miethke, D. Shirasaki, R.R. Loo, S.S. Merchant, J.A. Loo

BIOL **205.** Examination of latent structure in an intrinsically disordered protein and the thermodynamics of its binding to a target molecule. **A. Zidell**, S.A. Showalter

BIOL **206.** Chemical tools to study ubiquitin and ubiquitin-like activating E1 enzymes. **A.V. Statsyuk**, H. An

BIOL **207.** Azinomycin biosynthesis: Probing the mechanism of azabicycle biosynthesis. K. Nepal, S. Mori, D. Simkhada, V. Sharma, G.T. Kelly, C. Bryant, D. Delgado, Y. Rezenom, **C. Watanabe**

BIOL **208.** Discovery of lead macrocycle series from DNA-encoded libraries. **W. Connors**

BIOL **209.** Regulation of metabolic enzymes by lysine succinylation. **O.D. Nelson**, S. Sadhukhan, H. Lin

BIOL **210.** Study of iron metal oxides and metal-organic frameworks against Chinese hamster ovarian cell lines. **S. Bashir**, B. Martinez, X. Du, J.L. Liu

BIOL **211.** Synthesis, characterization, and antibacterial bioassay and molecular modeling studies of novel (E)-N-(5-chloro-2-(2-oxoazetidin-1-yl)benzylidene)benzohydrazide derivatives. **P. Tigulla**, P. Sureka, B. Ram, B. Balaram, V. Srinivasarao

BIOL **212.** Thiol-X reactions in action: Making oligonucleotide analogs in a click. **S. Pattanayak**, W. Xi, T. Gong, C.J. Kloxin, C. Bowman

BIOL **213.** Understanding catalytic outcome in a model monoterpene synthase: mutational analysis of (4*S*)-limonene synthase. **N. Srividya**, E.M. Davis, R.B. Croteau, B.M. Lange

BIOL **214.** Toward cellular and tissue selective inhibition of histone deacetylases (HDAC): Development of cellular- and isoform-selective HDAC probes. **P.A. Petukhov**, T. Hanigan, I. Kastrati, J. Frasor

BIOL **215.** Building a high definition breast tissue classifier: Applications in FT-IR histopathology. S. Leslie, **S. Mitttal**, D. Mayerich, A. Balla, R. Bhargava

BIOL **216.** Withdrawn.

BIOL **217.** Use of CRISPR-Cas 9 to develop a human embryonic stem cell line carrying the Trp64Arg mutation of the β3 adrenergic receptor. **J. Luna-Torres**

BIOL **218.** Examining the importance of backbone hydrogen bonding in the RGD-integrin interaction: Consequences for engineering degradable cell-adhesive biomaterials. **K. Eckes**, K. Baek, N.A. Hummell, L.J. Suggs

BIOL **219.** Discovery and characterization of human sORF-encoded polypeptides (SEPs). **J. Ma**, A. Saghatelian

Interfacial Biomolecular Recognition

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MONDAY MORNING

Section A

Hyatt Regency Denver at Colorado Convention Center

Capitol Ballroom 4

The Chemistry & Biology of Non-Natural Nucleic Acids

N. Richards, *Organizer, Presiding*

8:30 BIOL **220.** Exploring the sequence space from expanded genetic alphabets. L. Zhang, Z. Yang, K.M. Bradley, S. Hoshika, M. Kim, H. Kim, C. McLendon, C. Liu, W. Tan, **S.A. Benner**

9:15 BIOL **221.** Structural characterization of non-natural ZP base pairs in duplex DNA. **M.M. Georgiadis**, W.F. Kellett, I. Singh, S. Hoshika, S.A. Benner, N.G. Richards

10:00 BIOL **222.** Crystallization and structure of a functional riboswitch bearing an unnatural base pair. A. Hernandez, S. Hoshika, H. Kim, M. Kim, S.A. Benner, **J.A. Piccirilli**

10:45 BIOL **223. Award Address** (Nobel Laureate Signature Award for Graduate Education in Chemistry Sponsored by Avantor Performance Materials). Expansion of the genetic alphabet. **F.E. Romesberg**

MONDAY AFTERNOON

Section A

Hyatt Regency Denver at Colorado Convention Center

Capitol Ballroom 4

New Approaches to Investigating Chromatin Modifying Enzymes: Structure and Function

J. Meier, *Organizer, Presiding*

2:30 BIOL **224.** Protein methyltransferase inhibitors as personalized cancer therapeutics. **R. Copeland**

3:05 BIOL **225.** ChIP-less analysis of chromatin states and quantifying histone PTMs using data-independent acquisition mass spectrometry. Z. Su, K. Krautkramer, J. Dowell, **J. Denu**

3:40 BIOL **226.** Chemical probes to antagonize readers and writers methyl marks. **C. Arrowsmith**

4:15 BIOL **227.** Targeting MLL1 complex assembly for inhibition of H3K4 methyltransferase activity. **Y. Dou**

4:50 BIOL **228.** Unconventional chemical tools to interrogate protein methyltransferases. **M. Luo**

TUESDAY MORNING

Section A

Hyatt Regency Denver at Colorado Convention Center

Capitol Ballroom 4

Putting Chemical Biology in Context

Z. Gartner, *Organizer, Presiding*

8:30 BIOL **229.** Building small molecules to probe or perturb complex biological systems. **L.D. Lavis**

9:05 BIOL **230.** Chemistry-directed stem cell pluripotency and differentiation. **L.L. Kiessling**

9:40 BIOL **231.** Discovery of a class of endogenous mammalian lipids with antidiabetic and anti-inflammatory effects. **A. Saghatelian**, M.M. Yore, I. Syed, P.M. Moreas-Vieira, T. Zhang, M.A. Herman, E.A. Homan, J. Lee, S. Chen, O. Peroni, A. Hammarstedt, U. Smith, T.E. McGraw, B.B. Kahn

10:15 BIOL **232.** Nucleic acids as chemical probes of cell-cell interactions. **Z. Gartner**

10:50 BIOL **233.** Fluorogenic fluorescent probes reveal that the Hsp70-40-nucleotide exchange factor folding pathway hastens transthyretin folding and alters the resulting structure, rendering it more kinetically stable. X. Zhang, **J.W. Kelly**, A. Baranczak, P. Liu

Interfacial Biomolecular Recognition

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TUESDAY AFTERNOON

Section A

Hyatt Regency Denver at Colorado Convention Center

Capitol Ballroom 4

ACS Chemical Biology Award Symposium

L. L. Kiessling, *Organizer, Presiding*

2:30 BIOL **234.** Inositol pyrophosphates provide a link between metabolism and signaling. **D. Fiedler**

3:15 BIOL **235.** Chemical-proteomic strategies to investigate reactive cysteines. **E. Weerapana**

4:00 BIOL **236.** Use of chemical genetics to study mRNA splicing. **K.M. Shokat**

4:45 BIOL **237.** Engineering proteins for selective catalysis. H. Yang, C. Zhang, P. Srivastava, K. Ellis-Guardiola, **J.C. Lewis**

WEDNESDAY MORNING

Section A

Hyatt Regency Denver at Colorado Convention Center

Capitol Ballroom 4

In Vivo We Trust: Small Molecule Phenotypic Screening in Animals

R. Peterson, *Organizer, Presiding*

8:30 BIOL **238.** Reverse genetic analysis of restless legs syndrome in drosophila. N. Donelson, K. Trinh, **S. Sanyal**

9:00 BIOL **239.** Fly approach to cancer therapeutics. **R. Cagan**

9:30 BIOL **240.** Using *C. elegans* to identify novel small molecules that alter fat and feeding. **K. Ashrafi**

10:00 Intermission.

10:15 BIOL **241.** P7C3 and an unbiased approach to drug discovery for neurodegenerative diseases. **J. Ready**

10:45 BIOL **242.** Zebrafish screen identifies compounds that protect against chemotherapy-induced heart failure. Y. Liu, A. Asnani, L. Zou, V.L. Bentley, M. Yu, Y. Wang, G. Dellaire, K.S. Sarkar, H.H. Chen, D.E. Sosnovik, J.T. Shin, D.A. Haber, J.N. Berman, W. Chao, **R. Peterson**

11:15 BIOL **243.** Developmental vitamin D availability regulates hematopoietic stem cell production and expansion. M. Cortes, M. Chen, S.Y. Liu, W. Kwan, D.L. Stachura, T. Schlaeger, D. Traver, G.Q. Daley, W. Goessling, **T.E. North**

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WEDNESDAY AFTERNOON

Section A

Hyatt Regency Denver at Colorado Convention Center

Capitol Ballroom 4

Graduate Student & Postdoctoral Symposium

V. Bandarian, *Organizer, Presiding*

2:30 BIOL **244.** Novel genetic interactions with cell-envelope targeting antibiotics using ultrahigh density transposon libraries in *Staphylococcus aureus*. **M. Santiago**, T. Meredith, S. Walker

2:45 BIOL **245.** General approach to analysis of phosphatase activity in biological samples. J.R. Beck, **A. Lawrence**, A.S. Tung, E.N. Harris, C.I. Stains

3:00 BIOL **246.** Reconstitution and in-vitro activation of the prokaryotic pentameric ligand-gated ion channel ELIC. **O.S. Shafaat**, R. Rusinova, J.R. Winkler, O.S. Andersen, H.B. Gray, D.A. Dougherty

3:15 BIOL **247.** Nonenzymatic isomerization of acinetobactin, a siderophore from pathogenic *Acinetobacter baumannii*. **J.A. Shapiro**, T.A. Wencewicz

3:30 BIOL **248.** Controlling the phosphoproteome: Ligand-gated split-kinases and split-phosphatases. **J. Castillo-Montoya**, K. Camacho-Soto, B. Tye, L. Ogunleye, I. Ghosh

3:45 Intermission.

3:55 BIOL **249.** Dual small-molecule rheostat for precise control of protein concentration in mammalian cells. **Y. Lin**, M. Pratt

4:10 BIOL **250.** Repair of oxidized DNA in nucleosome core particles. **E.D. Olmon**, S. Delaney

4:25 BIOL **251.** Omics-based discovery of the rimosamides: A new class of nonribosomal peptide-polyketide hybrids. **R.A. McClure**, J.R. Doroghazi, A.W. Goering, Y. Chen, W.W. Metcalf, R.J. Thomson, N.L. Kelleher

4:55 BIOL **252.** Withdrawn.

Interfacial Biomolecular Recognition

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BMGT

Division of Business Development and Management

K. Allen and J. L. Bryant, *Program Chairs*

OTHER SYMPOSIA OF INTEREST:

Industrial Innovations in Polymer Chemistry *(see POLY, Mon)*

Best Practices for Success with SBIR & STTR Grants *(see SCHB, Sun)*

Kathryn C. Hach Award for Entrepreneurial Success: Symposium in Honor of Terry L. Brewer *(see SCHB, Mon)*

Chemical Angel Network: Chemists Investing in Chemical Companies *(see PROF, Mon)*

Chemical Tales of Success: Helpful Tips for Younger Chemists *(see YCC, Tue)*

SOCIAL EVENTS:

Reception: PNNL 50th Anniversary Reception 5:00 PM: Sun

Reception and Book Signing: Award for Industrial Chemistry 5:30 PM: Mon

MONDAY MORNING

Section A

Embassy Suites Denver–Downtown Convention Center

Crystal Ballroom B/C

ACS Award in Industrial Chemistry: Symposium in Honor of Thomas J. Colacot

Cosponsored by ANYL and I&EC

J. L. Bryant, *Organizer*

S. Chandrasekaran, *Presiding*

8:00 Introductory Remarks.

8:05 BMGT **1.** Metal-mediated and metal-catalyzed coupling for incorporation of fluorine into aromatic molecules. **J.F. Hartwig**

8:35 BMGT **2.** Metal catalyzed carbohalogenation reactions through reversible oxidative addition. **M. Lautens**

9:05 BMGT **3.** Understanding and design of organopalladium reactivity with experimental and computational tools. **F. Schoenebeck**

9:35 Intermission.

9:43 Remarks.

9:45 BMGT **4.** Carbon-carbon and carbon-heteroatom bond forming reactions in continuous flow. **T. Noël**

10:30 BMGT **5.** Applications of Pd and Ni catalysis to Pfizer's portfolio. **J. Magano**

11:00 BMGT **6.** Cross-coupling without redox changes at the metal – enantioselective eterodimerization of alkenes. **T. RajanBabu**

11:30 BMGT **7.** Asymmetric C-C bond formation in outer sphere Pd catalyzed processes. **B.M. Trost**

MONDAY AFTERNOON

Section A

Embassy Suites Denver–Downtown Convention Center

Crystal Ballroom B/C

ACS Award in Industrial Chemistry: Symposium in Honor of Thomas J. Colacot

Cosponsored by ANYL and I&EC

J. L. Bryant, *Organizer*

J. A. Gladysz, *Presiding*

1:15 Introduction of Plenary Address.

1:25 BMGT **8.** On the magical power of d-block transition metals as exemplified by ZACA (Zr-catalyzed asymmetric carboalumination of alkenes) – lipase-catalyzed acetylation – transition metal-catalyzed cross-coupling for highly enantioselective synthesis of various types of chiral organic compounds. **E. Negishi**, S. Xu, A. Oda, Y. Matsueda, H. Li, T.P. Bobinski

2:15 Intermission.

2:30 BMGT **9.** Photoinduced, copper-catalyzed coupling reaction. **G.C. Fu**

3:00 BMGT **10.** Connecting directed *ortho* metalation – transition metal catalyzed chemistries. **V.A. Snieckus**

3:30 BMGT **11.** Important catalytic transformations for drug development. **C. H. Senanayake**

4:00 BMGT **12.** ppm-Level Pd-catalyzed cross-couplings in water at room temperature. **B. H. Lipshutz**

4:30 Introductory Remarks of Award Recipient.

4:40 BMGT **13. Award Address** (ACS Award in Industrial Chemistry sponsored by the ACS Division of Business Development & Management and the ACS Division of Industrial & Engineering Chemistry). Story of Pd-catalyzed coupling: The reactions of the 21st century. **T. Colacot**

5:25 Concluding Remarks.

Innovations in Macromolecular Network Chemistry

Industrial Innovations in Polymer Chemistry

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CARB

Division of Carbohydrate Chemistry

E. Rozners, *Program Chair*

OTHER SYMPOSIA OF INTEREST:

Frontiers in Glycoscience *(see CELL, Mon, Tue)*

Ronald Breslow Award for Achievement in Biomimetic Chemistry *(see ORGN, Sun)*

Cellulose in Solid State and Solution - Structure, Chemistry and Reaction Mechanisms *(see CELL, Sun, Mon, Tue, Wed)*

ACS Chemical Biology Award Symposium *(see BIOL, Tue)*

Application of Computational Chemistry to Biomass Chemistry and Utilization *(see CELL, Sun, Mon)*

The Chemistry & Biology of Non-Natural Nucleic Acids *(see BIOL, Mon)*

BUSINESS MEETINGS:

Business Meeting, 5:00 PM: Sun

SUNDAY MORNING

Section A

Colorado Convention Center

Mile High Ballroom 1C

Wolfrom Award Symposium

N. L. Pohl, E. Rozners, *Organizers*

J. C. Paulson, *Presiding*

9:30 CARB **1.** Building on Wolfrom's legacy: From the Chemurgy of yesterday to the renewables of today. **K.B. Hicks**, A.A. Boateng, C.A. Mullen, Y. Elkasabi, A.T. Hotchkiss, M.P. Yadav

10:10 CARB **2.** Cranberries: From polyphenols to polysaccharides. **C. Khoo**

10:50 CARB **3.** Bioactive pectic oligosaccharides. **A.T. Hotchkiss**

SUNDAY AFTERNOON

Section A

Colorado Convention Center

Mile High Ballroom 1C

Isbell Award and Gin New Investigator Award Symposium

N. L. Pohl, E. Rozners, *Organizers*

J. C. Paulson, *Presiding*

1:00 CARB **4.** Recent studies on the synthesis of glycans from mycobacteria and campylobacters. **T.L. Lowary**

1:30 CARB **5.** Synthesis of heparan sulfate oligosaccharides and glycopeptide. **X. Huang**, S.B. Dulaney, Y. Xu, K. Yoshida, B. Yang, W. Yang, J. Liu

2:00 CARB **6.** Therapeutic in vivo synthesis by glycocarriers. **K. Tanaka**

2:30 Intermission.

2:50 CARB **7.** Split personality of human O-GlcNAc transferase. **S. Walker**

3:20 CARB **8.** Photocrosslinking approach to discover O-GlcNAc-interacting proteins. A. Rodriguez, S. Yu, B. Li, **J.J. Kohler**

3:50 CARB **9.** Chemical probes for the functional analysis of O-GlcNAc modifications. **M. Pratt**

MONDAY MORNING

Section A

Colorado Convention Center

Mile High Ballroom 1C

Glycomimetic Compounds: An Untapped Source of Novel Therapeutics

J. Magnani, *Organizer, Presiding*

9:00 CARB **10.** Hexosamine mimetics designed to reverse the Warburg Effect. **K.J. Yarema**

9:30 CARB **11.** Selectin antagonists: Acyclic tethers with a define conformational bias. **Y. Guindon**, C. Mickael, G. Tambutet, M. Prévost

10:00 CARB **12.** Toward the development of selective DC-SIGN antagonists. **A. Bernardi**

10:30 Intermission.

11:00 CARB **13.** Design and discovery of GMI 1070 (Rivipansel), a novel pan-selectin antagonist for the treatment of vaso-occlusive crisis in sickle cell disease. **J.M. Peterson**, A. Sarkar, J.T. Patton, M. Rahman, N. Karasanyi, B. Ernst, J.L. Magnani

11:30 CARB **14.** New NMR tools for unraveling the conformation, dynamics, and recognition properties of glycomimetics. **J. Jimenez-Barbero**

MONDAY AFTERNOON

Section A

Colorado Convention Center

Mile High Ballroom 1C

Glycomimetic Compounds: An Untapped Source of Novel Therapeutics

J. Magnani, *Organizer, Presiding*

1:30 CARB **15.** Galectin-ligand analogs and mimetics in intracellular vesicle damage and in angiogenesis. **U.J. Nilsson**, H. Leffler, N. Panjwani

2:00 CARB **16.** Druggability of lectins, using the example of a bacterial adhesin. **B. Ernst**, P. Frei, J. Bezencon, D. Eris, S. Rabbani, P. Zihlmann, R. Preston, B. Fiege

2:30 CARB **17.** Well-defined antibody-drug conjugates (ADCs) through site-specific conjugation. **G. Boons**

3:00 Intermission.

3:30 CARB **18.** Isoform selective inhibition of tumor-associated carbonic anhydrase IX using carbohydrate-based sulfamates for the treatment of several cancers. **B. P. Mahon**, J. Ladwig, L. Bornaghi, D. Vullo, S. Poulsen, C.T. Supuran, R. McKenna

4:00 CARB **19.** Synthesis and properties of polyfluorinated carbohydrates. **B. J. Linclau**

‡ *Cooperative Cosponsorship*

4:30 CARB **20.** Computational design of glycomimetic inhibitors — prospects and limitations. **M. Frank**, P. Nyholm

MONDAY EVENING

Section A

Colorado Convention Center
Halls C/D

Sci-Mix

E. Rozners, *Organizer*

8:00 - 10:00

32-33, 35-38, 43, 45-49, 51-52, 57- 60, 62. See subsequent listings.

TUESDAY MORNING

Section A

Colorado Convention Center
Mile High Ballroom 1C

Protein Glycosylation: Simulation, Synthesis, Characterization & Application

G. Beckham, *Organizer*
Z. Tan, *Organizer, Presiding*

9:15 CARB **21.** Sugars and proteins: Building glycoproteins. **B.G. Davis**

9:40 Discussion.

9:45 CARB **22.** New tools in glycoprotein chemical synthesis. **X. Li**

10:10 Discussion.

10:15 CARB **23.** Synthesis of homogeneous glycoproteins and application to biochemical studies and biosimilar comparability analysis. **T.J. Tolbert**

10:40 Discussion.

10:45 Intermission.

11:05 CARB **24.** Site-specific investigation of O-GlcNAc modifications using synthetic proteins. **M. Pratt**

11:30 Discussion.

11:35 CARB **25.** Chemical synthesis as a tool to study protein glycosylation. **Z. Tan**, X. Guan

12:00 Discussion.

TUESDAY AFTERNOON

Section A

Colorado Convention Center
Mile High Ballroom 1C

Protein Glycosylation: Simulation, Synthesis, Characterization & Application

Z. Tan, *Organizer*
G. Beckham, *Organizer, Presiding*

1:45 CARB **26.** Intracellular traffic of cell surface mimetic quantum dots-anchored glycopeptides. **S. Nishimura**, R. S. Tan, K. Naruchi, M. Amano, H. Hinou

2:10 Discussion.

2:15 CARB **27.** Protein glycosylation in the baculovirus-insect cell system. **D. L. Jarvis**

2:40 Discussion.

2:45 CARB **28.** Manipulating protein stability by glycosylation. **Y. Levy**

3:10 Discussion.

3:15 Intermission.

3:35 CARB **29.** Impact of glycosylation upon protein conformational tendencies. **W. G. Noid**

4:00 Discussion.

4:05 CARB **30.** Computational study of glycosylphosphatidyl-Inositol (GPI) anchor fragments embedded in phospholipid membranes. M. Wehle, R. Lipowsky, P.H. Seeberger, G. Brezesinski, C. Stefaniu, D. Varon-Silva, **M. Santer**

4:30 Discussion.

TUESDAY EVENING

Section A

Colorado Convention Center
Hall C

General Posters

E. Rozners, *Organizer*

7:00 - 9:00

CARB **31.** Withdrawn.

CARB **32.** Synthesis and antibacterial activity of antibiotic-functionalized graphite nanofibers. **R. M. Giuliano**, M. Rotella, A. Briegel, J. Hull, A.F. Lagalante

CARB **33.** Encapsulation and release of an active enzyme utilizing cobalt crosslinked chitosan nanoparticles. **J.B. Lampe**, G. Castillo, C.S. Morrison, D. Nguyen, R.J. Cavazos, R.A. Petros

CARB **34.** Reduction of flammability of cotton fabrics treated with phosphoryl piperazine derivatives. **T. Nguyen**, S. Chang, B. Condon, R. Slopek, E. Graves

CARB **35.** Synthesis of hyaluronic acid-based phototherapeutics. **R. A. Guerrieri**, **E. Xu**, R. D. Dolewski, R.G. Barkley, J.V. Ruppel, N.L. Snyder

CARB **36.** Synthesis of meso-substituted carbohydrate porphyrin and carbohydrate bacteriochlorin conjugates. **G.T. Mukosera**, R.D. Dolewski, J.V. Ruppel, N.L. Snyder

CARB **37.** Progress on the total synthesis of *Aspergillus fumigatus* galactosylaminoglycans for diagnostic and therapeutic applications. **E.J. Baker**, N.L. Snyder

CARB **38.** Progress on the synthesis of *N*-acetyllactosamine (LacNAc) probes for studying binding differences carbohydrate recognition domains of galectins-1, -3 and -9. **C. Tao**, N.L. Snyder

CARB **39.** Carbohydrate-based small molecules with immunostimulatory properties. **C.E. Marzabadi**, V. Basava, C. Bitsaktsis, E. Hanawa

CARB **40.** Synthesis of wooden based resource derived furanic diol and polymerization of PU via various isocyanate. **B. Kim**, S. Kim, J. Cho

CARB **41.** Selective hydrogenation of biomass-derived sugars using supported Ru nanoparticles based catalysts. **J. Hwang**, A.A. Dabbawala

CARB **42.** Hydrothermal treatment of eucalyptus using acidic ionic liquid as catalysis toward a biorefinery concept. **J. Xu**, R. Sun

CARB **43.** Carbohydrate polymer-coating chemistry for cellulose based bioassays. **R. Cao**, L. Guan, M. Li, W. Shen

CARB **44.** Synthesis of fluorogenic probes for selective biomass degradation by fungi. **Q. Zhang**, X. Peng, M. Grilley, J. Takemoto, C.T. Chang

CARB **45.** Synthesis and stability study of DNA duplexes with 1'-carboxamide residues. **W. Dong**, S.A. Woski

CARB **46.** Semisynthetic approach to cancer vaccines utilizing mimetics of natural and unnatural Tn antigens. **S. Nishat**, A.A. Shaik, P.R. Andreana

CARB **47.** Chemical synthesis and *O*-glycosidic linkage conformation in a ^{13}C-labeled βMan(1→4)βXyl(1→4)βMan(1→4)βXylOCH3 tetrasaccharide: Effects of linkage structure and context. **W. Zhang**, A.S. Serianni

CARB **48.** Quantitative evaluation of D-galactose–lectin binding properties via development of diversely presented carbohydrate surfaces. **B. Meng**, K. Tscherch, M.D. Best, D.C. Baker

CARB **49.** Lipase-mediated modification of peracylated macrolactonic sophorolipids. **A. Sembayeva**, J.A. Carr

CARB **50.** Optimization of autohydrolysis of bamboo for the production of low-DP xylo-oligosaccharides using response surface methodology. **X. Xiao**, J. Bian

CARB **51.** Facile synthesis of nested fragments of high-mannose *N*-glycans with lightly protected glycosyl acceptors. **Q. Pan**, S. Zhao, W. Zhang, Z. Zhang, A.S. Serianni

CARB **52.** Synthesis of 2-amino sugar building blocks and application for glycodiversification studies. C.M. Rojas, **A. Brown**, **G. Ezeude**, M. Miller, A. Scharnow, A. Oviatt

CARB **53.** Novel catalytic approach for the regioselective oxidation of carbohydrates under mild conditions. **W. Muramatsu**

CARB **54.** Using potatoes as a carbohydrate based additive in road salt. **R. Byrnes**, D. Szlosek, G. Smith, J. Walters, R. Tanous, D.A. Arris

CARB **55.** Amide-linked RNA: Synthesis, structure, and RNA interference activity. **E. Rozners**, D. Mutisya, C. Selvam, P. Tanui, B.D. Lunstad, S.D. Kennedy, P.S. Pallan, A. Haas, D. Leake, M. Egli

CARB **56.** Modification of glucose for targeted cellular delivery. H. Jacobs, **Z.J. Witczak**

CARB **57.** Targeted study of bacterial glycoproteins using metabolic oligosaccharide engineering. D.H. Dube, **E. Clark**

CARB **58.** Development of a cyclooctyne-based photodynamic antibiotic for targeting *Helicobacter pylori*'s surface sugars. D.H. Dube, **I. Kline**

CARB **59.** Analysis of *Helicobacter pylori* strains deficient in protein glycosylation. D.H. Dube, **S. Mikami**, H. Carol

CARB **60.** Synthesis of chitosan beads enclosed magnetic Fe_3O_4 nanoparticles endorsed several applications from environmental remediation to bio-nanocomposite integration in biomedicine interdisciplinary fields. **V. Fernandez-Alos**, A. Padilla, **C. Castro-Alvarado**, F.R. Roman

CARB **61.** Hybrid ceramide–gypsogenin triterpene saponin as a vaccine adjuvant. **V. Pathak**, A.K. Pathak

CARB **62.** Cell-surface engineering with biomimetic materials: Mucins and the cancer glycocalyx. **J. Kramer**, C.R. Bertozzi

CARB **63.** Structural characterization of a newly discovered trisaccharide in banana fruit ethanol extract. **M.A. Madson**

CARB **64.** Effect of conjugation and microwave treatment on structure and functional characteristics of gum karaya (*Sterculia urens*). **H. Mirhosseini**, E. Shekarforoush

CARB **65.** Synthesis, characterization, and application of soy protein flour-based additive to increase the dry strength of recycled and virgin paper furnish. **A. Salam**, L. Lucia, H. Jameel

CARB **66.** Structural insight into glycosylated human Notch1 EGF12 analogs. **S. Hayakawa**, H. Hinou, S. Nishimura

CARB **67.** Metabolism of four metabolic chemical reporters and their relative selectivity for different glycoproteins. **A. Batt**, M. Pratt

CARB **68.** Changes in metabolic chemical reporter structure yield a selective probe of O-GlcNAc modification. **K.N. Chuh**

CARB **69.** Efficient method for the incorporation of molecular probes at multiple/specific sites in RNA: Levulinyl protection for 2'-ACE®, 5'-silyl oligoribonucleotide synthesis. **M.O. Delaney**

CARB **70.** Aldehyde bearing triterpene saponins as vaccine adjuvants. V. Pathak, **A. K. Pathak**

CARB **71.** Xanthan: Conformation, degradation, and hydrophobic modification. I. Jenssen, A. Ulset, H. Schols, A. Roy, F. Renou, **B. Christensen**

CARB **72.** Alkali pretreatment of cellulose I to cellulose II with thiourea as an additive. **V. Uniyal**, P. Gupta, S. Naithani

CARB **73.** Immunomodulation of the linear b-(1,3)-glucan fr*Saccharomyces cerevisiae* through activation of mitogen-activated protein kinases and nuclear factor-kB in murine RAW264.7 macrophages. **X. Xu**

CARB **74.** *O*-mannosylated glycan induced conformational alteration of α-dystroglycan fragment. **H. Hinou**, S. Nishimura

CARB **75.** Efficient and α-selective glycosylation using 3-iodo Kdo (3-deoxy-D-*manno*-oct-2-ulosonic acid) fluoride donors. **B. Pokorny**, P. Kosma

CATL

Division of Catalysis Science and Technology

V. Schwartz, *Program Chair*

OTHER SYMPOSIA OF INTEREST:

E.V. Murphree Award in Industrial & Engineering Chemistry: Symposium in Honor of Joseph R. Zoeller *(see I&EC, Tue)*
Computational Pyrolysis and Upgrading of Bio-oils *(see COMP, Wed)*
ENFL Distinguished Researcher Award: Symposium in Honor of James Burrington *(see ENFL, Mon, Tue)*
Catalysis for Unconventional Energy Sources *(see ENFL, Sun, Mon)*
C1 Catalytic Chemistry *(see ENFL, Tue, Wed)*
Elucidation of Mechanisms & Kinetics on Surfaces *(see COLL, Wed)*

SUNDAY MORNING

Section A

Colorado Convention Center
Room 107

Electrocatalysis and Photocatalysis

Electrocatalysis

S. Ren, *Organizer*
K. Leonard, *Organizer, Presiding*

8:40 CATL **1.** Anodized silver plate electrode for carbon dioxide reduction. **L.Q. Zhou**, C. Ling, H. Jia

9:00 CATL **2.** Nanostructured Zn electrodes for electrochemical carbon dioxide reduction. **J. Rosen**, F. Jiao

9:20 CATL **3.** Mechanistic analysis of electrochemical oxygen reduction and development of economical silver alloy catalysts for low temperature fuel cells. **A. Holewinski**, S. Linic

9:40 Intermission.

10:00 CATL **4.** Molecular catalyst for water oxidation that binds to metal oxide surfaces and exhibits high activity without ligand degradation. **G.W. Brudvig**, S.W. Sheehan, J. Thomsen, U. Hintermair, R.H. Crabtree, C.A. Schmuttenmaer

10:40 CATL **5.** Synthesis of a fibrous MnOx catalytic film on FTO by dual-session cyclic voltammetry. **H. Yuan**, R.Y. Ofoli

11:00 CATL **6.** Mechanistic insight into water reduction provided by labile ligand variation at Rh(III) in Ru(II),Rh(III),Ru(II) supramolecular photocatalysts. **H.M. Rogers**, K.S. Brewer

11:20 CATL **7.** Perfluorinated phthalocyanines and other ligands for efficient co-catalyzed electrooxidation of water. **V.O. Rodionov**, N. Morlanes, B. Chen, K. Takanabe

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11:40 CATL **8.** Exploring earth-abundant chalcogenides and phosphides for catalytic hydrogen generation from water. **Y. Sun**

Section B

Colorado Convention Center
Room 109

Theoretical and Experimental Synergies at the Frontiers of Renewable Energy Catalysis

Challenges and Opportunities for Renewable Energy Catalysis

J. A. Keith, A. J. Morris, *Organizers, Presiding*

8:30 Introductory Remarks.

8:40 CATL **9.** Learning from nature how to make solar fuels. **G.W. Brudvig**

9:10 CATL **10.** Solar fuels: Thermodynamics, candidates, tactics, and figures of merit. **S. Bernhard**, A.C. Brooks, M. Li, H.N. Kagalwala, D.N. Chirdon

9:40 CATL **11.** Wavefunction embedding methods for the study of renewable energy catalysis. **T.F. Miller**

10:10 Intermission.

10:30 CATL **12.** Withdrawn.

10:50 CATL **13.** Theoretical modeling of excited-state processes for renewable energy: What do we need to make an impact? **A. Krylov**

11:20 CATL **14.** Decoding the zeolite genome and its application in understanding the active sites in the selective catalytic reduction of NO_x using NH_3 in Cu-SSZ13. **F. Goeltl**, R. Bulo, I. Hermans, P. Sautet

Section C

Colorado Convention Center
Room 111

New Catalysis Through Ligand Design

Energy and Catalysis

Financially supported by RSC Journal of Chemical Science

J. S. Figueroa, *Organizer*
A. S. Veige, *Organizer, Presiding*

8:10 Introductory Remarks.

8:12 CATL **15.** From light-triggered hydride transfer to photo(electro)catalysis. **A.J. Miller**, C.L. Pitman, S.M. Barrett, K.R. Brereton, S.A. Slattery, R.L. McCoy

8:34 CATL **16.** Water splitting with cobalt and nickel complexes: Core vs. ligand design. F. Evangelisti, R. Moré, F. Hodel, S. Luber, **G.R. Patzke**

8:56 CATL **17.** New ligands for multifunctional bimetallic catalysts. **B.M. Cossairt**, S. Flowers, D. Henckel

9:18 CATL **18.** Small molecule activation by platinum complexes containing bulky tin groups. **B. Captain**, A. Koppaka, L. Zhu, V. Yempally, G.C. Fortman, D. Isrow, C.D. Hoff

9:40 CATL **19.** Oxazolinylborate metal compounds and catalysis. **A.D. Sadow**

10:02 Intermission.

10:17 CATL **20.** Closing a cycle: Silver-heteroatom bonds in the heterolysis of dihydrogen. **J.P. Sadighi**, B. Tate, J.T. Nguyen, J. Bacsa, A.D. Royappa

10:39 CATL **21.** Nucleophilic CH activation of benzene and methane with Rh and Ir complexes in strongly basic solvents. **B.G. Hashiguchi**, M.M. Konnick, R.A. Periana

11:01 CATL **22.** Pincer ligand variations in catalysis of dehydrogenative borylation of terminal alkynes. **O. Ozerov**, C. Lee, J. Zhou, N. Bhuvanesh

11:23 CATL **23.** Improved catalysts for the telomerization of butadiene with methanol. J. Briggs, J. Klinkenberg, J. Patton, H. Launay, M. Van Engelen, H. Hagen, **D.C. Rosenfeld**

11:45 CATL **24.** Hemilabile N,O-chelating ligands: Dynamic coordination modes for promoting reactivity and hydroaminoalkylation catalysis. **L. Schafer**, E. Chong, J. Lauzon, M.W. Drover

Section D

Colorado Convention Center
Room 108

Symposium in Honor of Jens Rostrup-Nielsen

J. Hansen, *Organizer*
B. H. Davis, *Organizer, Presiding*

8:10 Introductory Remarks.

8:15 CATL **25.** Review of patent literature relating to synthesis gas production and Fischer-Tropsch tail gas processing aimed at the cost effective enhancement of the GTL process efficiency. **A.P. Steynberg**

8:50 CATL **26.** Branching pattern in Fischer-Tropsch synthesis. **H. Schulz**

9:25 CATL **27.** Improving Pt/zirconia WGS catalysts through doping by Y and electronic promotion with Na. **G. Jacobs**, M. Martinelli, W.D. Shafer, U. Graham, B.H. Davis

10:00 Intermission.

10:15 CATL **28.** Sulfur passivated reforming for production of syngas with low H_2/CO ratio. **N.R. Udengaard**

10:50 CATL **29.** Catalytic aspects of fuel processing for fuel cells and power to gas. **J.B. Hansen**

11:25 CATL **30.** First-principles study of Co-based catalysts for syngas conversion. **W. Li**

Catalysis for Un-conventional Energy Sources

Fuel Cell, Solar Cell and Solar Fuel

Sponsored by ENFL, Cosponsored by CATL and MPPG‡

SUNDAY AFTERNOON

Section A

Colorado Convention Center
Room 107

Electrocatalysis and Photocatalysis

Photocatalysis

S. Ren, *Organizer*
K. Leonard, *Organizer, Presiding*

1:30 CATL **31.** Using photoelectrochemistry to investigate visible light active photocatalytic materials. **J. Byrne**, J.W. Hamilton

1:50 CATL **32.** ZnO-SnO_2 photocatalyst: An in-depth study on morphologies affect on photocatalytic activity. **D.A. Ramirez**, L. Hope-Weeks

2:10 CATL **33.** Investigations of the role of surface metal catalysis and near surface nonmetal dopants in the photocatalytic activity of TiO2. **C. Muhich**, Y. Zhou, J.Y. Westcott, A. Holder, A.W. Weimer, C. Musgrave

2:30 CATL **34.** Synthesis and limits of *p*-$CuBi_2O_4$ nanocrystals as visible light photocatalyst for hydrogen evolution from water. **G. Sharma**, J. Wang, F.E. Osterloh

2:50 Intermission.

3:10 CATL **35.** Electrochemical synthesis of ternary oxide photoelectrodes for use in solar water splitting. T. Kim, D. Kang, **K. Choi**

3:50 CATL **36.** Nanohybrids based on semiconductors and Co_3O_4 or semiconductors/photosensitizers for photoassisted water oxidation and fuel generation. **O. Yehezkeli**, D. de Oliveira, A. Harguindey, J. Cha

4:10 CATL **37.** Charge carrier dynamics of photoexcited Co_3O_4 in methanol: Extending high harmonic transient absorption spectroscopy to liquid environments. **L. Baker**, C. Jiang, S.T. Kelly, J.M. Lucas, J. Vura-Weis, M.K. Gilles, P. Alivisatos, S.R. Leone

4:30 CATL **38.** Can we accurately model the key electronic properties of semiconductors for photocatalysis? **P. Sautet**, T. Le Bahers, M. Harb, K. Takanabe

4:50 CATL **39.** Overall photocatalytic water splitting using small organic shuttles. **J. Sommers**, N. Alderman, C.J. Viasus, C.H. Wang, S. Gambarotta

Section B

Colorado Convention Center
Room 109

Theoretical and Experimental Synergies at the Frontiers of Renewable Energy Catalysis

Challenges and Opportunities for Renewable Energy Catalysis

J. A. Keith, A. J. Morris, *Organizers, Presiding*

1:30 Introductory Remarks.

1:40 CATL **40.** New strategies for catalytic process design: Oxidative methane coupling with soft oxidants. **T.J. Marks**, M. Peter

2:10 CATL **41.** Mechanistic insights into catalytic conversion methane over supported catalysts. **M. Neurock**

2:40 CATL **42.** Significance of catalyst/support interactions for Pt nanoparticles on amorphous silica supports using density functional theory. C. Ewing, M.J. Hartmann, G. Veser, J.J. McCarthy, K. Johnson, **D. Lambrecht**

3:00 Intermission.

3:20 CATL **43.** Plasmon-enhanced chemistry. **G.C. Schatz**

3:50 CATL **44.** Plasmon-enabled hot carrier photocatalysis. **N.J. Halas**

4:20 Concluding Remarks.

Section C

Colorado Convention Center
Room 111

New Catalysis Through Ligand Design

New Frontiers in Catalysis

Financially supported by Exxonmobil

A. S. Veige, *Organizer*
J. S. Figueroa, *Organizer, Presiding*

1:20 Introductory Remarks.

1:22 CATL **45.** Development of molecular catalysts for the production of polyolefins. **J. Klosin**

1:44 CATL **46.** Micromanaging metal catalysts with structurally tunable acyclic carbene ligands. **L.M. Slaughter**, A.A. Ruch, S. Handa

2:06 CATL **363.** Terminal olefin-selective self-metathesis of 1,4-dienes using homogeneous Mo and W catalysts. **K.M. Wampler**, J. Uy, S.A. Cohen

2:28 CATL **47.** Carbazole-based coordination polymers to incorporate Lewis base functionality. **D.R. Manke**

2:50 CATL **48.** Ligand design toward functional materials. **J.M. Blackwell**

3:12 Intermission.

3:27 CATL **49.** Synthesis and reactivity of a molecular titanium nitride. **D.J. Mindiola**

3:49 CATL **50.** Reactivity of a dianionic 14-electron Pd(0) complex supported by charged carboranyl phosphine ligands. **V. Lavallo**

4:11 CATL **51.** Synthesis, characterization, and hydrogenation catalysis of a rhodium *NNN*-pincer complex. **P.G. Hayes**, M.M. Hänninen, C.S. MacNeil

4:33 CATL **52.** Selective ethylene oligomerization. **O.L. Sydora**

4:55 CATL **53.** Tailoring bimetallic catalysts with metal-metal interactions for small-molecule activation. **C.C. Lu**, R. Siedschlag, R.C. Cammarota, L.J. Clouston, K.D. Vogiatzis, V. Bernales, L. Gagliardi

5:17 Concluding Remarks.

Section D

Colorado Convention Center
Room 108

Symposium in Honor of Jens Rostrup-Nielsen

B. H. Davis, *Organizer*
J. Hansen, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CATL **54.** Importance of methane formation in determining overall selectivity of Fischer-Tropsch synthesis over cobalt-based catalyst. **B. Todic**, W. Ma, G. Jacobs, B.H. Davis, D. Bukur

2:05 CATL **55.** Structure-stability relationships for supported copper and nickel catalysts. **K.P. De Jong**

2:35 CATL **56.** Precious metal catalytic reforming of biosyngas. **J. Abbott**, A. Steele

3:05 Intermission.

3:20 CATL **57.** Coke management on zeolites: The benefits of hierarchization. **J. Gilson**, L. Lakiss, Z. Qin, V. Valtchev, K. Thomas, A. Vicente, C. Fernandez, F. Ngoye, S. Laforge, C. Canaff, Y. Pouilloux, L. Pinard

3:50 CATL **58.** Gas loop design incorporating water electrolysis. **A. De Klerk**

4:20 CATL **59.** Catalyst and process parameters for the gasification of rice husk with pure CO_2 and the gasification kinetics. **Z. Chen**, L. Zhang

Catalysis for Un-conventional Energy Sources

Biofuel and CO_2 Utilization

Sponsored by ENFL, Cosponsored by CATL and MPPG‡

MONDAY MORNING

Section A

Colorado Convention Center
Room 107

Surface Chemistry and Catalysis on Oxides

Oxide-Model Catalysts

Y. Xu, *Organizer*
W. Huang, Z. Wu, *Organizers, Presiding*

8:10 Introductory Remarks.

8:15 CATL **60.** Energetics of catalytically-relevant adsorbates on well-defined oxide surfaces. **C.T. Campbell**

8:50 CATL **61.** Oxidation reactions on PdO(101). **J.F. Weaver**

9:25 CATL **62.** CO oxidation over a Pt/Fe_3O_4(001) model catalyst: Watching Mars-van Krevelen at work. **R. Bliem**, J. van der Hoeven, P. de Jongh, M. Schmid, U. Diebold, G. Parkinson

9:45 CATL **63.** Water Interaction with model iron oxide surfaces. **S. Schauermann**, P. Dementyev, K. Dostert, C.P. O'Brien, H. Freund

10:05 Intermission.

10:15 CATL **64.** Model catalyst design: A material science perspective at the atomic level. **H. Freund**

10:50 CATL **65.** Electron transfer between single gold nanocrystals and oxide supports during hydrogen adsorption: A surface plasmon spectroscopy study. **S.S. Collins**, M. Cittadini, C. Pecharromán, A. Martucci, P. Mulvaney

11:10 CATL **66.** Electron transfer reactions at single crystal oxide surfaces as monitored by electron paramagnetic resonance spectroscopy: Alkaline earth oxide surfaces as exploratory examples. **T. Risse**, N. Richter, D. Cornu

11:30 CATL **67.** Determining the enantiomeric excess of epoxides at oxide surfaces using vibrational sum frequency generation. **F. Geiger**

11:50 CATL **68.** Enantioselectivity of chiral metal films grown on chiral oxide surfaces. **S.F. Yuk**, A.R. Asthagiri

Section B

Colorado Convention Center
Room 109

Electrocatalysis and Photocatalysis

Electrocatalysis

K. Leonard, *Organizer*
S. Ren, *Organizer, Presiding*

8:20 CATL **69.** Tuning core/shell nanoparticles for catalysis optimization. **S. Sun**

9:00 CATL **70.** Effect of measurement protocol and impurity levels on the oxygen reduction reaction activity of Pt/C using rotating disk electrode. **K. Shinozaki**, J.W. Zack, S. Pylypenko, R.M. Richards, B.S. Pivovar, S.S. Kocha

‡ *Cooperative Cosponsorship*

9:20 CATL **71.** Withdrawn.

9:40 CATL **72.** Designing catalysts for the development of low temperature direct methane fuel cells. **M.W. Joglekar**, V. Nguyen, S. Pylypenko, M.E. O'Reilly, Q. Li, T.S. Gray, T. Gunnoe, A.M. Herring, B.G. Trewyn

10:00 Intermission.

10:20 CATL **73.** Electrochemical confocal Raman microscopy: 3D characterization of bilirubine BOD oxidase SWCNT cryogel cathodes during the reduction of oxygen. **M. Reback**, N. Lalaoui, V. Mareau, L. Gonnon, A. Penicaud, M. Holzinger, V. Artero, P. Chenevier

10:40 CATL **74.** Oxygen reduction reaction electrocatalysts based on perovskite oxides. **J. Christ**, J. Tong, V. Stevanovic, A. Deml, R. O'Hayre, S. Pylypenko

11:00 CATL **75.** Comparative study of Fe<sub2N type Mo_2C electrocatalysts synthesized four different methods. **Y.N. Regmi**, C. Wan, K.D. Duffee, B.M. Leonard

11:20 CATL **76.** Electrocatalytic properties of delafossite $CuBO_2$ (B = Al and Ga) nanostructures. **Y. Mao**, J. Ahmed

11:40 CATL **77.** Modelling heterogeneous electrocatalytic CO_2 valorization. **S.N. Steinmann**, C. Michel, P. Sautet

Section C

Colorado Convention Center
Room 111

Theoretical and Experimental Synergies at the Frontiers of Renewable Energy Catalysis

Solid State and Heterogeneous Conversions Processes

J. A. Keith, A. J. Morris, *Organizers, Presiding*

8:30 Introductory Remarks.

8:40 CATL **78.** High-throughput strategies for the optimization of electrocatalysts for low temperature fuel cells. **B.E. Hayden**

9:10 CATL **79.** Electrocatalysis on metal alloys at the atomic scale. **J. Rossmeisl**

9:40 CATL **80.** Predicting the thermodynamic ability of materials to act as (water splitting) photocatalysts. P. Guiglion, C. Butchosa Robles, **M. Zwijnenburg**

10:00 Intermission.

10:20 CATL **81.** Experimental catalysis for the conversion of sugars and furans to renewable monomers and fuels. **P.J. Dauenhauer**, W. Fan, R.F. Lobo, R.J. Gorte

10:50 CATL **82.** Mechanisms and catalyst design principles in the conversion of sugars and furans to renewable monomers and fuels. **D.G. Vlachos**

11:20 CATL **83.** Structure-activity relationships for iono-covalent solid catalyst: Oxides, carbides, nitrides, sulfides, and phosphides in woody biomass deoxygenation to produce toluene and xylene. Y. He, G. Tate, **S. Laursen**

Section D

Colorado Convention Center
Room 108

George A. Olah Award in Hydrocarbon or Petroleum Chemistry: Symposium in Honor of Jingguang G. Chen

Catalysis and Spectroscopy

J. R. Kitchin, *Organizer*

D. Esposito, *Organizer, Presiding*

8:15 Introductory Remarks.

8:20 CATL **84.** Explorations with polyoxometalates. **M.A. Barteau**

8:50 CATL **85.** Design principles of bimetallic core-shell catalysts. **D.G. Vlachos**

9:20 CATL **86.** Structure of Pd-based bimetallic surfaces and their reactivities toward alcohol decomposition. J. Fu, X. Yang, **B.E. Koel**

9:50 Intermission.

10:05 CATL **87.** Understanding and controlling selectivity in heterogeneous catalysis of oxygenates. **J.W. Medlin**

10:35 CATL **88.** Bulk composition dependent H_2 dissociative adsorption energies on Cu_xPd_{1-x} alloy (111) surfaces. **J.R. Kitchin**, J. Boes, G. Gumuslu, J.B. Miller, A.J. Gellman

11:05 CATL **89.** Activation of metals on carbide surfaces: Novel catalysts for CO_2 hydrogenation and the low-temperature water-gas shift reaction. **J. Rodriguez**, P.J. Ramirez, P. Liu, J. Evans, F. Vines, F. Illas

Catalysis for Un-conventional Energy Sources

Novel Catalysts

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MONDAY AFTERNOON

Section A

Colorado Convention Center
Room 107

Surface Chemistry and Catalysis on Oxides

Oxide-Theory

W. Huang, Z. Wu, *Organizers*
Y. Xu, *Organizer, Presiding*
S. H. Overbury, *Presiding*

1:20 CATL **90.** Support effect in oxide catalysis: Methanol oxidation on vanadia/ceria compared to vanadia/silica. **J. Sauer**

1:55 CATL **91.** Theoretical studies of rare earth catalysis: From clean to supported CeO_2 surfaces. **X. Gong**, X. Wu, J. Zhang, L. Yin, G. Lu

2:30 CATL **92.** Roles of oxygen vacancy in the surface reactivity of CeO_2(111). **C. Zhao**, Y. Xu

2:50 CATL **93.** Dehydrogenation of methanol and formaldehyde by ceria. **M. Capdevila-Cortada**, N. Lopez

3:10 Intermission.

3:20 CATL **94.** Understanding the essential roles of metal oxides in heterogeneous catalysis. **P. Liu**, H. Kim

3:55 CATL **95.** Scaling relations and beyond in catalysis. **A. Vojvodic**

4:30 CATL **96.** DFT study of ethanol steam reforming on metallic and oxidized cobalt. **W. Luo**, A.R. Asthagiri

4:50 CATL **97.** Computational investigation of interfacial oxide activity and stability on Pd/CeO_2 catalysts. **T.P. Senftle**, A. Van Duin, M.J. Janik

Section B

Colorado Convention Center
Room 109

Electrocatalysis and Photocatalysis

Photocatalysis

K. Leonard, *Organizer*
S. Ren, *Organizer, Presiding*

1:30 CATL **98.** Controlling the titania-silica interface for enhanced (photo)catalytic performance. **T. Eaton**, H.L. Hinton, L. Sorokina, K.A. Gray, J.M. Notestein

1:50 CATL **99.** Isolating and controlling the nature of surface reaction sites of semiconductor photocatalysts: Selectivity in the photocatalytic reduction of CO_2 and H_2O to H_2 and reduced C_1 molecules. S. Poudyal, **S. Laursen**

2:10 CATL **100.** Thermally stable, crystalline, mixed phase (anatase/rutile) mesoporous titanium dioxide as excellent catalyst for photocatalytic organic pollutants degradation. **Z. Luo**, A. Poyraz, C. Kuo, Y. Meng, R. Miao, S. Chen, S.L. Suib

2:30 CATL **101.** One-pot synthesis of Cu-TiO_2 photocatalyst for photoreforming of alcohols, photoexcitation induced interfacial electron transfer, charging and discharging. M. Mehta, **A. Samokhvalov**

2:50 CATL **102.** Synproportionation reaction for the fabrication of Sn^{2+} self-doped SnO_{2-x} nanocrystals with tunable band structure and highly efficient visible light photocatalytic activity. **C. Fan**, A. Xu

3:10 Intermission.

3:30 CATL **103.** Withdrawn.

3:50 CATL **104.** Protection strategies for Si-based photoanode. **B. Mei**, B. Seger, T. Pederson, A. Permyakova, R. Frydendal, D. Bae, M. Malizia, P. Malacrida, I. Stephans, O. Hansen, P. Vesborg, I. Chorkendorff

4:10 CATL **105.** Electron-hole recombination controlled by doping sites in perovskite-structured photocatalysts: Sr-doped $NaTaO_3$. L. An, **H. Onishi**

4:30 CATL **106.** Mesoporous $W_{18}O_{49}$ hollow spheres as highly active photocatalyst. **Z. Huang**, J. Song, Z. Wang, **J. Zou**

4:50 CATL **107.** Carbazolic porous organic frameworks as green photoredox catalysts for organic synthesis. **J. Zhang**, J. Luo

Section C

Colorado Convention Center
Room 111

Symposium in Honor of Jens Rostrup-Nielsen

B. H. Davis, *Organizer*
J. Hansen, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CATL **108.** Migration of sulfur in prereforming catalysts during steaming conditions. **M. Oestberg**

2:05 CATL **109.** Nickel aluminate/α-alumina as catalysts for partial oxidation and steam reforming of methane and as support for cobalt Fischer-Tropsch catalysts. B.C. Enger, A. Holland Lillebø, E.A. Blekkan, **A. Holmen**

2:35 CATL **110.** Catalyst design principles: An application to the steam reforming of methane. **F. Abild-Pedersen**, T. Bligaard, F. Studt, J.K. Norskov

3:05 CATL **111.** Effects of metal oxide promoters on the activity, kinetics, and selectivity of co-based Fischer-Tropsch catalysts. **A.T. Bell**

3:35 Intermission.

3:50 CATL **112.** Evaluation of NiO-based oxygen transfer materials in chemical looping methane reforming. A. Antzara, E. Heracleous, L. Silvester, D. Ipsakis, D. Bukur, **A.A. Lemonidou**

4:20 CATL **113.** Activation of steam reforming catalysts: New fundamental insight into reduction of supported NiO. L.F. Lundegaard, R.R. Tiruvalam, F.M. Cano, **C.V. Ovesen**

4:50 CATL **114.** Time interrupted behavior of ammonia synthesis over ruthenium based catalysts. **D. Uner**, M. Aslan, N. Uner

Section D

Colorado Convention Center
Room 108

George A. Olah Award in Hydrocarbon or Petroleum Chemistry: Symposium in Honor of Jingguang G. Chen

Electrocatalysis and Solid/Liquid Catalysis

D. Esposito, *Organizer*
J. R. Kitchin, *Organizer, Presiding*

1:30 CATL **115.** Analysis of the mechanism of electrochemical oxygen reduction and development of Ag- and Pt-alloy catalysts for low temperature fuel cells. **S. Linic**

2:00 CATL **116.** Production of chemicals from dilute CO_2 and electricity. **A. West**, S. Banta

2:30 CATL **117.** Electrocatalysis for a distributed renewable electrochemical energy and mobility system. **Y. Yan**

3:00 Intermission.

3:15 CATL **118.** Nanoporous materials for energy applications. **F. Jiao**

3:45 CATL **119.** Metal-Insulator-Semiconductor (MIS) photoelectrodes as a platform for stable and efficient solar fuels production. **D. Esposito**

4:15 CATL **120.** Selective hydrogenation in liquid phase: A new catalytic process for the purification of alkynes. R. Hou, X. Lan, **T. Wang**

4:45 CATL **121.** Biomass conversion to high-purity hydrogen with integrated carbon fixation in the presence of group I & II hydroxides and a Ni/ZrO_2 catalyst. M. Stonor, **A. Park**

Section E

Colorado Convention Center
Room 207

Gabor A. Somorjai Award for Creative Research in Catalysis: Symposium in Honor of Maurice Brookhart

A. Goldman, *Organizer*
K. I. Goldberg, *Organizer, Presiding*

1:00 CATL **122.** Selective, catalytic functionalization of alkyl and aryl c-h bonds with silicon reagents. **J.F. Hartwig**

1:20 CATL **123.** Borane catalyzed selective deoxygenation of carbohydrate biomass. **M.R. Gagne**

1:40 CATL **124.** Synthesis of stereoregular polymers through ROMP. **R.R. Schrock**

2:00 CATL **125.** Insertion of olefins into aryl C-H bonds catalyzed by iridium complexes of hemilabile pincer ligands and bidentate derivatives. J.A. Flores, **A.S. Goldman**

2:20 CATL **126.** Aqueous olefin polymerization. A. Osichow, A. Tchernook, T. Wiedemann, F. Oelscher, P. Kenyon, I. Goettker gen. Schnetmann, **S. Mecking**

2:40 CATL **127.** Regioselective functionalization of sp^2 and sp^3 C-H bonds. **O. Daugulis**

3:00 Intermission.

3:10 CATL **128.** Unique C-H bond activations and functionalizations with ruthenium(II) catalysts. **P.H. Dixneuf**, F. Pozgan, P.B. Arockiam, B. Li, B. Sundararaju

3:30 CATL **129.** Selective reactions of olefins. **R.H. Grubbs**

3:50 CATL **130.** Hydrogermane and hydrogermoxane activation at ruthenium: Coordination chemistry and catalysis. K.A. Smart, E. Mothes-Martin, M. Grellier, R.N. Perutz, **S. Sabo-Etienne**

4:10 CATL **131.** Making hydrogen from water and fire: Alchemy lives. **R. Eisenberg**

4:30 CATL **132.** Pincer iron and cobalt complexes for cataltyic alkene hydrofunctionalizations. **Z. Huang**, L. Zhang, D. Peng, Z. Zuo

4:50 CATL **133. Award Address** (Gabor A. Somorjai Award for Creative Research in Catalysis sponsored by the Gabor A. and Judith K. Somorjai Endowment Fund). Catalysis using late transition metal complexes. **M. Brookhart**

MONDAY EVENING

Section A

Colorado Convention Center
Halls C/D

Sci-Mix

V. Schwartz, *Organizer*

8:00 - 10:00

12, 16, 26, 31-32, 34, 42, 54, 66, 72, 92, 115, 117-118, 120, 132. See previous listings.
183, 192-194, 227, 260, 272, 275, 281, 286, 300-301, 316, 320, 323, 328, 330, 336-337. See subsequent listings.

TUESDAY MORNING

Section A

Colorado Convention Center
Room 107

Catalytic Materials and Technologies for Upgrading of COx and Natural Gas

Oxidation

J. Bravo-Suarez, B. A. Kilos, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 CATL **134.** CH activation and functionalization of methane, ethane, and propane with main group cations. **R.A. Periana**

8:50 CATL **135.** Hydrocarbon oxidation reactivity in iron metal-organic frameworks. **D. Xiao**, E.D. Bloch, J.A. Mason, W. Queen, M.R. Hudson, N. Planas, P. Verma, D.G. Truhlar, L. Gagliardi, C.M. Brown, J.R. Long

9:20 CATL **136.** Catalytic conversion of methane to methanol and acetic acid on singly dispersed oxide species on internal surface of ZSM5. **F. Tao**, D. Xiao, A. Frenkel

9:50 CATL **137.** Ethylene epoxidation on metal-substituted silica mesopore catalysts: A combined experimental and theoretical investigation. **P.D. Patel**, W. Yan, A. Ramanathan, B. Subramaniam, B. Laird, W. Thompson

10:20 Intermission.

10:35 CATL **138.** General mechanistic role of reactive oxygen for the activation of alkanols, alkenes, and alkanes on dispersed metal clusters. **Y. Chin**, W. Tu, P. Lachkov

11:05 CATL **139.** Withdrawn.

11:35 CATL **140.** Biocatalytic polymer membrane system for selective partial oxidation of methane to methanol. **J. Stolaroff**, S.E. Baker, C. Blanchette, J.M. Lenhardt

12:05 Concluding Remarks.

Section B

Colorado Convention Center

Room 109

Surface Chemistry and Catalysis on Oxides

Oxide-Synthesis and Catalysis

Z. Wu, *Organizer*

W. Huang, Y. Xu, *Organizers, Presiding*

8:10 CATL **141.** Controllable synthesis and catalytic property of ceria-based nano- and mesoporous materials. **C. Yan**

8:45 CATL **142.** Structure sensitivity and reaction pathways in oxygenate reactions catalyzed by CeO_2. A.K. Mann, Z. Wu, D.R. Mullins, **S.H. Overbury**

9:20 CATL **143.** Advanced nanomaterials: Synthesis and catalytic applications. **M. Gawande**, R.S. Varma, L. Kvitek, R. Zboril

9:40 CATL **144.** On the surface dependent acid-base property of ceria nanoshapes. **Z. Wu**, A.K. Mann, S.H. Overbury

10:00 Intermission.

10:10 CATL **145.** Rod-shaped metal oxides: Structural control and catalytic properties. **W. Shen**

10:45 CATL **146.** Electronic and reaction study of doped CeO_2 with Fe cations for hydrogen production from water. **Y. Alsalik**, H. Idriss

11:05 CATL **147.** Withdrawn.

11:25 CATL **148.** Controlling the selectivity of metal oxide catalysts using silanes and phosphonates for polyol dehydration. **L. Ellis**, D.K. Schwartz, J.W. Medlin

11:45 CATL **149.** Surface modification of silica-supported Ti(IV) and Nb(V) oxides for understanding reactivity and stability in the epoxidation of alkenes with H_2O_2. **N.E. Thornburg**, R.E. Franks, J.M. Notestein

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Section C

Colorado Convention Center

Room 111

Symposium in Honor of Jens Rostrup-Nielsen

B. H. Davis, *Organizer*

J. Hansen, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 CATL **150.** Role of alkali in heterogeneous catalysis for gas cleaning in stationary and mobile applications. P. Haghighi Moud, J. Granestrand, S. Dahlin, M. Nilsson, K. Andersson, L. Pettersson, **K. Engvall**

9:05 CATL **151.** Electron microscopy advances for catalysis. **S. Helveg**

9:35 CATL **152.** Fischer-Tropsch synthesis: A time resolved study evidences changes in the product distribution during the initial steps on cobalt catalysts. **G. Melaet**, W. Ralston, W. Liu, G.A. Somorjai

10:05 Intermission.

10:20 CATL **153.** Withdrawn.

10:50 CATL **154.** Effect of metal on the reduction and reoxidation characteristics of ceria under ethanol steam reforming conditions. **U.S. Ozkan**, H. Sohn, I. Soykal, J.T. Miller, F. Tao

11:20 CATL **155.** Fischer-Tropsch synthesis in coal-to-liquids: Old technology with a bright future? **J.W. Niemantsverdriet**

Section D

Colorado Convention Center

Room 108

George A. Olah Award in Hydrocarbon or Petroleum Chemistry: Symposium in Honor of Jingguang G. Chen

Heterogeneous Catalysis

D. Esposito, J. R. Kitchin, *Organizers*

M. A. Barteau, *Presiding*

8:30 CATL **156.** Oxygen removal and chain growth pathways in the catalytic upgrading of oxygenates. **E. Iglesia**

9:00 CATL **157.** Alkane activation over molybdenum carbide nanoparticles supported on nonacidic zeolites. E.P. Schreiner, S. Teketel, **R.F. Lobo**

9:30 CATL **158.** Single-atom-catalysts: New opportunities in selective hydrogenation reactions. **T. Zhang**

10:00 Intermission.

10:15 CATL **159.** Spectator or Intermediate? Simultaneous MS/FTIR studies of methanol catalysis. **C. Mims**, C.H. Peden, C.T. Campbell, Y. Yang, J.H. Kwak

10:45 CATL **160.** Metal catalysts on silica: issues and opportunities. **S. Soled**, S. Miseo, J.E. Baumgartner

11:15 CATL **161. Award Address** (George A. Olah Award in Hydrocarbon or Petroleum Chemistry sponsored by the George A. Olah Award Endowment). Carbide and bimetallic catalysts for hydrocarbon transformation reactions. **J.G. Chen**

E.V. Murphree Award in Industrial & Engineering Chemistry: Symposium in Honor of Joseph R. Zoeller

Sponsored by I&EC, Cosponsored by CATL

TUESDAY AFTERNOON

Section A

Colorado Convention Center

Room 107

Catalytic Materials and Technologies for Upgrading of COx and Natural Gas

Oxidation and Oxidative Coupling

J. Bravo-Suarez, B. A. Kilos, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 CATL **162.** Insights in confinement effects in methane-to-methanol conversion over Fe-SSZ-13. **F. Goeltl,** C. Michel, P. Andrikopoulos, I. Hermans, P. Sautet

2:05 CATL **163.** Methane to methanol conversion on copper-containing small-pore aeolites. **B. Ipek**, M.J. Wulfers, S. Teketel, J.P. Smith, K.S. Booksh, R.F. Lobo

2:35 CATL **164.** Ethylene epoxidation in metal-substituted mesopore catalysts: Multiscale insights from experiment and molecular simulation. **J.L. Kern**, K.G. Steenbergen, W. Yan, A. Ramanathan, B. Subramaniam, W. Thompson, B.B. Laird

3:05 Intermission.

3:20 CATL **165.** Methane coupling reaction in an oxysteam stream via an OH radical pathway. **K. Takanabe**

3:50 CATL **166.** Effects of transition metal doping in TiO_2 nanowire catalysts for oxidative coupling of methane. **R.T. Yunarti**, J. Ha, D. Suh, J. Choi, Y.J. Hwang

4:20 CATL **167.** Efficient removal of formaldehyde by layered double hydroxides at room temperature. F. Liu, **P. Zhang**

4:50 CATL **168.** Withdrawn.

5:20 Concluding Remarks.

Section B

Colorado Convention Center

Room 109

Surface Chemistry and Catalysis on Oxides

Metal-Oxide Interface: Oxidation Reactions

W. Huang, Z. Wu, Y. Xu, *Organizers*

X. Gong, S. H. Overbury, *Presiding*

1:20 CATL **169.** Identification of reaction sites for the oxidation of NO on a mixed Fe+Cr oxide surface. **M.A. Henderson**, M.H. Engelhard

2:30 CATL **171.** Selectivity changes at interfaces between Pt and oxide nanoparticles in catalytic alcohol oxidation. **K. An**, G.A. Somorjai

2:50 CATL **172.** Remarkable enhancement of dichloromethane oxidation over potassium - promoted Pt/Al_2O_3 catalysts. **J. Lu**

3:10 Intermission.

3:20 CATL **173.** Reactivity of water and hydroxyls on oxide surfaces. **W. Huang**

3:55 CATL **174.** On the interface confinement effect in the oxide-on-metal inverse catalysts. **Q. Fu**

4:30 CATL **175.** Catalysis by HBEA zeolite in aqueous media: The impact of water on reaction pathways and catalyst performance. **A. Vjunov**, J.L. Fulton, D.M. Camaioni, M.A. Derewinski, J.A. Lercher

4:50 CATL **176.** Toward improved catalytic low-temperature CO removal in H_2 rich streams. **J. Saavedra**, C.J. Pursell, B.D. Chandler

5:10 CATL **177.** Direct simulation evidence of generation of oxygen vacancies at the golden cage Au_{16} and TiO_2(110) interface for CO oxidation. **L. Li**, X.C. Zeng

Section C

Colorado Convention Center

Room 111

Symposium in Honor of Jens Rostrup-Nielsen

J. Hansen, *Organizer*

B. H. Davis, *Organizer, Presiding*

1:20 Introductory Remarks.

1:25 CATL **178.** Hot electron surface chemistry at oxide-metal interfaces: The foundation of acid-base catalysis. **G.A. Somorjai**

1:55 CATL **179.** Enhanced activity and selectivity of Fischer-Tropsch synthesis catalysts in water/oil emulsions. **D.E. Resasco**

2:25 CATL **180.** Insights into emission and capture of atoms during Ostwald ripening. **A.K. Datye**, T.R. Johns, C. Carillo, S. Challa, A. DeLaRiva, B. Kiefer, C.H. Kim, M.P. Balogh, J.W. Niemantsverdriet

2:55 CATL **181.** Withdrawn.

3:25 Intermission.

3:40 CATL **182.** Critical role of isolation effect in solid solution catalysts for CO_2 reforming of methane. **Y.H. Hu**

4:10 CATL **183.** Coking- and sintering- resistant core-shell nanoparticles for dry reforming of methane. **N. Almana**, P. Laveille, K. Takanabe, J.M. Basset

4:40 CATL **184.** ECUST coal gasification updates: New projects and operations experience. **J. Xu**

5:10 Concluding Remarks.

Section D

Colorado Convention Center

Room 108

Theoretical and Experimental Synergies at the Frontiers of Renewable Energy Catalysis

Solid State and Heterogeneous Conversions Processes

J. A. Keith, A. J. Morris, *Organizers, Presiding*

1:30 Introductory Remarks.

1:40 CATL **185.** Ab initio approaches to modeling catalysis on solid oxide fuel cell cathodes. **D.D. Morgan**

2:10 CATL **186.** Oxygen reduction mechanisms on perovskite oxides and the effects of dissimilar interfaces. **B. Yildiz**

2:40 CATL **187.** Investigating CuO catalyzed oxidation of glucose to gluconic acid using an integrated computational and experimental approach: Insights into the role of lattice oxygen. Q. Thang Trinh, P. N. Amaniampong, Y. Yang, **S. Mushrif**

3:00 Intermission.

3:20 CATL **188.** Promotion and poisoning of hydrogen evolution by co-adsorbed CO on transition-metal electrodes. **Y. Zhang**, V. Sethuraman, R. Michalsky, A.A. Peterson

3:40 CATL **189.** Critical role of water in catalytic CO oxidation over Au/TiO_2 catalysts: Part 1 — experiment. J. Saavedra, H. Doan, C.J. Pursell, L. Grabow, **B.D. Chandler**

4:10 CATL **190.** Critical role of water in catalytic CO oxidation over Au/TiO_2 catalysts: Part 2 — theory. H. Doan, J. Saavedra, C.J. Pursell, B.D. Chandler, **L. Grabow**

4:40 Concluding Remarks.

E.V. Murphree Award in Industrial & Engineering Chemistry: Symposium in Honor of Joseph R. Zoeller

Sponsored by I&EC, Cosponsored by CATL

TUESDAY EVENING

Section A

Colorado Convention Center

Hall C

General Poster Session

I. I. Soykal, *Organizer*

6:00 - 8:00

CATL **191.** Growth of carbon nanofibers synthesized from electrocracking gas on a Ni/Al_2O_3 catalyst: Thermodynamic and kinetic analyses. **A.S. Ismail**

CATL **192.** Influence of ligand substitution on electronic properties in bis(diphosphine) nickel (I) catalysts used in hydrogen catalysis. **T.L. Brown**, **A. Pitts-Mccoy**, J. Niklas, O. Poluektov, K. Mardis

CATL **193.** Characterization of amine-treated zeolites by methanol chemisorption. **A.D. D'Amico**, C. Baker, J.L. Gole, J.I. Brauer, S. Graham, J.Z. Hu, J.C. Kenvin, M.G. White

CATL **194.** Metal-oxide sites for facile methane dissociation. A. Trinchero, A. Hellman, **H. Grönbeck**

CATL **195.** Hydrodesulphurization of the DBT using low ratio nickel-molybdenum sulfide catalysts. **I.A. Montemayor**, J.S. Sollner, D.F. Gonzalez, J.G. Parsons

CATL **196.** Direct oxidative carboxylation of olefins for the synthesis of cyclic organic carbonates. **A. Sathe**, R.M. Rioux

CATL **197.** Chiral carbazolic porous framework as asymmetric heterogeneous organocatalyst. **X. Zhang**, A. Kormos, J. Zhang

‡ *Cooperative Cosponsorship*

CATL **198.** High pressure STM studies on carbon monoxide adsorption on copper and cobalt sites. **Y. Hao**, B. Eren, M. Salmeron, G.A. Somorjai

CATL **199.** Highly efficient visible light-induced active oxygen generation by carbazolic porous organic frameworks and their use in organic synthesis. **J. Luo**, J. Zhang

CATL **200.** Hydrodesulfurization of dibenzothiohene using tungsten, cobalt and nickel. **D.F. Gonzalez**, K. Williams, J.S. Sollner, J.G. Parsons

CATL **201.** Hydrodesulphurization of DBT using CoMoS2 catalyst. **J.S. Sollner**, D.F. Gonzalez, J.G. Parsons

CATL **202.** Water's effect on the nucleation and growth of nickel nanoparticles on ceria thin films. **E.W. Peterson**, J. Zhou

CATL **203.** Secretive world of copper substituted zeolites in NH_3-SCR investigated by EPR. **A. Godiksen**, S.B. Rasmussen, T.V. Janssens, H. Falsig, L.F. Lundegaard, P. Moses, F. Giordanino, E. Borfecchia, K. Lomachenko, C. Lamberti, S. Bordiga, P. Beato, S. Mossin

CATL **204.** Withdrawn.

CATL **205.** Structure and catalytic activity of Mo and Cr nanoparticle in ZSM-5 for natural gas conversion to aromatics. **J. Gao**, Y. Zheng, J. Jehng, Y. Tang, J. Gallagher, J.T. Miller, I.E. Wachs, S. Podkolzin

CATL **206.** Methanol conversion to dimethyl ether over Fe-embedded graphene. A. Thivasasith, J. Sirijaraensre, P. Khongpracha, C. Warakulwit, **J. Limtrakul**

CATL **207.** Role of acid strengths and confinement effects on the conversion of propan-2-ol: MFI zeolites vs. Keggin polyoxometalates. S. Choomwattana, J. Sirijaraensre, **J. Limtrakul**

CATL **208.** Preparation of di- and triglycerol using acetate salts. **J. Lee**, T. Han, S. Park, M. Cheong

CATL **209.** Preparation of di- and triglycerol using heterogeneous catalysts. **J. Lee**, S. Park

CATL **210.** Cross-selectivity in the catalytic decarboxylative ketonization. A. Ignatchenko, **V. Marino**, **J. DeRaddo**

CATL **211.** Condensation of ketones with carboxylic acids: Extending kinetic scheme for the mechanism of ketonic decarboxylation. **T. DiProspero**, H. Patel, A. Ignatchenko

CATL **212.** Efficient catalytic conversion of cellulose into levulinic acid by sulfonated hyperbranched poly(arylene oxindole)s with chloro substituents. **F. Yu**, J. Thomas, S. Van de Vyver, M. Smet, W. Dehaen, B.F. Sels

CATL **213.** Photocatalytic production of H_2O_2 and its further utilization for Baeyer-Villiger oxidation. **L. Liu**, A. Corma

CATL **214.** Synthesis, characterization of Ag/SiO_2 and Ag/Co_3O_4 hierarchically porous monoliths and evaluation for hydrogenation of dyes. Y. Hakat, T. Kotbagi, **M.G. Bakker**

CATL **215.** Evaluation of Ag/SiO_2 and Ag/Co_3O_4 Hierarchically porous monoliths for epoxidations. **Y. Hakat**, T. Kotbagi, M.G. Bakker

CATL **216.** Aerobic oxidation reaction catalyzed by graphene oxide. **J. Park**, F. Raza, D. Yim, J. Kim

CATL **217.** Zeolite-templated Ni nanostructure for methanol oxidation reaction. **D. Aldhayan**

CATL **218.** Preparation of C60 nanowhiskers — WO_3 nanocomposites and kinetics for photocatalytic degradation of organic dyes. K.H. Kim, H.S. Park, J.W. Ko, **W.B. Ko**

CATL **219.** Investigation of structure, composition, and catalytic activity of AuPd bimetallic nanoparticles of variable Au/Pd ratio. **T.A. G. Silva**, E. Teixeira-Neto, L.M. Rossi

CATL **220.** Picking up the pace: Improving oxygen evolution reaction catalysts. **M. Hinojos**, S. Jin, L. Li

CATL **221.** Preparation of SAPO-34 by vapor-phase crystallization. **W. Wang**, H. Liu, W. Yang

CATL **222.** Silver nanoparticle-functionalized 2D nanosheets as a plasmonic photocatalyst for reduction of nitroaromatic compounds. **H. Lee**, J. Park, F. Raza, D. Yim, J. Kim

CATL **223.** Investigation of metal xanthates as latent thermal epoxy resin curing catalysts. **T.C. Vagvala**, S.S. Pandey, Y. Ogomi, S. Hayase

CATL **224.** Multiwalled carbon nanotubes supported palladium-Iridium alloy nanoparticles with enhanced electrocatalytic activity for the formic acid oxidation. **F. Wang**, F. Wang, J. Bao, H. Liu

CATL **225.** Sb-doped SnO_2 supported platinum catalyst with high stability for proton exchange membrane fuel cells. **M. Dou**, M. Hou, F. Wang

CATL **226.** Nitrogen-doped hierarchical porous carbon fabricated from food waste as the support material for Pt electrocatalyst toward the oxygen reduction reaction. **F. Wang**, Y. Huang, H. Liu, Y. Cao

CATL **227.** Comparison of hydrogen peroxide decomposition in the presence of N_2, H_2 and C_3H_6 over supported Pd catalysts. **T. Chen**, E. Kertalli, A. Nijhuis, S.G. Podkolzin

CATL **228.** Effect of Hydrogen and Propylene Presence on Hydrogen Peroxide Decomposition over Pd. **T. Chen**, E. Kertalli, A. Nijhuis, S.G. Podkolzin

CATL **229.** Learning from microbial systems to develop biomimetic catalysts for hydrocarbon oxidation. **S.S. Yu**, S.I. Chan

CATL **230.** Hydrodesulfurization of thiophene using phosphomolybdic acid and nickel substituted phosphomolybdic as catalyst. **A.M. Alsalme**, M.H. Siddiqui

CATL **231.** Catalytic ozone membrane reactor for treatment of EDCs in water. T. Corbet, **L. Li**, Y. Li, W. Han, K. Yeung

CATL **232.** Role of surface chemistry on the photoactivity of C-doped TiO_2 derived from TiC. W. Ching, **S.A. Ferdousi**, K.L. Yeung

CATL **233.** Pd@V-P oxide core-shell nanoparticels supported on MWCNTs as selective electrocatalyst for the ORR. **H. Liu**, J. Bao, F. Wang

CATL **234.** Homogenous Ir-catalyzed asymmetric hydrogenation of pyridinium Salts: High throughput experimentation approach, scope and preliminary mechanistic studies. **Y. Huang**, Y. Chen, Y. Liu, S.W. Krska, I.W. Davies, M. Chang, S. Liu, X. Zhang

CATL **235.** Hydrogen generation via sodium borohydride hydrolysis using graphene supported platinum-cobalt catalysts prepared by microwave-assisted synthesis. K. Antanaviciute, A. Matuseviciute, **L. Tamasauskaite-Tamasiunaite**, I. Stalnioniene, A. Zieliene, L. Naruskevicius, B. Simkunaite-Stanyniene, E. Norkus

CATL **236.** N-Heterocyclic carbene-based materials for CO_2 activation. **E. Kaley**, E. Finney

CATL **237.** Graphene supported PtAuCeO_2 nanocomposites as electrocatalysts for fuel cells. M. Urbonas, **L. Tamasauskaite-Tamasiunaite**, V. Kepeniene, A. Matuseviciute, R. Kondrotas, R. Juskenas, V. Pakstas, E. Norkus

CATL **238.** Aqueous phase CO_2 reduction with sodium borohydride: An ab initio molecular dynamics and nudged-elastic band mechanistic study. **M.C. Groenenboom**, K.A. Grice, **J.A. Keith**

CATL **239.** Tandem isomerization-decarboxylation of unsaturated fatty acids to olefins via Ruthenium metal-as-ligand catalysts. **R.E. Murray**, E.L. Walter, K.M. Doll

WEDNESDAY MORNING

Section A

Colorado Convention Center
Room 107

Novel Catalytic Materials for Renewable Fuels/Chemicals

M. Foston, J. C. Hicks, *Organizers, Presiding*

8:15 Introductory Remarks.

8:20 CATL **240.** Supported metal catalysts for lignin hydrogenolysis. **S.L. Scott**, Z. Jones, X. Wu

8:40 CATL **241.** Lignin depolymerization by rhodium phosphine complexes and water-stable Lewis acids. **R. Jastrzebski**, B.M. Weckhuysen, P.C. Bruijnincx

9:00 CATL **242.** Designing active and stable Ru catalysts for the aqueous-phase hydrogenation levulinic acid. **J. Bond**, O.A. Abdelrahman

9:20 CATL **243.** Promotion of activity and selectivity by alkanethiol monolayers for Pd-catalyzed benzyl alcohol hydrodeoxygenation. **C. Lien**, J.W. Medlin

9:40 CATL **244.** Direct catalytic conversion of Ethanol stream to hydrocarbon blend-stock: Approaches to increase liquid hydrocarbon production. **Z. Li**, E. Casbeer, B.H. Davison, C.K. Narula

10:00 Intermission.

10:10 CATL **245.** One-pot conversion of Kraft lignin into high-valued small-molecular chemicals over nanostructured molybdenum based catalyst. **Y. Li**

10:30 CATL **246.** Mechanism and kinetics of acetic acid ketonization over zeolites. **S. Crossley**, A. Gumidyala, . Godavarthy

10:50 CATL **247.** Catalytic pathways and periodic trends for the hydrogenation of acetic acid in aqueous phase. J. Shangguan, **Y. Chin**

11:10 CATL **248.** Nitrate-Intercalated Layered double-hydroxide catalysts for lignin depolymerization. **J.S. Kruger**, N.S. Cleveland, M.J. Biddy, G. Beckham

11:30 CATL **249.** Effects of Brønsted acid strength and site environment for C=C bond formation and hydrogen transfer reactions. **F. Lin**, Y. Chin

Section B

Colorado Convention Center
Room 109

Catalytic Materials and Technologies for Upgrading of COx and Natural Gas

Hydrogenation and Dehydroaromatization

J. Bravo-Suarez, B. A. Kilos, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 CATL **250.** Mechanistic insights into the activation of CO and hydrocarbon chain growth in Fischer Tropsch synthesis. **M. Neurock**, D. Hibbitts, B. Loveless, C. Buda, T. Lawlor, E. Dybeck

8:50 CATL **251.** Quantum mechanical analysis of CO_2 and CO hydrogenation on metal-doped Cu(111) surfaces. **Y. Santiago-Rodriguez**, M. Curet-Arana

9:20 CATL **252.** Catalytic light olefin upgrading: Using natural gas for gasoline quality improvement. **P. He**, H. Song

9:50 CATL **253.** Natural gas to chemicals via reactive separation. **P. Chitta**

10:20 Intermission.

10:35 CATL **254.** Topsøe aromatics synthesis catalysts. **L.J. Lemus-Yegres**, B. Temel, X. Yang, F. Joensen, P.H. Nielsen

11:05 CATL **255.** Structure and regeneration of Mo/ZSM-5 catalysts for natural gas conversion. J. Gao, Y. Tang, I.E. Wachs, **S.G. Podkolzin**

11:35 CATL **256.** High selectivity of zinc and phosphorus modified ZSM-5 for MTA. **J. Qiao**, J. Teng, Y. Wang, W. Yang

12:05 Concluding Remarks.

Section C

Colorado Convention Center
Room 111

Surface Chemistry and Catalysis on Oxides

Metal-Oxide Interface: Others

W. Huang, Y. Xu, *Organizers*
Z. Wu, *Organizer, Presiding*
Q. Fu, *Presiding*

8:10 CATL **257.** Role of surface oxygen vacancies in heterogeneous Au catalysis. **J. Behm**

8:45 CATL **258.** Role of TiO_2 defects and the Ru/TiO_2 interface on the conversion of phenolics. **S. Crossley**, T. Omotoso

9:05 CATL **259.** Investigation of Pd-Cu single atom alloy catalysts for selective hydrogenation of acetylene in ethylene. **X. Cao**, A. Mirjalili, W. Xie, **B. Jang**

9:25 CATL **260.** Selective hydrogenation of phenol catalyzed by palladium on high surface ceria at room temperature and ambient pressure. **N. Nelson**, A.D. Sadow, I.I. Slowing

9:45 Intermission.

9:55 CATL **261.** Importance of the metal-oxide interface in catalysts for the water-gas shift and methanol synthesis. **J. Rodriguez**, D.J. Stacchiola, P. Liu, S.D. Senanayake, J. Graciani, J.F. Sanz

10:30 CATL **262.** Kinetically stabilized Pd@Pt core-shell nanocubes with thin Pt layers for enhanced catalytic hydrogenation performance. **P. Zhang**, S. Zhou

10:50 CATL **263.** Investigating the function of metal oxide promoters on supported Rh catalysts for syngas conversion to oxygenates through surface and interface modification. **N. Yang**, S. Fleischman, P. Wang, S.F. Bent

11:10 CATL **264.** Preparation of 3D ordered macroporous SiO_2-supported $K_{xx}MnCeO_2$ catalysts for soot combustion. **X. Yu**, Z. Zhao

11:30 CATL **265.** Modeling acrolein hydrogenation on constrained platinum nanoparticles. **C. Engelhardt**, D. Ellis, K.R. Poeppelmeier, R. Kennedy

Section D

Colorado Convention Center
Room 108

Theoretical and Experimental Synergies at the Frontiers of Renewable Energy Catalysis

CO_2 Reductions

J. A. Keith, A. J. Morris, *Organizers, Presiding*

8:30 Introductory Remarks.

8:40 CATL **266.** Design principles for reversible CO_2 chemistries. **W.F. Schneider**, T. Lee

9:10 CATL **267.** Electrocatalytic conversion carbon dioxide to fuels promoted by 1,3-dialkylimidazolium based ionic liquids. J. DiMeglio, J. Medina-Ramos, R.C. Pupillo, **J. Rosenthal**

9:40 CATL **268.** Toward electrochemical carbon dioxide reduction by porous coordination networks. W. Maza, S. Ahrenholtz, **A.J. Morris**

10:00 Intermission.

10:20 CATL **269.** Hydrogen evolution in the context of electrochemical CO_2 reduction. **R.J. Nielsen**, S. Johnson, Y. Lam, W.A. Goddard, D.W. Shaffer, J. Yang

10:50 CATL **270.** Thermodynamic considerations in the design of molecular electrocatalysts for selective CO_2 reduction. **J. Yang**, D.W. Shaffer, S. Poteet, J. Ritter

11:20 CATL **271.** First-principles quantum chemical investigations on the selectivity of borohydride for carbon dioxide and bicarbonate reduction in protic conditions. M.C. Groenenboom, K.A. Grice, **J.A. Keith**

WEDNESDAY AFTERNOON

Section A

Colorado Convention Center
Room 107

Novel Catalytic Materials for Renewable Fuels/Chemicals

M. Foston, J. C. Hicks, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 CATL **272.** Synthesis of glycal-based bolaamphiphiles tethered to cobalt-Schiff base complexes for catalyst delivery to lignocellulose biomass. **J.J. Bozell**, C. Njiojob, B.K. Long

1:55 CATL **273.** Anion catalysis: A novel pathway for C-O activation. **M. Emmert**

2:15 CATL **274.** Role of defect sites in the hydrolysis of cellulose over activated carbon catalysts. G. Foo, **C. Sievers**

2:35 CATL **275.** Catalytic depolymerization of lignin extracted from Kraft black liquor and lignin model compound 4-phenoxyphenol. **B.D. Carter**, D.A. Bruce

2:55 CATL **276.** Natural inorganic catalysts in eellulose pyrolysis. **C. Zhu**, A. Paulsen, P. Dauenhauer

3:15 Intermission.

3:25 CATL **277.** Reaction mechanism and active site location for the hydrodeoxygenation of phenolics over Ru/TiO_2. B. Baek, **L. Grabow**

3:45 CATL **278.** Progress toward the mild and selective hydrogenolysis of lignin to produce chemicals. **M.B. Foston**, Y. Gao

4:05 CATL **279.** Selective conversion of xylose to furfural in γ-valerolactone using novel catalysts. **S.M. Bruce**, M.A. Carreon, S.G. Wettstein

4:25 CATL **280.** Surface chemistry of oxygenates on molybdenum-modified platinum. **A. Robinson**, J. Hensley, J.W. Medlin

4:45 CATL **281.** Hydrodeoxygenation of lignocellulosic biomass and lignin model compounds with bimetallic phosphide catalysts. **D.J. Rensel**, M. Abbott, J.C. Hicks

Section B

Colorado Convention Center
Room 109

Catalytic Materials and Technologies for Upgrading of COx and Natural Gas

Dehydrogenation

J. Bravo-Suarez, B. A. Kilos, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 CATL **282.** Light alkane dehydrogenation over Pt and PtSn alloys: A density functional theory investigation. A. Hook, J.D. Massa, **F.E. Celik**

2:05 CATL **283.** Theoretical study looking into the role of different gallium species in catalytic alkane dehydrogenation. **U. Das**, A.B. Getsoian, J. Bunquin, B. Hu, G. Zhang, A. Hock, P.C. Stair, L.A. Curtiss, J.T. Miller

2:35 CATL **284.** Supported nickel catalysts for propane dehydrogenation. **D.C. Rosenfeld**, P. Dellinger, J. Chen, B.A. Kilos, L. Luo

3:05 Intermission.

3:20 CATL **285.** Dry method synthesis of efficient Ni-Nb oxide catalysts for low temperature oxidative dehydrogenation of ethane to ethylene. H. Zhu, D. Rosenfeld, **J.M. Basset**

3:50 CATL **286.** Controlled synthesis of supported metal oxide catalysts. A. Love, S. Conrad, C.A. Carrero, **I. Hermans**

4:20 CATL **287.** Mixed metal oxide catalysts at sub-monolayer and monolayer coverage for natural gas upgrading. J. Grant, F. Huang, **C.A. Carrero**, I. Hermans

4:50 Concluding Remarks.

Section C

Colorado Convention Center
Room 111

Surface Chemistry and Catalysis on Oxides

Metal-Oxide Interface: Others

Z. Wu, Y. Xu, *Organizers*
W. Huang, *Organizer, Presiding*
J. Lu, *Presiding*

1:30 CATL **288.** Theory driven design of MnOx-modified TiO_2 for solar driven CO_2 activation. M. Nolan, K. Schwartzenberg, **J.M. Notestein**, K.A. Gray

2:05 CATL **289.** Withdrawn.

2:25 CATL **290.** Comparison of catalytic ozonations in the structural and functional groups changes of the filtered water. **W. Qun**, Y. Zhichao, G. Mingkun, C. Bin, X. He, C. Shuang

2:45 CATL **291.** Ternary metal oxide catalysts for electrochemical oxidation and reduction of oxygen. **J. Kim**, X. Yin, K. Tsao, P. Shih, X. Chen, H. Yang

3:05 Intermission.

3:15 CATL **292.** Synthesis of layer birnessite with different structure of water for formaldehyde removal at room temperature. **J. Wang**, P. Zhang

3:35 CATL **293.** Recyclable ionic liquid as soft template: Synthesis of mesoporous La-based transition metal perovskites. **H. Lu**, P. Zhang, **S. Dai**, Z. Qiao

3:55 CATL **294.** One-pot synthesis of ferrite aerogels via epoxide addition method. **R. Baghi**, D. Ua Cearnaigh, L. Hope-Weeks

4:15 CATL **295.** Polymer brushes: Modular hybrid nanostructures for supported catalysis. **A.E. Fernandes**, Q. Ye, B. Nysten, O. Riant, A.M. Jonas

4:35 Concluding Remarks.

Section D

Colorado Convention Center
Room 108

General Papers

V. Schwartz, *Organizer*
A. K. Mann, *Organizer, Presiding*

1:10 Introductory Remarks.

1:15 CATL **296.** Different catalytic oxidation behaviors of 1-propanol on size-controlled platinum nanoparticles at solid-gas and solid-liquid interfaces. **F. Liu**, A. Sapi, H. Wang, K. An, G.A. Somorjai

1:35 CATL **297.** Partial oxidation of surrogate Jet-A fuel over SiO_2 supported nanoparticle MoO_3. **S. Shah**, S. Ha, M.G. Norton, K. Chinnathambi

1:55 CATL **298.** Influence of sulfur on carbon deposition on Pt/Al_2O_3 catalysts during alkane oxidation. **C. O'Brien**, D.T. Tran, I. Lee

2:15 CATL **299.** Withdrawn.

2:35 CATL **300.** Catalytic deoxygenation of model and algal lipids to fuel-like hydrocarbons over supported nickel alloy catalysts. **R. Loe**, T. Morgan, E. Santillan-Jimenez, M. Crocker

2:55 CATL **301.** Reaction study of model bimetallic CoM_x catalysts for Fischer-Tropsch synthesis. **W. Ralston**, G. Melaet, W. Liu, S. Alayoglu, G.A. Somorjai

3:15 Intermission.

3:30 CATL **302.** Plasma-derived nanometric Co/C and Fe/C catalysts for Fischer-Tropsch synthesis. **J. Aluha**, N. Braidy, Y. Hu, A. Dalai, N. Abatzoglou

3:50 CATL **303.** Actinide-amido complexes as switchable catalysts for linear oligomerisation and [2+2+2] cycloaddition of terminal alkynes. **R. Batrice**, J. McKinven, P.L. Arnold, M.S. Eisen

4:10 CATL **304.** Theoretical insights into development of bio-inspired catalysts for peptide hydrolysis. **R. Prabhakar**

4:30 CATL **305.** Improving the catalytic performance of HZSM-5 by alkaline and acid treatments for the alkylation of benzene with methanol. **J. Lv**, X. Huang

4:50 CATL **306.** Inducing chemical interaction via in situ polymerization for graphene-reinforced ion-exchange resin catalyst design and application. **Y. Li**, . He, W. Yang

5:10 CATL **307.** Synergism between anatase and rutile: Effect of Initial particle size of TiO_2 for photocatalytic water splitting. **K. Ahmed**, M. Al-Oufi, S. Muhammad Bashir, H. Idriss

5:30 CATL **308.** Photocatalytic hydrogen production from water over Au-Pd/TiO_2 and Ag-Pd/TiO_2. **S. Muhammad Bashir**, K. Ahmed, M. Al-Oufi, H. Idriss

THURSDAY MORNING

Section A

Colorado Convention Center
Room 107

Novel Catalytic Materials for Renewable Fuels/Chemicals

M. Foston, J. C. Hicks, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 CATL **309.** Studies of the reductive disassembly of lignocellulose to value-added chemicals. **P.C. Ford**, C.M. Bernt, M.A. Chui, Z. Jones, G. Bottari, F. Brunner, H. Maneesuwan, K. Barta, A. Iretski, S.L. Scott

8:55 CATL **310.** Hierarchical ZSM-5 for the production of renewable aromatics from biomass via Diels Alder cyclo-addition of 2,5-dimethylfuran with ethylene. J. McGlone, P. Priecel, **J. Lopez-Sanchez**

9:15 CATL **311.** Renewable feedstocks via olefin metathesis: A high throughput workflow for the discovery of novel homogeneous olefin metathesis catalysts. **D.R. Romer**, V.J. Sussman, K. Miller

9:35 CATL **312.** Highly dispersed SiO_2/Al_2O_3 materials: Catalytic relevance of the isolated silanol site. **A. Mouat**, C. George, T. Kobayashi, R.P. Van Duyne, T.J. Marks, P.C. Stair

9:55 Intermission.

10:05 CATL **313.** Upgrading renewable feedstocks to fatty alcohols, esters, and paraffins via novel single stage hydroprocessing. **C. Chen**, A.E. Kuperman, W.J. Cannella

10:25 CATL **314.** Novel polymeric acid catalysts for biomass hydrolysis and dehydration. **X. Qian**, A. Vu

10:45 CATL **315.** Modified silicas as solid acid catalysts for esterification reactions: Convenient materials for deacidification of biodiesel feedstocks. **A. Puente-Urbina**, G. Valle-Bourrouet

11:05 CATL **316.** Mechanistic insights on glycerol decomposition on PtMo bimetallic catalysts from first-principles methods. **B. Liu**, J.P. Greeley

Section B

Colorado Convention Center
Room 109

Catalytic Materials and Technologies for Upgrading of COx and Natural Gas

Carbonylation, Metathesis, Reforming

J. Bravo-Suarez, B. A. Kilos, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 CATL **317.** Revisiting and reimaging C2 carbonylation to propionates. **J.M. Notestein**, C. Yang, S. Yacob, S. Park, R. Watson, L.R. McCullough, E. Weitz, H.H. Kung, B.A. Kilos, D.G. Barton

8:50 CATL **318.** How do oxide catalyst structure and composition dictate the rate and selectivity of light olefin metathesis? Z. Cheng, **C. Lo**

9:20 CATL **319.** Alkane and olefin metathesis with well-defined $W(Me)_6$ supported on silica/silica-alumina catalysts. M. Samantaray, E. Callens, N. Riache, R. Dey, A. Hamieh, A. Dery, N. Kharbatia, M. Atiqullah, **J.M. Basset**

9:50 CATL **320.** Effect of oxidant and hydrocarbon-type on syngas production over $Ba_{0.75}Ni_xAl_{12-x}O_{19-\delta}$ reforming catalysts. **T.H. Gardner**, J.J. Spivey, E.L. Kugler

10:20 Intermission.

10:35 CATL **321.** Ni-Ce-O catalysts for the reforming of ethanol and methane: Importance of metal-support interactions. **J. Rodriguez**

11:05 CATL **322.** Vapor phase ethanol carbonylation over supported rhodium catalysts. **S. Yacob**, B.A. Kilos, D.G. Barton, J.M. Notestein

11:35 CATL **323.** Transition metal sulfide catalysts for ethylene carbonylation. **R. Watson**, B.A. Kilos, D.G. Barton, J.M. Notestein, H.H. Kung

12:05 Concluding Remarks.

Section C

Colorado Convention Center
Room 111

General Papers

V. Schwartz, *Organizer*
A. K. Mann, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 CATL **324.** Monolithic flow microreactors using silver supported on hierarchically porous silica and cobalt oxide: Activity and stability. T. Kotbagi, Y. Hakat, **M.G. Bakker**

8:25 CATL **325.** Consistent reaction mechanism for the selective catalytic reduction of NO with NH_3. **S. Mossin**, A. Godiksen, T.V. Janssens, H. Falsig, L.F. Lundegaard, P.N. Vennestrøm, S.B. Rasmussen, P. Moses, F. Giordanino, E. Borfecchia, K. Lomachenko, C. Lamberti, S. Bordiga, P. Beato

9:05 CATL **326.** Pyrene-based porous organic framework for efficient heterogeneous visible-light photocatalysis. **J. Lu**, J. Zhang

9:25 CATL **327.** Tripodal titanium silsesquioxanes: Selective catalysts for alkene epoxidation. **S. Peak**

9:45 Intermission.

10:00 CATL **328.** Catalytic consequences of MgAlO rate of hydration: An in-situ XRD study. **K. Goulas**, E. Sacia, S. Rengshausen, D. Toste, A.T. Bell

10:20 CATL **329.** In-situ atomic force microscopy study of metal surfaces for catalytic hydrogenation membrane reactors. **M.J. Young**, P.H. Pfromm, M.E. Rezac, B.M. Law

10:40 CATL **330.** Au, Ag, and Au-Ag catalysts supported on SBA15 for the selective hydrogenation of butadiene. **N. Masoud**, L. Delannoy, K. De Jong, C. Louis, P. de Jongh

11:00 CATL **331.** Enhanced catalytic hydrogenation performance over size-controlled Pt-NiO@SiO_2 mesoporous core-shell nanocatalysts. **H. Liu**, Y. Hu, P. Zhang, S. Zhou, C. Xiong, H. Jiang

11:20 CATL **332.** Catalytic hydrogenation of isophthalonitrile (IPN) over supported monometallic and bimetallic Ni catalysts. C. Liu, **T. Wang**

11:40 CATL **333.** Metal deposition on TiO_2 using potassium iodide as an anchoring element to enhance hydrogen production via photocatalytic water splitting. **H. AlGhamdi**, T. Ahmed, K. Katsiev, H. Idriss

Section D

Colorado Convention Center
Room 108

Theoretical and Experimental Synergies at the Frontiers of Renewable Energy Catalysis

CO_2 Reductions

J. A. Keith, A. J. Morris, *Organizers, Presiding*

8:30 Introductory Remarks.

8:40 CATL **334.** Inverse design and characterization of catalytic systems for CO_2 reduction. **V.S. Batista**

9:10 CATL **335.** Molecular electrocatalytic reduction of CO_2 — mechanistic insights. **C. Costentin**, J. Savéant

9:40 CATL **336.** Reduction of CO_2 to methanol catalyzed by a biomimetic organo-hydride produced from pyridine. **C. Lim**, A. Holder, J.T. Hynes, C. Musgrave

10:00 Intermission.

10:20 CATL **337.** Carbon dioxide reduction by earth abundant catalysts in artificial photosynthesis: Mechanistic insights and challenges. **C.P. Kubiak**

10:50 CATL **338.** Mechanisms of rhenium- and manganese-catalyzed electrochemical reduction of CO_2 from theory. **E.A. Carter**

11:20 Concluding Remarks.

THURSDAY AFTERNOON

Section A

Colorado Convention Center
Room 107

Novel Catalytic Materials for Renewable Fuels/Chemicals

M. Foston, J. C. Hicks, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 CATL **339.** Platinum-cobalt-graphene catalysts for alkaline fuel cells. J. Jablonskiene, **L. Tamasauskaite-Tamasiunaite**, K. Antanaviciute, A. Balciunaite, V. Kepeniene, A. Zieliene, L. Naruskevicius, R. Kondrotas, R. Juskenas, E. Norkus

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1:55 CATL **340.** Nanostructured nickel and cobalt phosphides as electrocatalysts for the hydrogen evolution reaction. **E.J. Popczun**, R.E. Schaak, C.G. Read

2:15 CATL **341.** Withdrawn.

2:35 CATL **342.** Theoretical investigation of thermodynamic and kinetic properties of dihydropyridines in the catalytic reduction of CO_2 and various unsaturated functional groups. **Y. Kuo**, C. Lim, A. Holder, J.T. Hynes, C. Musgrave

2:55 Intermission.

3:05 CATL **343.** Gold nanowires as an efficient and durable catalyst for CO_2 reduction. **W. Zhu**, Y. Zhang, H. Zhang, H. Lv, Q. Li, A.A. Peterson, S. Sun

3:25 CATL **344.** Design of visible light activated TiO_2 photocatalysts from first principles simulations. **M. Nolan**

3:45 CATL **345.** Carbon negative, renewable energy compatible electrochemical process for converting CO_2 and water into CO and H_2. **D. Kauffman**, C. Matranga, D. Alfonso, J. Thakkar, R. Jin

Section B

Colorado Convention Center
Room 109

Catalytic Materials and Technologies for Upgrading of COx and Natural Gas

CO_2 Activation

J. Bravo-Suarez, B. A. Kilos, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 CATL **346.** Electrochemical reduction of CO_2 to fuels. **A.T. Bell**

2:05 CATL **347.** CO_2 splitting in a packed-bed dielectric barrier discharge reactor. **K.J. Nordheden**, A.M. Banerjee, J. Billinger, S.M. Stagg-Williams, B. Subramaniam

2:35 CATL **348.** Carbon depositions and kinetic study over Ni-based catalysts in steam-CO_2 reforming of methane. **Y. Park**, Y. Kim, D. Moon

3:05 Intermission.

3:20 CATL **349.** Functionality and topology dependence of CO_2/CH_4 adsorption and selectivity in zeolitic imidizolate frameworks (ZIFs). **B.B. Laird**

3:50 CATL **350.** Conversion of CH_4 and CO_2 into acidic acid on zinc-modified H-ZSM-5 zeolite. **W. Wang**, J. Wu, S. Yu

4:20 CATL **351.** Simultaneously converting carbonate/bicarbonate and biomass to value-added carboxylic acid salts by aqueous-phase hydrogen transfer. **H. Lin**, J. Su

4:50 CATL **352.** Engineering Co-exposed (001) and (101) facts and defects in TiO_2 nanocrystals for enhanced CO_2 photoreduction. **L. Liu**

5:20 Concluding Remarks.

Section C

Colorado Convention Center
Room 111

General Papers

V. Schwartz, *Organizer*
A. K. Mann, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CATL **353.** Colloidal supported metal nanoparticles (CSMNs) as novel intermediate nanocatalysts for the Suzuki and Heck reactions. **R. Narayanan**, K. Gude

1:55 CATL **354.** Model nanoparticle and zeolite catalysts for high selectivity hydrocarbon reforming. **N. Musselwhite**, S. Alayoglu, K. Na, K. An, G.A. Somorjai

2:15 CATL **355.** Stability and phase transfer of catalytically-active nanoparticle suspensions. **I. Sriram**, K. Jeerage

2:55 CATL **356.** Cu and CoCu surfaces in equilibrium with CO at Torr pressures. **B. Eren**, M. Salmeron, G.A. Somorjai

3:15 Intermission.

3:30 CATL **357.** Identify the active species in ligand and base-free Cu-catalyzed aerobic homo-coupling of alkynes. **L. Liu**, A.L. Perez, **A. Corma**

3:50 CATL **358.** Metal-ligand cooperation in methanol/water dehydrogenation. **M. Trincado**

4:10 CATL **359.** New composite catalyst for trioxane production: Dramatic salt effect on trioxane synthesis. **L. Yin**, Y. Hu, Z. Yang, J. Qi

4:30 CATL **360.** Surface-bound ligands modulate chemoselectivity and activity of a bimetallic nanoparticle catalyst. **V.O. Rodionov**, B. Vu, K. Bukhriakov

4:50 CATL **361.** Controlled synthesis of Pd-NiO@SiO_2 mesoporous core-shell nanoparticles and their enhanced catalytic performance for *p*-chloronitrobenzene hydrogenation with H_2. **S. Zhou**, H. Liu, K. Tao

5:10 CATL **362.** Ti^{3+}- and V-doped TiO_2 quantum dots loaded on MCM-41 for photocatalytic degradation of organic dyes and isomerization of norbornadiene. **L. Pan**, **J. Zou**, S. Wang, Z. Huang, L. Wang, X. Zhang

CELL

Division of Cellulose and Renewable Materials

C. Frazier, *Program Chair*

OTHER SYMPOSIA OF INTEREST:

Next Generation Smart Materials *(see POLY, Sun, Mon, Wed, Thu)*

Water Our Most Critical Resource *(see AGFD, Wed, Thu)*

Biofuels & Sustainable Energy: Biomass Pretreatment & Hydrolysis *(see BIOT, Tue, Wed, Thu)*

Colorado Biotechnology: The Science of Colorado's Craft Beer, Wine & Spirits Industries *(see BIOT, Sun)*

Nanoscale Spectroscopic and Microscopic Characterization *(see PMSE, Tue, Wed)*

SOCIAL EVENTS:

Dinner, 6:30 PM, Tue

BUSINESS MEETINGS:

CELL Division Business Meeting, 5:00 PM: Wed

CELL Division Executive Committee Meeting, 5:00 PM: Sat

SUNDAY MORNING

Section A

Colorado Convention Center
Room 403

Cellulose in Solid State and Solution — Structure, Chemistry and Reaction Mechanisms: Anselme Payen Award Symposium in Honor of Thomas Rosenau

Structural Aspects of Cellulose and NMR Studies

F. Liebner, L. Lucia, A. Potthast, *Organizers*
P. Kosma, J. Ralph, *Presiding*

8:00 Introductory Remarks.

8:05 CELL **1.** Thomas Rosenau, playful explorer of the mysteries of cellulose. **A.D. French**

8:35 CELL **2.** Imperfections in higher plant cellulose: Crystal stacking faults and structure of crystal-crystal interfaces. **C. Driemeier**

9:05 CELL **3.** Fabrication and characterization of cellulose nanoanemone. **T. Kondo**

9:35 CELL **4.** Cellulose nanocrystals: New preparation routes, and the relationship to the structure of native cellulose. **E. Kontturi**

10:05 Intermission.

10:20 CELL **5.** Structural characteristics influencing the reactivity of isolated cellulose **I. T. Larsson**

10:50 CELL **6.** Identifying different hydroxyl populations in cellulose by ^{2}H MAS NMR. **E. Lindh**, C. Terenzi, I. Furó, L. Salmén

11:20 CELL **7.** High-resolution solution-State NMR of wood and pulp in ionic liquid electrolytes. A.J. Holding, V. Mäkelä, K.J. Helminen, I. Kilpelainen, **A.W. King**

11:50 CELL **8.** NMR analysis of periodate-oxidation products of 5-*N*-acetylneuraminic acid methyl glycosides and 2,8-polysialic acid (PSA). **P. Kosma**

Section B

Colorado Convention Center
Room 404

Functional Lignocellulosics and Nanotechnology

I. Filpponen, S. Spirk, *Organizers*
T. Nypelö, M. S. Peresin, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 CELL **9.** Pickering foams from cellulose nanofibrils. **L. Wagberg**, N. Tchang Cervin

8:35 CELL **10.** Inhibition of alphavirus infection with tyrosine sulfate mimetic cellulose nanocrystals. **J.O. Zoppe**, V. Ruottinen, J. Ruotsalainen, S. Rönkkö, L. Johansson, A. Hinkkanen, K. Järvinen, J. Seppälä

8:55 CELL **11.** Modification of nanocellulose with natural molecules: A green perspective for cellulose based materials with active properties. **A. Garcia**, A. Gandini, N. Belgacem, J. Bras

9:15 CELL **12.** Size exclusion nanocellulose based paper filter for virus removal. **A. Mihranyan**

9:35 CELL **13.** Antibacterial surface modification of nanocellulosic materials. **J. Henschen**, J. Illergård, P. Larsson, M. Ek, L. Wågberg

9:55 Intermission.

10:15 CELL **14.** Tuning the properties and yield of cellulose nanocrystals in the production space. **J. Zhu**

10:35 CELL **15.** Properties of nanocellulose from wood pulp and bacterial cellulose obtained by different methods. **L. Vikele**, I. Sable, L. Rozenberga, R. Treimane, A. Treimanis, P. Semjonovs

10:55 CELL **16.** Nanocrystalline cellulose from agricultural waste for optical devices. **L. Steiner**, A.G. Dumanli, D. Reid, M. Duer, S. Vignolini

11:15 CELL **17.** Characterisation and reinforcing properties of cellulose nanocrystals esterified in water. **B. Dhuiege**, G. Sèbe

11:35 CELL **18.** Control of the surface properties of cellulose nanocrystals by transesterification of vinyl esters. **J. Brand**, G. Sèbe

11:55 CELL **19.** One step polymer grafting of poly(methyl methacrylate) from cellulose nanocrystals for composite applications. **S. Kedzior**, L. Graham, E.D. Cranston

Section C

Colorado Convention Center
Room 405

Advances in Lignocellulosic Materials and Chemistry: A Tribute to W.G. Glasser

Green Chemicals from Lignocellulosics

G. Garnier, S. Kelley, *Organizers*
T. G. Rials, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 CELL **20.** Mechanisms of biogenic formaldehyde generation in wood. **C.E. Frazier**, G. Wan, M. Tasooji, H. Wise

8:35 CELL **21.** Amphipathic lignin derivatives for enzymatic saccharification and fermentation of lignocellulosics. **Y. Yamamoto**, N. Cheng, K. Igarashi, K. Koda, Y. Uraki

9:05 CELL **22.** Homogeneous tosylation of agarose as an approach towards functional bio-based materials. **M. Gericke**, T.J. Heinze

9:35 Intermission.

9:50 CELL **23.** From sustainable chemical blocks to fuel: Synthesis of hydrocarbons from isoprene and acrolein. **Z. Tong**, F. Wang

10:20 CELL **24.** Development of an efficient polymer analogous reaction in ionic liquids and its application to chemical modification of lignocellulose. **R. Kakuchi**, Y. Shibata, M. Yamaguchi, K. Takahashi

10:50 CELL **25.** Fundamental approaches to multiscale, multiphase phenomena in cellulose pyrolysis chemistry. **C. Krumm**, A. Paulsen, P.J. Dauenhauer

11:20 CELL **26.** Valorization of lignin to renewable fuels and chemicals through biological funneling and chemical catalysis. **D. Vardon**, M. Franden, C. Johnson, E. Karp, M. Guarnieri, J. Linger, P. Pienkos, T.J. Strathmann, G. Beckham

Section D

Colorado Convention Center
Room 406

Lignin Biosynthesis, Characterization and Modifications

Lignin Biosynthesis and Biotechnical Conversion

T. Tamminen, *Organizer*
C. Crestini, *Organizer, Presiding*

8:00 CELL **27.** β-O-4 -type quinone methides in lignin biosynthesis and in pulping. **J. Sipila**, A. Haikarainen, P. Nousiainen, M. Muuronen

8:30 CELL **28.** Molecular models of milled-wood lignin. **P. Schiffels**, H. Lange, C. Crestini

9:00 CELL **29.** Mechanical properties of bamboo nanofibers: An atomistic simulation study. S. Youssefian, **N. Rahbar**

9:30 CELL **30.** Impact of changes in the lignin synthetic pathway on cell wall architecture. **J. Liu**, J.C. Cusumano, J. Kim, C. Chapple, L. Makowski

10:00 Intermission.

10:15 CELL **31.** Diastereoselective fungal lignolysis. **D.J. Yelle**, A.N. Kapich, C. Houtman, F. Lu, V. Tymokhin, R.C. Fort, J. Ralph, K. Hammel

10:45 CELL **32.** Exquisite sensitivity of Acridine Orange to lignocellulosic oxidation and mechanistic investigation. P. Kitin, J. Worple, J. Houtman, K.E. Hammel, **C.G. Hunt**, C.J. Houtman

11:15 CELL **33.** Lipoxygenase: A new oxidative enzyme for lignin biorefinery. **C. Crestini**, H. Lange, P. Giannì, E. Bartzoka

11:45 CELL **34.** Quantitation of S/G ratio in woods using 1064 nm FT-Raman spectroscopy. **U.P. Agarwal,** S. Ralph

Section E

Colorado Convention Center
Room 407

Application of Computational Chemistry to Biomass Chemistry and Utilization

Synthesis and Molecular-level Interactions of Cellulose

S. C. Chmely, T. J. Elder, *Organizers*
P. Ramakrishnan, *Presiding*

8:00 CELL **35.** Synthesizing cellulose. **B.C. Knott**, M.F. Crowley, M. Himmel, J. Zimmer, G. Beckham

8:30 CELL **36.** QM/MM and MD study on catalytic mechanism of bacterial CESA. **H. Yang**, J. Lee, J. Zimmer, Y.G. Yingling, J.D. Kubicki

9:00 CELL **37.** Molecular dynamics simulation study of the AxCeSD octamer compelxed with cellulose chains. **T. Yui**, T. Uto, Y. Ikeda, K. Tajima, M. Yao

9:30 CELL **38.** Molecular basis for cellulose twist. **M.F. Crowley**, L. Bu, M. Himmel

10:00 Intermission.

10:10 CELL **39.** DFT calculations on the thermodynamics of PCW component interactions. **J.D. Kubicki**, V. Gibilterra, T. Weiss, H. Watts, L. Petridis, P. Langan, L. Zhong

10:40 CELL **40.** Can crystal structure conformations help validate conformational analyses of isolated molecules? **A.D. French**

11:10 CELL **41.** Hydration control of the mechanical and dynamical properties of cellulose. **L. Petridis**, H.M. ONeill, M. Johnsen, B. Fan, E. Mamontov, J.K. Maranas, R. Schulz, P. Langan, J.C. Smith

11:40 CELL **42.** Modeling graphene-cellulose-water interactions. **S.J. Eichhorn**, R.A. Bryce, R. Alqus

SUNDAY AFTERNOON

Section A

Colorado Convention Center
Room 403

Cellulose in Solid State and Solution — Structure, Chemistry and Reaction Mechanisms: Anselme Payen Award Symposium in Honor of Thomas Rosenau

Plant Cell Walls and Biorefineries

F. Liebner, L. Lucia, A. Potthast, *Organizers*
H. Sixta, A. Van Heiningen, *Presiding*

1:30 CELL **43.** Recent progress on oxygen delignification of softwood Kraft pulp. **A. Van Heiningen**

2:00 CELL **44.** BLN hot water extraction process — taking forest biomass fractionation to a totally new level. **S. Willför**, L. Vähäsalo, S. von Schoultz

2:30 CELL **45.** Full utilization of wood in the future pulp mill bio-refinery. **P. Axegård**

3:00 CELL **46.** Influence of pectinase treatments on the dissolution abilities of cellulose pulps in NaOH-water. **P.R. Navard**, N. Dos Santos, J. Puls, B. Saake

3:30 Intermission.

3:45 CELL **47.** Nanoporous cellulose: A new form of cellulose with novel properties. **R.H. Atalla**, R.S. Atalla

4:15 CELL **48.** New model of plant cell wall cellulose elementary fibril. **U.P. Agarwal**

4:45 CELL **49.** Effect of cellulose polymorphism on the TEMPO-based oxidation and further grafting by amidation. **D. Da Silva Perez**, **Y. Habibi**, A. Guillemain, J. Puteaux, L. Heux

5:15 CELL **50.** Porosity development of dissolving pulp during mechanical and enzymatic processing. **S. Grönqvist**, T. Hakala, T. Kamppuri, M. Vehviläinen, T. Liitiä, T. Maloney, A. Suurnäkki

Section B

Colorado Convention Center
Room 404

Functional Lignocellulosics and Nanotechnology

T. Nypelö, M. S. Peresin, S. Spirk, *Organizers*
I. Filpponen, *Organizer, Presiding*
T. Tammelin, *Presiding*

1:30 CELL **51.** Functionalising micro/nano-fibrillated cellulose with TEMPO-based approaches: From laboratory to pilot scale. **D. Da Silva Perez**, A. Guillemain, S. Tapin-Lingua, V. Meyer, B. Fabry, P. Huber

1:50 CELL **52.** Structurally colored films using nanocellulose fiber. **S.J. Eichhorn**, P. Vukusic, D. Hewson, J.C. Grunlan, P. Tzeng

2:20 CELL **53.**
Architecture and properties of hybrid cellulose nanocrystals/Gibbsite nanoplatelets multilayered films. **C. Martin**, R. Barker, E.D. Cranston, L. Heux, B. Jean

2:40 CELL **54.** Functional cellulose nanocrystals for ATRP and click chemistry-preparation and characterization. **A. Carlmark**, A. Boujemaoui, S. Mongkhontreerat, E.E. Malmstrom

3:00 CELL **55.** Surfactant and polymer-enhanced CNC Pickering emulsions, gels, and oil powders. Z. Hu, R.H. Pelton, **E.D. Cranston**

3:20 Intermission.

3:40 CELL **56.** Cellulose nanocrystals with CO_2-switchable aggregation and redispersion properties. H. Wang, J. Bouchard, P.G. Jessop, P. Champagne, **M.F. Cunningham**

4:00 CELL **57.** Nanocellulose composites for electronic paper displays. **A.G. Dumanli**, H. Yuan, U. Steiner

4:20 CELL **58.** Withdrawn.

4:40 CELL **59.** Composite fibers from cellulose nanofibril emulsions. **T. Nypelö**, C.A. Carrillo, O.J. Rojas

5:00 CELL **60.** Structure and properties of carboxylated nanocellulose with various counter-ions. **M. Shimizu**, T. Saito, A. Isogai

5:20 CELL **61.** Thermoresponsive TOCN films: Influence of PNIPAm on film properties. **N. Lavoine**, J. Bras, T. Saito, A. Isogai

Section C

Colorado Convention Center
Room 405

Advances in Lignocellulosic Materials and Chemistry: A Tribute to W.G. Glasser

Fundamentals of Cellulosic Materials

S. Kelley, T. G. Rials, *Organizers*
G. Garnier, *Organizer, Presiding*

1:30 CELL **62.** Contributions of computational chemistry to understanding cellulose. **A.D. French**

2:00 CELL **63.** Pros and cons of various cellulose crystallinity estimation methods: 380-Raman, ^{13}C NMR, and Segal-WAXS. **U.P. Agarwal**

2:30 CELL **64.** Interactions between rod-shaped nanoparticles and polymer chains in aqueous solutions. **H. Oguzlu**, Z. Khalili, Y. Boluk

3:00 CELL **65.** Synthesis and properties of fatty acid esters of technical lignins for biorefinery applications. K. Koivu, H. Sadeghifar, P. Nousiainen, D. Argyropoulos, **J. Sipila**

3:30 Intermission.

3:45 CELL **66.** Single step functionalization of cellulose to produce bacterial cellulose-reinforced derivatised all-cellulose nanocomposites. K. Lee, **A. Bismarck**

4:15 CELL **67.** Polymer-grafting or adsorption of amphiphilic block copolymers — different approaches to compatibilization in CNF-based nanocomposites. **E.E. Malmström**, C. Bruce, L. Fogelström, M.K. Johansson, A. Carlmark

4:45 CELL **68.** Cellulose surfaces modified by latex particles prepared via RAFT-mediated emulsion polymerization. **A. Carlmark**, L.K. Carlsson, E.E. Malmstrom, L. Wagberg, J. Engström, F. Hatton, M. Jawerth, C. Freire, F. D'Agosto, M. Lansalot

5:15 CELL **69.** Model cellulose surfaces to characterize (bio)polymer interaction: Designing the interphase. **G. Garnier**, J. Su, C. Garvey, W. Batchelor, W. Raverty

Section D

Colorado Convention Center
Room 406

Lignin Biosynthesis, Characterization and Modifications

Lignin Characterization

C. Crestini, *Organizer*
T. Tamminen, *Organizer, Presiding*

1:30 CELL **70.** Why "laboratory standard" is not good enough in GPC-analyses of lignins. **H. Lange**, F. Rulli, C. Crestini

2:00 CELL **71.** Enzyme surface hydrophobicity predicts enzyme adsorption to lignin films. **D. Sammond**, J. Yarbrough, E. Mansfield, Y.J. Bomble, M. Resch, J.J. Bozell, M.E. Himmel, M.F. Crowley

2:30 CELL **72.** Comparing different approaches to measure molar mass of lignin: SEC, DOSY and AsFlFFF. **I. Sulaeva**, I. Sumerskii, M. Bacher, G. Zinovyev, U. Henniges, T. Rosenau, A. Potthast

3:00 CELL **73.** Exploring the use of pulsed field gradient (PFG) NMR to extract molecular weight distributions of lignin. J.O. Thomas, **C.F. Clewett**, T.M. Alam

3:30 Intermission.

3:45 CELL **74.** Analysis of lignin hydroxyl groups by NMR spectroscopy. **E.A. Capanema**

4:15 CELL **75.** Characterization of alkaline lignin by thermal desorption and pyrolysis methods. **K. Voeller**, A. Kubatova, E.I. Kozliak

4:45 CELL **76.** Low-field NMR study of interactions between lignin and cellulase. M. Li, J. Yang, M. Tu, **T.J. Elder**

5:15 CELL **77.** Facile quantification of biomass lignin using acidic lithium bromide (ALB) method. **N. Li**, J. Alexander, X. Pan

Section E

Colorado Convention Center
Room 407

Application of Computational Chemistry to Biomass Chemistry and Utilization

Cellulose Degradation and Conversion

S. C. Chmely, T. J. Elder, *Organizers*
P. Ciesielski, *Presiding*

1:30 CELL **78.** Solvation dynamics and energetics of hydride transfer reactions in cellulosic biomass conversion. **S. Mushrif**, C. BK, J.J. Varghese

2:00 CELL **79.** Frequency filtration to obtain realistic thermal vibrations in crystal from molecular dynamics. **Y. Ogawa**, Y. Nishiyama, K. Mazeau

2:30 CELL **80.** Mechanism of alkyl and alkaline earth chloride-enhanced hydrolysis of cellulose in acid solutions. **P. Chen**, B. Rabideau, A.E. Ismail

3:00 CELL **81.** Computational targets for reaction pathways and energetics of cellulose conversion to fuels and chemicals. **P.J. Dauenhauer**

3:30 Intermission.

3:40 CELL **82.** Interference trinity: Lignins' role in biomass recalcitrance explored through petascale simulation. **J.V. Vermaas**, X. Qi, R. Schulz, L. Petridis, J.C. Smith

4:10 CELL **83.** Unmasking the mystery base employed by the *T. reesei* Cel6A cellulase. **H. Mayes**, B. Knott, M.F. Crowley, A.W. Goetz, J. Ståhlberg, L.J. Broadbelt, G. Beckham

4:40 CELL **84.** Role of water on metal catalyst performance for ketone hydrogenation: A joint experimental and theoretical study on levulinic acid conversion into gamma-valerolactone. **C. Michel**, J. Zaffran, A.M. Ruppert, J. Matras-Michalska, M. Jedrzejczyk, J. Grams, P. Sautet

5:10 CELL **85.** Multiscale modeling of the interfacial structure in xylan/cellulose nanocomposites. **K. Mazeau**, P. Perre, I. Li, X. Frank

SUNDAY EVENING

Section F

Colorado Convention Center
Hall C

Advances in Lignocellulosic Materials and Chemistry: A Tribute to W.G. Glasser

Posters

G. Garnier, S. Kelley, T. G. Rials, *Organizers*

6:00 - 8:00

CELL **86.** Macroalgae as filler in thermoplastic composites: Opportunities and weaknesses. **M. Bulota**, T. Budtova

CELL **88.** Where are the *gauche-gauche*-CH_2OH groups in cellulose I materials? **U.P. Agarwal**

CELL **90.** Study of nitrogen fixation by condensation of urea on hydrothermally treated corncob. **J.A. Cordoba Arias**, E. Salcedo Pérez, R. Manriquez Gonzalez, E. Delgado

CELL **93.** Analysis of recalcitrant lignin structures to understand the impact of alkaline hydrothermal pretreatment on enzyme digestibility. **L. Xiao**, Y. Bai, X. Chen, Z. Xue, R. Sun

CELL **94.** Synthesis and characterization of novel green wood adhesives from biorefinery lignin. **P.S. Dongre**, **M. Driscoll**, J. Smith, T. Amidon, **B. Bujanovic**

CELL **96.** Properties of regenerated bamboo fibers prepared from raw materials with different hemicellulose content. **J. Chen**, K. Wang, F. Xu, R. Sun

CELL **99.** Structural characterization of annealed bacterial cellulose by SFG, FTIR and XRD. **Y. Weng**, K. Kafle, S.H. Kim, J.M. Catchmark

CELL **101.** Microwave-assisted carbonization of bamboo by wet torrefaction in diluted acid. **M. Li**, Y. Shen, J. Sun, C. Chen, X. Li, R. Sun

CELL **102.** Production of furfural from hemicelluloses in biphasic system by highly efficient and recyclable magnetic solid acid from glucose. **Y. Bai**, L. Xiao, X. Chen, R. Sun

CELL **105.** Systematic evaluation on degradation products during hydrothermal pretreatment of sweet sorghum basis for biorefinery. **S. Sun**

CELL **107.** Sustainable bitumen. **T. Slaghek**, D.V Vliet, I. Haaksman, C. Giesen

CELL **109.** Physical and structural changes in cellulose microfibrils responsible for enzymatic hydrolysis rate deactivation studied by FTIR, XRD, XPS and SFG. **K. Kafle**, C. Lee, H. Shin, S.H. Kim, S. Park

CELL **111.** Impact of fractionation time on thermal and chemical properties of organosolv lignins. **J. Tao**, O. Hosseinaei, P. Kim, D.P. Harper, J.J. Bozell, T.G. Rials, N. Labbe

CELL **112.** In situ catalytic fast pyrolysis of lignin for production of phenols using oxide catalysts. **V. Nair**, V. R

CELL **115.** All-cellulose composites from partial periodate oxidation and thermal crosslinking. **N. Guigo**, A. Codou, L. Heux, N. Sbirrazzuoli

Section F

Colorado Convention Center
Hall C

General Posters

Cosponsored by CARB

C. E. Frazier, *Organizer*

6:00 - 8:00

CELL **87.** Use of micro-structured cellulose from soybean hulls as coating additives for paper. **A. Ferrer**, C.L. Salas, T.W. Theyson, O.J. Rojas

CELL **89.** Bioinspired xyloglucan-containing films as responsive smart materials. **A. Villares**, C. Moreau, **B. Cathala**

CELL **91.** Cellulose nanoparticles from new sources – agricultural wastes: Apple tree (*Malus domestica*) pruning residues and pea (*Pisum sativum*) stalks. **A. Garcia**, A. Gandini, J. Labidi, N. Belgacem, J. Bras

CELL **92.** Hybrid composites with microcrystalline cellulose, lignin, and polyethylene. **A. Treimanis**, M. Laka, J. Ganster, J. Erdmann, L. Ziegler

CELL **95.** Sulfite pretreatment of post-enzymatic hydrolysis softwood residue to enhance saccharification and produce lignosulfonates. **B. Jeuck**, O.J. Rojas, H. Jameel

CELL **97.** Process simulation of biomass fast-pyrolysis into transportation fuels: Model sensitive to variations in biomass chemical composition. **C.E. Aizpurua**, H. Kim, H. Jameel, M. Wright, S.S. Kelley, S. Park

CELL **98.** Characterization and evaluation of the lignin from one-pot HDA process for chemical transformation of biomass into hydrocarbons. **C. Yoo**, S. Zhang, H. Kim, J. Zeng, J. Ralph, Z. Tong, X. Pan

CELL **100.** Study on the characteristics of two marine oil-degraded yeasts and their utilization for carbon source spectrum of crude oil. **C. Ma**, J. Liu, N. Ma, X. Mou, N. He

Technical program information known at press time. The official technical program for the 249th ACS National Meeting is available at: www.acs.org/denver2015

‡ *Cooperative Cosponsorship*

CELL **103.** Novel production of furfural from biomass based on hot water extracted pentoses. **C.D. Wood**, B. Bujanovic, T. Amidon

CELL **104.** Cooxidant-free TEMPO-mediated oxidation of highly crystalline *Cladophora* nanocellulose. **D.O. Carlsson**, J. Lindh, L. Nyholm, M. Stromme, A. Mihranyan

CELL **106.** Potential for enhancement of enzymatic hydrolysis of sugar maple (*Acer saccharum*). M.A. Uygut, M. Zelie, C.D. Wood, **D.B. Corbett**, P.S. Dongre, B. Bujanovic

CELL **108.** Structures of carboxylated cellulose fibers – fates of S1, S2, and S3 layers. **G. Sim**, M.N. Alam, L. Godbout, T.G. van de Ven

CELL **110.** Development of 3 drug combination formulations with cellulose esters for the effective oral treatment of HIV. **H. Arca**, D. Dahal, K.J. Edgar

CELL **113.** Magnetic responsive hybrid paper materials that react to external magnetic fields. **H. Wang**, M. Biesalski

CELL **114.** Effect of different ratio of CMC and Eu(III) on the fluorescence properties and structures of CMC/Eu nanocomposites. B. Wang, J. Ye, **J. Xiong**

CELL **116.** One-pot formation of 2,3-dialdehyde cellulose (DAC) beads. **J. Lindh**, D.O. Carlsson, C. Ruan, M. Stromme, A. Mihranyan

CELL **117.** Interactions between cellulose surfaces and cellulases from different origins studied by QCM. **J. Song**, Y. Li, O.J. Rojas

CELL **118.** Isolation and structural analysis of novel sulphur-free lignin fraction from non-wood plant materials. **J. Sipila**, J. Kontro, P. Nousiainen, Y. Mälkki

CELL **119.** Vibrational sum-frequency-generation (SFG) spectroscopy study of cellulose microfibril orientation and assembly in onion epidermis and reaction woods. **K. Kafle**, X. Xi, R. Shi, C. Lee, A. Mittal, S. Park, B.R. Tittmann, V. Chiang, D. Cosgrove, Y. Park, S.H. Kim

CELL **120.** Determination of the molecular weight distribution of highly oxidized dialdehyde cellulose by size exclusion chromatography. I. Sulaeva, T. Rosenau, A. Potthast, **K. Klinger**

CELL **121.** Nanofibrillation of dried pulp in NaOH solutions and their regenerations. **K. Abe**

CELL **122.** Characterization of cellulose nanofibrils sheet mixed with synthetic or natural pulp fiber. **K. Sim**, H. Youn, J. Lee, H. Lee

CELL **123.** Theoretical models of electron transfer processes in LPMOs and model peptide systems. **L. Berstis**, M.F. Crowley, G. Beckham

CELL **124.** Continuous hydrolysis of carboxymethyl cellulose with cellulase aggregates trapped inside membranes. **L. Nguyen**, K. Yang

CELL **125.** Novel materials from wood component. **L.K. Carlsson**, P. Martirez, M. Helander, A. Lopéz Cabezas, O. Schmidt

CELL **126.** Production of nanocellulose through hydrolysis without mineral acids using sub-critical water. **L. Pereira Novo**, A. Garcia, A. da Silva Curvelo, N. Belgacem, J. Bras

CELL **127.** New nanohybrid materials from sugar cane bagasse: The role of acid hydrolysis. **L. Diaz**, R. Hernandez Ortiz, M. Tete, E. Mata, E. Sosa, R. Atencio

CELL **128.** Imaging cellulose nanocrystals by transmission electron spectroscopy. **M. Kaushik**, W. Chen, T.G. Van De Ven, A.H. Moores

CELL **129.** Evaluation of various parameters in the production of whey protein concentrate-based films. **M. Víquez**, M. Molina Cordoba, M. Esquivel Alfaro, M. Montero Calderon

CELL **130.** Immobilization of *glucose oxidase* in cellulose supports. **M.L. Auad**, R.A. Ballestero, O. Nordness, M. Arugula, A.L. Simonian

CELL **131.** Thermal protection of vitamins B1, B2, B3, B6 and B12 with bacterial nanocellulose. **M. Osorio Delgado**, D. Sanchez, J. Velásquez-Cock, R. Zuluaga Gallego, P. Gañán, C. Jiménez, O.J. Rojas, L. Velez-Acosta, B. Gómez, C. Castro Herazo

CELL **132.** Effects of time, temperature, and pH on the Interconversion of cellulose I to cellulose II. **M. Islam**, C.J. Huntley, W.E. Collier, M.L. Curry

CELL **133.** Polymeric functionalized beads from alginate for targeted release of auxin into water. **M. Li**, G. Buschle-Diller, T.J. Elder

CELL **134.** Moisture and solvent responsive cellulose/SiO_2 nanocomposite materials. **M. He**, B. Duan, L. Zhang

CELL **135.** Paper-based microfluidics for typing of primary and secondary human blood groups in "text". **M. Li**, W. Then, J. Tian, W. Shen

CELL **136.** In vitro synthesis of cellulose under various conditions. **P.A. Penttilä**, J. Sugiyama, T. Imai

CELL **137.** Method for studies of oxidoreductase catalyzed oxidation of synthetic lignin in presence of co-oxidants. **P. Nousiainen**, J. Kontro, H. Manner, A. Hatakka, J. Sipila

CELL **138.** Regenerated cellulosic fiber from ionic liquid-waste cotton solution by dry-jet wet spinning. **S. Asaadi**, M. Hummel, H. Sixta

CELL **139.** Evaluation of nanocelluloses as flooding additives for the petroleum industry. **S.N. Molnes**, K. Syverud, S. Strand, K.G. Paso

CELL **140.** Modification and optimization of cellulose nanocrystal-latex interactions. **S. Kedzior**, Z. Dastjerdi, M.A. Dubé, E.D. Cranston

CELL **141.** Structural stability of the molecular chain sheets composing the crystal structures of cellulose allomorphs: A theoretical study. **T. Uto**, T. Yui

CELL **142.** Characterization of noncrystalline regions in regioselectively methylated cellulosic films using vapor-phase deuteration and generalized 2D correlation infrared spectroscopy. Y. Hishikawa, **T. Kondo**

CELL **143.** Density functional theory calculations on concerted lignin pyrolysis mechanisms. **T.J. Elder**, A. Beste

CELL **144.** Effect of urea as an additive in the alkali pretreatment of cellulose I to cellulose II. **V. Uniyal**, P. Gupta, S. Naithani

CELL **145.** Iridescent 3D structures produced by evaporation of droplets of cellulose nanocrystal suspensions. **X. Mu**, D.G. Gray

CELL **146.** 3D nanofiber scaffolds of bacterial cellulose and chitosan generated from solution blowing spinning using an airbrush. **X. Yin**, L.A. Lucia, A. Nandgaonkar

CELL **147.** Hydrophobic functionalization of jute fabric via enzymatic grafting of octadecylamine. **X. Fan**, A. Dong, Q. Wang, P. Wang, J. Yuan

CELL **148.** Textile fibers from recycled waste materials. **Y. Ma**, S. Asaadi, M. Maattanen, A. Sarkilahti, M. Hummel, A. Harlin, H. Sixta

CELL **149.** Hemicellulose-based hydrogel containing Ag nanoparticles for antibacterial application. **Y. Guan**, F. Peng, R. Sun

CELL **150.** Antibacterial cellulose acetate films containing N-halamine modified nanocrystalline cellulose. **Y. Liu**, X. Ren, G. Buschle-Diller

CELL **151.** Direct chemical modificationand separation of biomass components using ionic liquids based organocatalysts. **Y. Shibata**, R. Kakuchi, K. Takahashi

CELL **152.** Preparation of butyl levulinate through the acid catalysed solvolysis of cellulose using a single reaction process. **Y. Hishikawa**, M. Yamaguchi, S. Kubo, T. Yamada

CELL **153.** Effect of molecular weight and chain length on surface and interfacial tension, emulsification and cleaning properties of polysaccharide-based surfactants derived from pectin. **Z. Mohd Aris**, V. Bavishi, N. Tchirkova, R. Nagarajan

MONDAY MORNING

Section A

Colorado Convention Center
Room 403

Cellulose in Solid State and Solution — Structure, Chemistry and Reaction Mechanisms: Anselme Payen Award Symposium in Honor of Thomas Rosenau

Advances in Lignin Chemistry and Analysis of Polysaccharides

F. Liebner, L. Lucia, A. Potthast, *Organizers*
D. O. Klemm, M. Tenkanen, *Presiding*

8:00 CELL **154.** Update on Zip-lignins™: Lignins designed for deconstruction. **J. Ralph**, F. Lu, S.D. Karlen, D. Padmakshan, M. Regner, R. Smith, H. Kim, Y. Zhu, J. Rencoret, J. Grabber, C.G. Wilkerson, J.C. Sedbrook, S. Mansfield

8:30 CELL **155.** Cross-coupling and oxidation of novel lignin monomers with conventional monolignols. **T.J. Elder**, J. Ralph

9:00 CELL **156.** Recent advances in lignin chemistry. **M. Balakshin**

9:30 CELL **157.** Multistep lignin degradation method for the isolation of lignin-carbohydrate-complex (LCC) bonding sites. **D. Ando**, F. Nakatsubo, T. Takano, H. Yano

10:00 Intermission.

10:15 CELL **158.** Determination of molecular mass and molecular mass distribution of TEMPO-oxidized celluloses (TOCs) and TOC nanofibrils (TOCNs) using SEC-MALLS. R. Hiraoki, Y. Ono, T. Saito, **A. Isogai**

10:45 CELL **159.** Recent advances in biorefinery process stream analysis. **A. Potthast**

11:15 CELL **160.** Mass spectrometry analysis of structural details in *O*-acetylglucuronoxylans. S. Chong, P. Tuomainen, M. Juvonen, M. Derba-Maceluch, E. Mellerowicz, **M. Tenkanen**

11:45 CELL **161.** Cellulose degradation during deformation processing and analytics. **T. Roeder**, G. Kliba, W. Milacher, G. Kraft, A. Potthast, T. Rosenau

Section B

Colorado Convention Center
Room 404

Functional Lignocellulosics and Nanotechnology

T. Nypelö, S. Spirk, *Organizers*
I. Filpponen, M. S. Peresin, *Organizers, Presiding*

8:00 CELL **162.** Functionalization of nanocelluloses by supramolecular motifs to combine competing properties. J.R. McKee, E. Appel, E. Janacek, H. Tenhu, E. Kontturi, O.A. Scherman, **O.T. Ikkala**

8:30 CELL **163.** Controlling the elastic modulus of cellulose nanofibril hydrogels – scaffolds with potential in tissue engineering. **K. Syverud**, S.R. Pettersen, K.I. Draget, G. Chinga-Carrasco

8:50 CELL **164.** Aerogels and foams from cellulose nanocrystals as superabsorbents, shape recovery materials, and templates. X. Yang, Z. Hu, **E.D. Cranston**

9:10 CELL **165.** Biocompatible cellulose-based cell scaffolds: Generation of interconnected micron-size pores embedded in frameworks of nanoporous PMMA-reinforced cellulose struts. **N. Pircher**, D. Fischhuber, L. Carbajal Galan, C. Strauβ, J. Nedelec, C. Kasper, T. Rosenau, F. Liebner

9:30 CELL **166.** Photoactive materials for wound care purposes based on bacterial cellulose. **H. Hettegger**, S. Sortino, A. Potthast, T. Rosenau

9:50 Intermission.

10:10 CELL **167.** Functionalization of cellulose nanofibril surfaces to enhance crystallization and mechanical properties of poly-l-lactide. **S. Fujisawa**, T. Saito, A. Isogai

10:30 CELL **168.** Phase behavior of water-in-oil emulsions stabilised solely by hydrophobised bacterial cellulose nanofibrils. **K. Lee**, J. Blaker, R. Murakami, J.Y. Heng, A. Bismarck

10:50 CELL **169.** Withdrawn.

11:10 CELL **170.** Silver nanoparticles synthesis mediated by cellulose nanocrystals: Role of surface chemistry in nucleation phenomena. **K. Uddin**, A.R. Lokanathan, J. Laine, O.J. Rojas

11:30 CELL **171.** Nanocomposites from holocellulose and silver with enhanced antimicrobial activity. **L. Fu**, F. Deng, M. Ma

Section C

Colorado Convention Center
Room 405

Advances in Lignocellulosic Materials and Chemistry: A Tribute to W.G. Glasser

Advanced Materials from Lignocellulosics

G. Garnier, T. G. Rials, *Organizers*
S. Kelley, *Organizer, Presiding*

8:00 CELL **172.** Biobased materials from lignocellulosic fibers: A brief overview. **E. Frollini**, B. Rodrigues, E. Ramires, F. de Oliveira, I. Razera, R. Passos de Oliveira Santos

8:30 CELL **173.** Efficient adsorbents based on nanoporous carbon fibers from cellulosic precursors. **D. Berek**, I. Novak, K. Munka

9:00 CELL **174.** Curing behavior and bond performance of wood adhesive from enzymatic hydrolysis residues of lignocellulosic biomass. **I. Hafez**, H. Yang, W.T. Tze

9:30 CELL **175.** Electrospinning of lignin based composite nanofibers with nanocrystalline celluloses. **M. Cho**, F.K. Ko, S.H. Renneckar

10:00 Intermission.

10:15 CELL **176.** Preparation and properties of composite Lyocell fibers using hemicelluloses as regulator. **J. Chen**, Y. Guan, K. Wang, F. Xu, R. Sun

10:45 CELL **177.** Repeated homogenization, a route for decreasing the energy consumption in the nanofibrillated cellulose manufacturing process? **A. Naderi**, T. Lindström

11:15 CELL **178.** Recent advances in cellulose ester performance and applications. **J.D. Goodrich**

11:45 CELL **179.** Biopolymer modification: Converting biopolymers into processable thermoplastics. **W.G. Glasser**

12:15 Concluding Remarks.

Section D

Colorado Convention Center
Room 406

Lignin Biosynthesis, Characterization and Modifications

Degradative Routes for Lignin Valorisation

C. Crestini, T. Tamminen, *Organizers*
R. Gosselink, *Presiding*

8:00 CELL **180.** Willow as a potential source of lignin raw material. **T. Tamminen**, A.M. Koskinen, T. Vuorinen

8:30 CELL **181.** New mutiplexed assay for lignin depolymerization. **M. Kent**, I. Avina, N. Rader, V. Chavez, M. Busse

9:00 CELL **182.** Sub- and supercritical water liquefaction of alkali lignin in presence of carbon dioxide and ammonia. **A. Numan-Al-Mobin**, C. Lynde, P. Kolla, D.J. Dixon, A. Kubatova, A. Smirnova

9:30 CELL **183.** Lignin oxidation depolymerization using graphene oxide as a metal-free catalyst. **J. Zeng**, Z. Tong

10:00 Intermission.

10:15 CELL **184.** Catalytic hydrogen-free conversion of lignin in key aromatics. **R. Gosselink**

10:45 CELL **185.** Metal-organic frameworks as selective catalysts for carbon-oxygen bond cleavage in lignin model compounds. **V. Stavila**, K. Leong, R. Parthasarathi, K. Sale, R. Davis, M. Allendorf

11:15 CELL **186.** Comparative separation and characterization of lignin by catalytic hydrothermal pretreatment with metal chlorides. **M. Wu**, X. Zhang, R. Sun

11:45 CELL **187.** Correlating structural features of lignin with physical properties: Toward a descriptive-predictive database. **H. Lange**, O. Sevastyanova, C. Crestini

Section E

Colorado Convention Center

Room 407

Frontiers in Glycoscience

Synthesis and Functions

Cosponsored by CARB‡ and DAC‡

K. J. Edgar, L. Wang, *Organizers*

L. C. Hsieh-Wilson, *Presiding*

8:00 Introductory Remarks.

8:15 CELL **188.** Integrated approach to uncover ligands for heparan sulfate binding proteins. **G. Boons**

8:45 CELL **189.** Proteoglycan mimics: Glycoscience opportunities in nanobiomaterials. **M. Kipper**

9:15 CELL **190.** Gagomers: Safe, lipid-based-nanoparticle clusters coated with a glycosaminoglycan for systemic delivery of therapeutic payloads. **D. Peer**

9:45 Intermission.

10:15 CELL **191.** Carbohydrate signaling in the brain. **L.C. Hsieh-Wilson**

10:45 CELL **192.** Carbohydrate biosynthetic enzymes for one-pot multienzyme (OPME) chemoenzymatic synthesis of glycans and glycoconjugates. **X. Chen**

11:15 CELL **193.** Using chemistry to identify and characterize O-GlcNAcylated proteins. **M. Pratt**

Biomass to Fuel and Products

Sponsored by SOCED, Cosponsored by CELL, ENFL and MPPG

MONDAY AFTERNOON

Section A

Colorado Convention Center

Room 403

Cellulose in Solid State and Solution — Structure, Chemistry and Reaction Mechanisms: Anselme Payen Award Symposium in Honor of Thomas Rosenau

Novel Cellulosic Materials and Medical Applications

L. Lucia, A. Potthast, *Organizers*

F. Liebner, *Organizer, Presiding*

D. G. Gray, *Presiding*

1:30 CELL **194.** Nanoscale natural recourses important to life: Surface design of biotech nanocellulose hydrogels for applications as medical implants and tissue engineering scaffolds. **D.O. Klemm**, W. Fried, F. Kramer, S. Nietzsche, K. Petzold-Welcke, T. Richter, U. Udhardt

2:00 CELL **195.** Preparation of nanocellulosic biointerfaces. **E.I. Filpponen**, H. Orelma, L.O. Morales, M. Vuoriluoto, O.J. Rojas

2:30 CELL **196.** Functional cellulose microspheres for pharmaceutical applications. **P.E. Fardim**

3:00 CELL **197.** Surface modification of nanocellulose to rngineer responsive materials. Y. Zhang, J.O. Zoppe, **O.J. Rojas**

3:30 Intermission.

3:45 CELL **198.** Ioncell-F: A high-strength regenerated cellulose fiber. **H. Sixta**, L.K. Hauru, S. Asaadi, Y. Ma, A. King, M. Hummel, I. Kilpelainen

4:15 CELL **199.** Revisiting regenerated cellulose fibers. **S.J. Eichhorn**, S. Rahatekar, T. Welton, K.D. Potter, A. Bismarck, N. Wanasekara

4:45 CELL **200.** Cellulose man-made fibers reinforcing bio-based thermoplastics – the role of fiber diameter and fiber-matrix interphase. **J. Ganster**, E. Jens, H. Fink

5:15 CELL **201.** Polysaccharides and blends for enhanced drug delivery. **X. Meng**, J.A. Marks, H. Liu, G. Ilevbare, L. Taylor, **K.J. Edgar**

Section B

Colorado Convention Center

Room 404

Functional Lignocellulosics and Nanotechnology

I. Filpponen, M. S. Peresin, S. Spirk, *Organizers*

T. Nypelö, *Organizer, Presiding*

C. A. Carrillo, *Presiding*

1:30 CELL **202.** High consistency fibrillation of pulps with enzymes — benefits and application foresights. **J.J. Pere**

1:50 CELL **203.** Customizing the mechanical performance of water stable TEMPO oxidized cellulose nanofibril films. **M. Hakalahti**, A. Salminen, J. Seppälä, T. Tammelin, T.A. Hanninen

2:10 CELL **204.** Polyelectrolyteinterdigitation across interfaces and wet adhesion: Influence of polyvinylamine on wet adhesion between cellulose model surfaces modified with carboxymethylcellulose. **E. Gustafsson**, L. Wagberg, R.H. Pelton

2:30 CELL **205.** Versatile modification of cellulose by UV-induced surface-initiated ATRP. **E.E. Malmström**, E. Larsson, T. Kaldéus, S. Pendergraph, A. Carlmark

2:50 CELL **206.** Nanomechanical properties of single pulp fibers. **N. Nordgren**, V. Wallqvist, M. Fredlund

3:10 CELL **207.** Assessment of paper topography by confocal laser scanning microscopy and image analysis. **R. Kargl**, D. Horvat, A. Dobaj-Štiglic, A. Kornherr, G. Drexler, D. Mongus, B. Zalik, K. Stana-Kleinschek

3:30 Intermission.

3:50 CELL **208.** Agroindustrial residues as alternative sources for nanocellulose production. **M.S. Peresin**, P. Lahtinen, J. Vartiainen, T. Hänninen, S. Liukkonen, J.J. Pere, T. Tammelin

4:10 CELL **209.** Microwave-assisted synthesis of cellulose and alkali earth metal fluorides (MF_2, M=Ca, Mg, Sr, Ba) nanocomposites. **F. Deng**, L. Fu, M. Ma

4:30 CELL **210.** Electrospun cellulose acetate fibers used as templates of fabrication of tubular micro-meso silica materials for controllable drug release. **J. Song**, C. Jia, Y. Jin, Q. Cheng, Y. Li

4:50 CELL **211.** Carbon fibers from polyacrylonitrile (PAN)/cellulose nanocrystals (CNCs). **H. Chang**, A. Chien, H.C. Liu, B.A. Newcomb, P. Wang, S. Kumar

5:10 CELL **212.** CNT incorporated lignin/PAN composite carbon fibers. **H.C. Liu**, A. Chien, B.A. Newcomb, Y. Liu, S. Kumar

Section C

Colorado Convention Center

Room 405

Application of Computational Chemistry to Biomass Chemistry and Utilization

S. C. Chmely, T. J. Elder, *Organizers*

B. Knott, *Presiding*

1:30 CELL **213.** Understanding lignin acidolysis with aryl-ether model compounds: A combined DFT and microkinetic study. **A. Pelzer**, M. Sturgeon, A. Yanez-McKay, G. Chupka, M. O'Brien, R. Katahira, G. Beckham, L.J. Broadbelt

2:00 CELL **214.** Modifications to the structure and dynamics of lignin under THF-water co-solvent systems. **M.D. Smith**, X. Cheng, L. Petridis, B. Mostofian, J.C. Smith

2:30 CELL **215.** Modeling coupling reactions for upgrading biomass pyrolysis vapor. **M.R. Nimlos**, S. Kim, L. Bu, D. Robichaud, G. Beckham, G.A. Ferguson

3:00 CELL **216.** Mesoscale simulations of biomass conversion processes using particle models with explicit, species-specific microstructure. **P. Ciesielski**, M.F. Crowley, M.R. Nimlos, B. Donohoe, T. Foust

3:30 Intermission.

3:40 CELL **217.** Catalyst support effects in the carbon-oxygen bond cleavage of lignin degradation products. **G.A. Ferguson**, M. Griffin, S. Habas, D. Ruddy, J.A. Schaidle, M. Biddy, G. Beckham

4:10 CELL **218.** Dissolution and reaction of lignin in ionic liquids: A computational mechanistic study. **B.G. Janesko**

4:40 CELL **219.** Theoretical understanding of biomass dissolution and dissociation in acidic and basic ionic liquids. **P. Ramakrishnan**

5:10 CELL **220.** Molecular simulation of hydrolysis reactions to engineer more efficient biomass conversion. **K. Fleming**, J. Pfaendtner

Section D

Colorado Convention Center

Room 406

Lignin Biosynthesis, Characterization and Modifications

Value-added Products from Lignin

C. Crestini, T. Tamminen, *Organizers*

D. Da Silva Perez, *Presiding*

1:30 CELL **221.** Structural characteristics of industrial lignins in respect to their valorization. **T. Liitiä**, S. Rovio, R. Talja, T. Tamminen, J. Renocoret, A. Gutiérrez, J. del Río, B. Saake, K. Schwarz, J. Gravitis, M. Orlandi

2:00 CELL **222.** Features of different lignin sources for adhesives and aromatic chemicals production. **D. Da Silva Perez**, V. Rousseau-Popa, F. Ham-Pichavant, S. Grelier, A. Guillemain, S. Tapin-Lingua, C. Crestini

2:30 CELL **223.** Methyl isobutyl ketone/ethanol organosolv lignin: Characterization and conversion to carbon fiber. **O. Hosseinaei**, D.P. Harper, J.J. Bozell, T.G. Rials

3:00 CELL **224.** Macromolecular characterization of plastics with 85–100% levels of methylated native softwood lignin. Y. Wang, Y. Chen, **S. Sarkanen**

3:30 Intermission.

3:45 CELL **225.** Laccase-catalyzed synthesis of conducting polyaniline-lignosulfonate composite. **Q. Wang**, Y. Zhang, X. Fan, P. Wang, J. Yuan

4:15 CELL **226.** Preparation of water-soluble lignin polyoxyethylene ether by epoxidation and etherification. **C. Chen**, X. Li, **M. Li**, R. Sun

4:45 CELL **227.** Utilization of biorefinery technical lignins on lignin-phenol-formaldehyde resin adhesives. **S. Yang**, T. Yuan, R. Sun

5:15 CELL **228.** Novel functional lignins as building blocks in preparation of polyurethane materials. **J. Dietz**, M. Biesalski, M. Duetsch, O. Ringena, S. Valkonen

Section E

Colorado Convention Center

Room 407

Frontiers in Glycoscience

Control of Sequence and Regiochemistry

Cosponsored by CARB‡ and DAC‡

L. Wang, *Organizer*

K. J. Edgar, *Organizer, Presiding*

1:30 CELL **229.** Sugars and proteins: Exploring and exploiting sugar chemical biology. **B.G. Davis**

2:00 CELL **230.** Synthesis and properties of end-functionalized methyl cellulose derivatives: Bridging the gap between oligo- and polysaccharides. **H. Kamitakahara**, A. Nakagawa, R. Suhara, M. Yamagami, H. Kawano, T. Takano

2:30 CELL **231.** Regioselective synthesis of polysaccharide derivatives. X. Zheng, R. Zhang, J. Pereira, **K.J. Edgar**

3:00 CELL **232.** Synthesis and biological evaluation of carbohydrate-functionalized polymers. **H.M. Nguyen**

3:30 Intermission.

4:00 CELL **233.** Bioengineering of third generation chitosans. **B.M. Moerschbacher**

4:30 CELL **234.** Understanding and manipulating cellulase glycosylation. **Z. Tan**

5:00 CELL **235.** Glycosynthase technology for enzymatic synthesis of functional polysaccharides. **A. Planas**

Polymeric Biomaterials

Novel Polymeric Biomaterials: Synthesis, Modification and Fabrication

Sponsored by PMSE, Cosponsored by CELL

MONDAY EVENING

Section A

Colorado Convention Center

Halls C/D

Sci-Mix

C. E. Frazier, *Organizer*

8:00 - 10:00

87, 90, 93-96, 98, 100, 103, 105, 109, 110-112, 115, 116, 119-120, 126-127, 130, 133, 135-136, 145, 148, 153. See previous listings.

TUESDAY MORNING

Section A

Colorado Convention Center

Room 403

Cellulose in Solid State and Solution — Structure, Chemistry and Reaction Mechanisms: Anselme Payen Award Symposium in Honor of Thomas Rosenau

Aerogels and Nanostructured Celluloses

F. Liebner, L. Lucia, A. Potthast, *Organizers*

T. J. Heinze, A. Isogai, *Presiding*

8:00 CELL **236.** Highly porous cellulose: Aerogels vs. cryogels. N. Buchtova, **T. Budtova**

8:30 CELL **237.** Photoluminiscent and transparent cellulose-based aerogels and films carrying covalently immobilized core-shell quantum dots. **F. Liebner**, H. Wang, S. Plappert, S. Quraishi, N. Pircher, T. Rosenau

9:00 CELL **238.** Novel insights into the development of nanocomposites based on cellulose nanofibers. **C. Freire**, A. Silvestre, C. Pascoal Neto

9:30 CELL **239.** Honeycomb-patterned cellulose films as a promising tool to investigate deformation of wood crossSection and wood cell wall formation. **Y. Uraki**, Q. Li, T.B. Bardant, K. Koda

10:00 Intermission.

10:15 CELL **240.** High-added value materials with cellulose nanocrystals. **C. Weder**

10:45 CELL **241.** Effects of structure of cellulose in solid state on functions and properties of composite materials. **L. Zhang**, Q. Wang, J. Guo, A. Lu

11:15 CELL **242.** Surface chemistry and characterisation of cellulose nanocrystals. S. Eyley, **W. Thielemans**

11:45 CELL **243.** Formation of chiral nematic films from cellulose nanocrystal suspensions is a two-stage process. X. Mu, **D.G. Gray**

Section B

Colorado Convention Center

Room 404

Functional Lignocellulosics and Nanotechnology

I. Filpponen, T. Nypelö, S. Spirk, *Organizers*

M. S. Peresin, *Organizer, Presiding*

T. Tammelin, *Presiding*

8:00 CELL **244.** Advanced polysaccharide materials for biomedical applications. **M. Kurečič**, U. Maver, T. Mohan, R. Kargl, S. Spirk, V. Ribitsch, **K. Stana-Kleinschek**

8:20 CELL **245.** Construction of functional biomaterials of hemicellulose-chitosan. **Y. Du**, S. Wu, X. Shi, H. Deng, A. Lu, L. Zhang

8:40 CELL **246.** Thermal inducing self-assemble nanofibrils to construct chitin microspheres for tissue engineering. **B. Duan**, L. Zhang

9:00 CELL **247.** Antibacterial wound dressing electrospun nanofibers from chitosan - iodoacetamide. **A.M. Abdelgawad**, S. Hudson, O.J. Rojas

‡ *Cooperative Cosponsorship*

9:20 CELL **248.** Surface phthaloylation of chitin nanofiber in aqueous media to improve dispersibility in and ultraviolet protection properties. **S. Ifuku**, N. Suzuki

9:40 CELL **249.** Chitosan modification via nitroxide-mediated polymerization and "grafting to" approach in homogeneous media. O. García-Valdez, S. George, E. Saldivar, M.F. Cunningham, **P. Champagne**

10:00 Intermission.

10:20 CELL **250.** Synthesis of functional sponges from nanofibrillated cellulose using a silylation process in water. **P. Tingaut**, T. Zimmermann, G. Sèbe

10:40 CELL **251.** Functionalization of nanofibrillated cellulose with alkoxysilanes in water and reinforcing properties in PDMS networks. **G. Sèbe**, T. Zimmermann, P. Tingaut

11:00 CELL **252.** Tailoring barrier-properties of paper substrates using fiber-immobilized polyvinyl acetate copolymer. **M. Graf**, M. Biesalski

11:20 CELL **253.** Photocatalytic papers with enhanced chemical stability in wet conditions. **M.A. Biesalski**, F. Loyal

11:40 CELL **254.** Functionalization of nanofibrillated cellulose for improved wet strength and biomedical applications. **H. Mertaniemi**, O.T. Ikkala

Section C

Colorado Convention Center
Room 405

Smart and Responsive Composites from Renewable Building Blocks

Cues from Nature: Environmentally-Triggered Functionality in Biopolymers

Cosponsored by PMSE

Y. Habibi, Q. Lin, *Organizers*
L. A. Lucia, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 CELL **255.** Smart and responsive molecular ensembles from renewable building blocks: Assemblies and properties. **G. John**

8:35 CELL **256.** Multiresponsive polymer-grafted cellulose nanocrystals. F. Azzam, E. Siqueira, J. Putaux, F. Pignon, **B. Jean**

9:05 CELL **257.** Withdrawn.

9:35 CELL **258.** CO_2-switchable polysaccharide graft copolymers. **Y. Huang**, N. Che, **R. Liu**

10:05 Intermission.

10:20 CELL **259.** High strength chitosan hydrogels fabricated from alkaline aqueous solution. **J. Duan**

10:50 CELL **260.** From a terminal olefin to functional groups: Olefin cross-metathesis and hydroboration-oxidation in the synthesis of novel cellulose esters. **X. Meng**, K.J. Edgar

11:20 CELL **261.** Softwood hemicelluloses promote the physical stability of oil-in-water emulsions. **K.S. Mikkonen**, C. Berton-Carabin, C. Xu, M. Tenkanen, K. Schroën

11:50 CELL **262.** Recycled thermoset waste/polypropylene composites with enhanced stiffness and impact resistance. **O. Oguz**, E. Simsek, K. Bilge, Y.Z. Menceloglu

Section D

Colorado Convention Center
Room 405

Renewable Resources for Materials and Energy: Recent Research and Developments in Ibero-America

Adding Value to Lignin and Renewable Resources

M. L. Auad, J. Campos-Teran, D. Petri, *Organizers*
O. El Seoud, O. J. Rojas, *Organizers, Presiding*

8:00 CELL **263.** Ionic liquid/molecular solvent mixtures as tailored media for cellulose derivatization: Uncatalyzed- and imidazole-catalyzed acylation. **O. El Seoud**, T.C. Teixeira, P.R. Pires, H. Nawaz, T.A. Bioni

8:25 CELL **264.** Lignin-soy protein aerogels. **C.L. Salas**, I.C. Hoeger, M. Ago, O.J. Rojas

8:50 CELL **265.** Reinforcing capability of cellulose nanofibrils (NFC) on nanopapers from soybean hulls forms: Study of the synergetic effects on the mechanical and barrier properties. **A. Ferrer**, C.L. Salas, T.W. Theyson, O.J. Rojas

9:15 CELL **266.** Mill wood lignin interactions with monocomponent cellulases. **A. Pereira Gonzalez**, I.C. Hoeger, A. Ferrer, J. Renocoret, J. del Río, A.T. Martinez, A. Gutiérrez, O.J. Rojas

9:40 Intermission.

9:55 CELL **267.** Strategy for multidimensional understanding of lignocellulose conversion processes. **C. Driemeier**, M.T. Pimenta

10:20 CELL **268.** Gelatin as renewable source for new material production. **C. Peña-Rodriguez**, G. Mondragon, A. Arbelaiz, R. Ruseckaite, A. Eceiza

10:45 CELL **269.** Lignin-additives-enzymes interactions studied by QCM-D. **C. Fritz**, A. Ferrer, C.L. Salas, H. Jameel, O.J. Rojas

11:10 CELL **270.** Withdrawn.

11:35 Concluding Remarks.

Section E

Colorado Convention Center
Room 407

Frontiers in Glycoscience

Characterization and Applications

Cosponsored by CARB‡ and DAC‡

K. J. Edgar, L. Wang, *Organizers*
J. H. Prestegard, *Presiding*

8:00 CELL **271.** Glycosylated proteins and glycan binding: Insight into function using NMR. **J.H. Prestegard**, Q. Gao, C. Chen

8:30 CELL **272.** Photoregenerated cellulose: From 2D patterns to 3D microfabrication. A. Wolfberger, A. Petritz, V. Schmidt, R. Kargl, B. Stadlober, K. Niegelhell, T. Griesser, **S. Spirk**

9:00 CELL **273.** Glycan maps and quantitation of glycoproteins. **C.B. Lebrilla**

9:30 Intermission.

10:00 CELL **274.** Well-defined sugar-based amphiphilic copolymers: From controlled architectures to nanostructured materials. **S. Halila**, I. Otsuka, R. BORSALI

10:30 CELL **275.** Wood hydrolysates: From fractions to products. **A. Albertsson**, U.M. Edlund

11:00 CELL **276.** Proteomics analysis of sialylated glycoproteins identifies substrates for sialyltransferases and sialidases. Y. Wang, J. McCombs, **J.J. Kohler**

Polymeric Biomaterials

Novel Polymeric Biomaterials: Synthesis, Modification and Fabrication

Sponsored by PMSE, Cosponsored by CELL

TUESDAY AFTERNOON

Section A

Colorado Convention Center
Room 403

Cellulose in Solid State and Solution — Structure, Chemistry and Reaction Mechanisms: Anselme Payen Award Symposium in Honor of Thomas Rosenau

Organic Synthesis in Cellulose Science

F. Liebner, L. Lucia, *Organizers*
A. Potthast, *Organizer, Presiding*
K. J. Edgar, *Presiding*

1:00 CELL **277.** Aligned cellulose nanowhisker-based high-performance polymeric proton conductors. **M.M. Hasani-Sadrabadi**, E. Dashtimoghadam, F.S. Majedi, P. Renaud, K.I. Jacob

1:30 CELL **278.** Cellulose carbontes – a platform for novel cellulose derivatives. **T.J. Heinze**

2:00 CELL **279.** Synthesis, characterization, and properties of cellulose derivatives having an annular structure in the side chains. C. Chang, Y. Teramoto, **Y. Nishio**

2:30 CELL **280.** Preparation and properties of photosensitizer-bounded cellulose derivatives. **T. Takano**, Y. Saito, H. Kamitakahara

3:00 CELL **281.** Synthetic strategies for cellulosic diblock copolymers. **H. Kamitakahara**

3:30 CELL **282.** Topochemical considerations controlling the dynamics of cellulose nanocrystal brush polymerization. C. Tian, S. FU, Y. Habibi, **L.A. Lucia**

4:00 Intermission.

4:15 CELL **283.** Cellulose in solid state and solution: Structure, chemistry, and reaction mechanisms. **T. Rosenau**

5:00 Concluding Remarks.

Section E

Colorado Convention Center
Room 407

Frontiers in Glycoscience

Medicine

Cosponsored by DAC‡

K. J. Edgar, *Organizer*
L. Wang, *Organizer, Presiding*

1:30 CELL **284.** From biological glycosylation to universal vaccine development. **C. Wong**

2:00 CELL **285.** Entirely carbohydrate-based cancer vaccines for disease prevention and treatment. **P.R. Andreana**

2:30 CELL **286.** SELMA and glycopeptide mRNA display: Directed evolution of multivalent glycoclusters in HIV vaccine design. **I.J. Krauss**

3:00 CELL **287.** Site-specific chemoenzymatic glycoengineering of therapeutic antibodies. **L. Wang**

3:30 Intermission.

4:00 CELL **288.** Fighting cancer with a sweet bullet: The development of carbohydrate based anticancer vaccines. **X. Huang**

4:30 CELL **289.** Mapping the glycome with systems-based analysis. **L.K. Mahal**

5:00 CELL **290.** Targeting immune cells with glycan ligands of siglecs. **J.C. Paulson**, M.S. Macauley, R. McBride, C. Nycholat, F. Pfrengle, W. Peng, S.L. Ingale, C. Rademacher, C. Rillahan

Polymeric Biomaterials

Drug Delivery and Controlled Release

Sponsored by PMSE, Cosponsored by CELL

WEDNESDAY MORNING

Section A

Colorado Convention Center
Room 403

Cellulose in Solid State and Solution — Structure, Chemistry and Reaction Mechanisms: Anselme Payen Award Symposium in Honor of Thomas Rosenau

Biomaterials, Cellulose Dissolution and Analytical Aspects

F. Liebner, A. Potthast, *Organizers*
L. Lucia, *Organizer, Presiding*
T. Roeder, *Presiding*

8:00 CELL **291.** Synthesis of cellulosic bottlebrushes with regioselectively substituted side chains and their self-assembly. **K. Sakakibara**, Y. Kinose, Y. Tsujii

8:25 CELL **292.** Withdrawn.

8:50 CELL **293.** Preparation of cross-linked cellulose nanofibril aerogel with water absorbency and shape recovery. **C. Kim**, H. Lee, H. Youn

9:15 CELL **294.** Making fiber-fiber bonds visible. **J. Belle**, S. Kleemann, J. Odermatt, A. Olbrich

9:40 CELL **295.** Zinc nitrate influences for promoting the dissolution of cellulose in NaOH based aqueous solvent at low temperature. S. Wang, **A. Lu**, L. Zhang

10:05 Intermission.

10:20 CELL **296.** Requirements for successful cellulose fiber spinning from ionic liquid solutions. **M. Hummel**, A. Michud, S. Asaadi, Y. Ma, L.K. Hauru, H. Sixta

10:45 CELL **297.** Degree of acetylation in biopolymers: a novel analytical method. **T. Zweckmair**, M. Becker, K. Ahn, H. Hettegger, P. Kosma, T. Rosenau, A. Potthast

11:10 CELL **298.** Reaction mechanisms in pulp bleaching: H_2O_2 degradation of 2,5-dihydroxy-[1,4]-benzoquinone as a key chromophore in aged cellulosics. **T. Hosoya**, U. Henniges, A. Potthast, T. Rosenau

11:35 CELL **299.** One-pot synthesis of levulinic acid from cellulose in SO_3H-functionalized ionic liquids. **Y. Shen**, J.K. Sun, B. Wang, F. Xu, R. Sun

Section B

Colorado Convention Center
Room 404

Functional Lignocellulosics and Nanotechnology

T. Nypelö, M. S. Peresin, *Organizers*
I. Filpponen, S. Spirk, *Organizers, Presiding*

8:00 CELL **300.** Affibody functionalized bacterial cellulose tubes for biofiltration applications. **H. Orelma**, L.O. Morales, L. Johansson, I.C. Hoeger, I. Filpponen, C. Castro, J. Laine, O.J. Rojas

8:30 CELL **301.** Triggering protein adsorption on tailored cationic cellulose surfaces. **K. Niegelhell**, T. Mohan, C. Zarth, R. Kargl, S. Köstler, V. Ribitsch, T.J. Heinze, K. Stana-Kleinschek, **S. Spirk**

8:50 CELL **302.** Modification of cellulose with PDMAEMA-block-POEGMA copolymers to control protein affinity for detection and separation. **M. Vuoriluoto**, H. Orelma, M. Poutanen, A. Walther, J. Laine, O.J. Rojas

9:10 CELL **303.** Detection of human neutrophil elastase with fluorescent peptide sensors conjugated to nanocellulosic solid supports targeting wound care diagnostics. **K. Fontenot**, J. Edwards, N. Prevost, D. Haldane

9:30 CELL **304.** Interaction of biomolecules with micro- and nanostructured polysaccharide interfaces. **R. Kargl**, M. Hribar, M. Kolar, C. Cerny, T. Mohan, S. Spirk, V. Ribitsch, K. Stana-Kleinschek

9:50 Intermission.

10:10 CELL **305.** Lignin esters in cellulose bicomponent thin films. **S. Strasser**, S. Spirk, C. Slugovc, M. Kaschowitz, K. Niegelhell, T. Mohan

10:30 CELL **306.** Valorization of lignins with applications in nanostructured films. **B.M. Cerrutti**, S.V. Harb, M.L. Moraes, P. Hammer, S.H. Pulcinelli, C.V. Santilli

10:50 CELL **307.** Flexibility of cellulose nanocrystal networks in response to water vapor. **E. Niinivaara**, M. Faustini, T. Tammelin, H. Ehmann, S. Spirk, E. Kontturi

11:10 CELL **308.** Deuterated cellulose thin films — challenges and surprises. **D. Reishofer**, R. Kargl, H. Ehmann, R. Schennach, S. Hribernik, A. Kornherr, K. Stana-Kleinschek, **S. Spirk**

11:30 CELL **309.** Cellulose thin films meet a synchrotron beam: In situ observation of rearrangement during regeneration and drying using grazing incidence small angle X-ray scattering. **H. Ehmann**, O. Werzer, T. Mohan, A. Kornherr, K. Stana-Kleinschek, H. Amenitsch, R. Resel, E. Kontturi, **S. Spirk**

11:50 CELL **310.** Model wound dressing materials – thin films vs. electrospun fibers. U. Maver, **M. Kurečič**, T. Maver, T. Pivec, Z. Peršin, L. Gradišnik, **K. Stana-Kleinschek**

Section C

Colorado Convention Center
Room 405

Smart and Responsive Composites from Renewable Building Blocks

Innovative Film & Ordered Assemblies/ Advanced Nanoreactor Systems

Cosponsored by PMSE

Q. Lin, L. A. Lucia, *Organizers*
Y. Habibi, *Organizer, Presiding*

8:00 CELL **311.** Nanocelluloses as versatile platform of interactions for smart and tunable thin films. **B. Cathala**, C. Moreau, F. Azzam, P. Bertoncini, O. Chauvet

8:30 CELL **312.** Synergistic templated self-assembly of cellulose nanocrystals (CNCs) in thin block copolymer films. **D. Grolman**, J. Gilman, A. Karim

9:00 CELL **313.** New concepts for molecular engineering of macroscopic adhesion between cellulose surfaces. **A. Trager**, S. Pendergraph, A. Carlmark, L. Wagberg

9:30 CELL **314.** Improved interfacial bonding in cellulosic biocomposites with humins-based furanic resins. **N. Guigo**, J. Pin, A. Mija, L. Vincent, N. Sbirrazzuoli, J.C. van der Waals, E. de Jong

10:00 Intermission.

10:15 CELL **315.** Spray-dried microencapsulation of tea tree oil with a complex of methyl cellulose/chitosan/alginate. J. Chen, **X. Yin**, X. Wang, J. Chen, L. Zhu, L.A. Lucia

10:45 CELL **316.** Photocatalytic and biocatalytic degradation of dye solution using laccase and titanium dioxide loaded on bacterial cellulose. **A. Nandgaonkar**, Q. Wang, W. Krause, Q. Wei, L. Lucia

11:15 CELL **317.** Enzymatic bio-fuel cells based on bacterial cellulose (BC)/MWCNT/laccase (Lac) and bacterial cellulose / MWCNT/ glucose oxidase (GOD) electrodes. **Q. Wang**, A. Nandgaonkar, L. Lucia, Q. Wei

11:45 CELL **318.** Improved antibacterial noatings with Nanotitania and cyclic N-halamine. **X. Ren**, J. Li, L. Li, T. Huang

Section D

Colorado Convention Center

Room 406

Renewable Resources for Materials and Energy: Recent Research and Developments in Ibero-America

Composites and Nanomaterials

J. Campos-Teran, O. El Seoud, D. Petri, O. J. Rojas, *Organizers*

M. L. Auad, *Organizer, Presiding*

R. Christoph, J. Vega-Baudrit, *Presiding*

8:00 CELL **319.** Renewable resources as precursors of biobased thermosetting resins. **M.L. Auad**, B. Sibaja

8:25 CELL **320.** Sisal pulp as raw material for magnetic hybrid films and sugars. **E. Frollini**, L. Varanda, A. de Oliveira, Â. Faceto, B. Rodrigues, D. Furlan, D. de Moraes, J. Kaschuk

8:50 CELL **321.** Biopolymers from tomato agro-industrial residual wastes. **M.B. Gómez-Patiño**, J. Méndez-Méndez, M. Jaramillo-Flores, **J. Campos-Terán**, **D. Arrieta-Baez**

9:15 CELL **322.** Formation and characterization of 10,16-dihydroxyhexadecanoic acid thin films extracted from tomato residues. J. Hernández-Ortíz, M.B. Gómez-Patiño, C. Ramos-Torres, D. Arrieta-Baez, **J. Campos-Terán**

9:40 Intermission.

9:55 CELL **323.** Functional lignins used as curing agent in fiber-reinforced epoxy-materials. **M.A. Biesalski**, M. Baaske, S. Mehlhase, R. Klein, S. Valkonen, M. Duetsch

10:20 CELL **324.** Deconstructing a natural fiber: Physicochemical and structural properties of cellulose nanofribils and nanocrystals from Colombian fique plants. S.A. Ovalle-Serrano, L.F. Jaimes-Cote, C.P. García-Villamizar, F.N. Gómez-Jaimes, C. Blanco-Tirado, **M.Y. Combariza**

10:45 CELL **325.** Collection and evaluation of blended polypropylene banana tree rachis fibers (Musa AAA). **R. Zamora**

11:10 CELL **326.** Surface active materials from functionalized fique's nanocrystalline cellulose. F.N. Gómez-Jaimes, M.M. Gonzáles-Bernal, C.F. Medina-Sandoval, J. Valencia, M.Y. Combariza, **C. Blanco-Tirado**

11:35 CELL **327.** QCM/SPR to study the oxidation and removal of unsaturated fatty acids from NFC and PET surfaces by lipooxygenase treatment. **A. H M.Tayeb**, O.J. Rojas, C.L. Salas, K.D. Wing

12:00 Concluding Remarks.

Section E

Colorado Convention Center

Room 407

Cellulose Dissolution: New Solvents and Mechanisms

N. Abidi, E. L. Quitevis, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 CELL **328.** Recent developments in solvents for cellulose. **T.J. Heinze**

8:35 CELL **329.** Interactions between cellulose and small molecules. **R. Liu**, C. Zhang, Z. Liu, Z. Jiang, **Y. Huang**

9:05 CELL **330.** Mechanism and kinetics of advantaged biofuels synthesis from D-fructose. **T. Flannelly**, S. Dooley, J. Leahy

9:35 CELL **331.** Biphasic process using molten salt hydrates for chemical transformation of lignocellulosic biomass into furan-based chemicals. **C. Yoo**, S. Zhang, X. Pan

10:05 Intermission.

10:20 CELL **332.** Homogeneous saccharification of lignocellulosic biomass in molten salt hydrates. **N. Li**, X. Pan

10:50 CELL **333.** Energetically favored alternative hydrogen bond of cellulose II and cellulose III^{I}. **P. Chen**, Y. Ogawa, Y. Nishiyama, M. Bergenstråhle-Wohlert, K. Mazeau

11:20 CELL **334.** Probing particle – particle interactions in swollen cellulose nanocrystal thin films by surface plasmon resonance spectroscopy. **M.S. Reid**, M. Villalobos, E.D. Cranston

11:50 CELL **335.** On the combination of NaOH activation and DMAc/ LiCl dissolution of cellulose from cotton fibers during different stages of fiber development. **S.P. Liyanage**, N. Abidi

12:20 Concluding Remarks.

Polymeric Biomaterials

Sensors and Medical Devices

Sponsored by PMSE, Cosponsored by CELL

WEDNESDAY AFTERNOON

Section A

Colorado Convention Center

Room 403

ACS Award for Affordable Green Chemistry: Symposium in Honor of John Frye, Todd Werpy, and Alan Zacher

Cosponsored by MPPG

C. E. Frazier, L. A. Lucia, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 CELL **336.** Chemical functionalization and characterization of crystalline cellulose derived from agricultural waste products. **C.J. Huntley**, K.D. Crews, M.L. Curry

2:00 CELL **337.** Isomerization of glucose to fructose by magnetic organic basic catalysts in aqueous media. **Q. Yang**, T. Runge

2:25 CELL **338.** Direct thermal processing of cellulose plasticized with ionic liquids and its composites as polymer electrolytes. J. Wu, Y. Liao, Y. Ye, X. Zhou, B. Brycki, **X. Xie**

2:50 CELL **339.** Fabrication and characterization of cellulose functional materials using ionic liquid 1-ethyl-3-methylimidazolium acetate (EmimAc). **J. Pang**, **X. Zhang**, **Q. Zhang**, **M. Wu**, **R. Sun**

3:15 CELL **340.** Flexible route for solely biomass-derived *p*-xylene and terephthalic acid. **F. Wang**, Z. Tong

3:40 Intermission.

3:55 CELL **341.** Cellulose nanocrystals as reinforcing agent in melt-spinning of polypropylene. **X. Lu**

4:20 CELL **342.** Continuous hydrothermal liquefaction of cellulosic and lignocellulosic biomass. **J. Billing**, A. Schmidt, T. Hart, G. Maupin, R.T. Hallen, D.C. Elliott

4:45 CELL **343.** Overview of the catalyst and process research and development efforts related to the PNNL glycerol to propylene glycol process. **J. Frye**, A. Zacher, T. Werpy

5:15 CELL **344. Award Address** (ACS Award for Affordable Green Chemistry sponsored by The Dow Chemical Company and endowed by Rohm and Haas). Scale up challenges of first of a kind renewable chemicals. **T. Werpy**, J. Frye, A. Zacher

5:45 Concluding Remarks.

Section B

Colorado Convention Center

Room 404

Functional Lignocellulosics and Nanotechnology

I. Filpponen, S. Spirk, *Organizers*

T. Nypelö, M. S. Peresin, *Organizers, Presiding*

1:30 CELL **345.** Withdrawn.

1:50 CELL **346.** Defined cellulose-polymer hybrid materials by synthesis under homogeneous reaction conditions. **M.W. Ott**, M. Biesalski

2:10 CELL **347.** Carbon dot (CD) modified cellulose nanocrystals (CNC) for biosensing and -imaging. **J. Guo**, I. Filpponen, O.J. Rojas

2:30 CELL **348.** Carbon quantum dots from biomass: Synthesis and functionalization. **X. Wang**, Z. Liang, R. Sun

2:50 Intermission.

3:10 CELL **349.** Inkjet printed paper-based sensing device for colorimetric determination of contaminants in drinking water. **P. Gasparic**, A. Kornherr, S. Hribernik, K. Stana-Kleinschek

3:30 CELL **350.** Improving the redispersability of cellulose nanofibrils. **E.I. Filpponen**, A. Anttila, O.J. Rojas

3:50 CELL **351.** Carboxymethylated lignin (CML) in liquid and solid foams. **S. LI**, O.J. Rojas

4:10 Concluding Remarks.

Section C

Colorado Convention Center

Room 405

Smart and Responsive Composites from Renewable Building Blocks

Advanced Nanoreactor Systems/New Paradigms to Smart Material Chemistry & Engineering

Cosponsored by PMSE

Y. Habibi, Q. Lin, *Organizers*

L. A. Lucia, *Organizer, Presiding*

1:30 CELL **352.** Cellulose nanocrystals as 2D chiral inducers: Enantioselective catalysis and transmission electron microscopy 3D characterization. **M. Kaushik**, C. Benoit, C.M. Cirtiu, A.H. Moores

2:00 CELL **353.** Reinforcing piezoelectric films with cellulose nanocrystals. **M. Shir** Mohammadi, J. Simonsen, j. Nairn

2:30 CELL **354.** Two-stage separation and alignment of cellulose nanocrystals. **Y. Hu**, N. Abidi

3:00 Intermission.

3:15 CELL **355.** Life cycle assessment of high performance nanocellulose-reinforced advanced fibre composites. **H. Martin**, S. Evangelisti, P. Lettieri, K. Lee

3:45 CELL **356.** Regioselective preparation of curdlan derivatives aminated at the C-6 position for biomedical applications. **R. Zhang**, K.J. Edgar

4:15 CELL **357.** Macroscopic cellulose probes for contact adhesion. **S.A. Pendergraph**, C. Carrick, L. Wagberg, A. Carlmark, M.K. Johansson, G. Klein, A. Trager

4:45 Concluding Remarks.

Section D

Colorado Convention Center

Room 406

Renewable Resources for Materials and Energy: Recent Research and Developments in Ibero-America

Fundamental Aspects in Processing and Energy

M. L. Auad, J. Campos-Teran, O. El Seoud, O. J. Rojas, *Organizers*

D. Petri, *Organizer, Presiding*

S. Madrigal, *Presiding*

1:30 CELL **358.** Determination of useful parameters to decide the suitability of a biomass to be used as raw material for thermochemical processes. **A. Puente-Urbina**

1:55 CELL **359.** Performance of a low-cost portable carbonizer for the valorization of lignocellulosic wastes. **E. Perez**

2:20 CELL **360.** New organic composites for FDM applications. **R. Christoph**, J. Vega-Baudrit

2:45 CELL **361.** Strategies for the utilization of cellulosic residues generated from the pineapple cultivation. **M. Esquivel Alfaro**, G. Moreno Cento, D. Rojas Fonseca, K. Ramírez Amador, G. Jiménez Villalta

3:10 Intermission.

3:25 CELL **362.** Carbonize it or not? A simple test method for biomassic materials. **J.F. Quesada-Kimzey**

3:50 CELL **363.** Emulsified systems containing cellulose nanofibrils (CNF). **C.A. Carrillo**, T. Nypelö, O.J. Rojas

4:15 CELL **364.** Adsorption of inorganic photo-active nanoparticle/enzyme hybrid systems on surfaces modified with cellulose obtained from natural and industrial residues: A QCM study. **I. Iñarritu**, A. Topete, R. López-Simeon, E. Torres, J. Campos-Teran

4:40 CELL **365.** Drying kinetics as a convenient method to determine relative diffusivity of water in woody biomasses. **A. Puente-Urbina**, J. Morales-Aymerich, Y. Kim, J.F. Mata

5:05 Panel Discussion.

5:30 Concluding Remarks.

Section E

Colorado Convention Center

Room 407

Cellulose Dissolution: New Solvents and Mechanisms

Ionic Liquids

N. Abidi, E. L. Quitevis, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 CELL **366.** Enzymatic pretreatment to improve cellulose solubility in a green solvent of NaOH/urea. **L. Zhang**, T. You, L. Zhang, F. Xu

2:05 CELL **367.** Development and characterization of compatible cellulose and cellulose blended with soy protein membranes using a novel solvent system. **E.F. Douglass**, R. Kotek

2:35 CELL **368.** Withdrawn.

3:05 CELL **369.** Effective dissolution of cellulose for making electrically-responsive films. **S. Acharya**, Y. Hu, N. Abidi

3:35 Intermission.

3:50 CELL **370.** Cellulose/PVA composite films prepared by NaOH/urea solvent: Structure and properties. **M. Xu**, H. Ge, X. Wang

4:20 CELL **371.** Facile ionic liquid-mediated technology for cellulose nanocrystals production directly from wood. **H. Abushammala**, I. Krossing, M.G. Laborie

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‡ *Cooperative Cosponsorship*

4:50 CELL **372.** Ionic liquids: Not always innocent solvents for cellulose. **M.T. Clough**, K. Geyer, P. Hunt, S. Son, U. Vagt, T. Welton

5:20 CELL **373.** How ionic liquids effect glucose and cellobiose solvation: Insights from enhanced sampling molecular dynamics techniques. **V.S. Bharadwaj**, T. Ashurst, T. Schutt, C.M. Maupin

5:50 Concluding Remarks.

Polymeric Biomaterials

Instructive Tissue Engineering Matrices

Sponsored by PMSE, Cosponsored by CELL

THURSDAY MORNING

Section A

Colorado Convention Center
Room 403

Conservation Science of Cellulosic Materials - Recent Developments

Degradation of Paper: Analysis and Approaches to Prevent It

A. Potthast, *Organizer*
U. Henniges, *Organizer, Presiding*

8:00 CELL **374.** Degradation of paper under adverse environmental conditions: Modeling considerations. J. Tétreault, P. Bégin, **A. Dupont**

8:30 CELL **375.** Ancient paper as a multicomponent system: A novel approach to the kinetics of its degradation. **S. Zaccaron**, P.F. Calvini, R. Ganzerla

9:00 CELL **376.** Cellulose as a detector for assessing storage materials for cultural heritage objects. **E. Breitung**, M. Wiggins, L. Nguyen

9:30 CELL **377.** Durability and permanency of formulated traditional Malay black ink on European handmade paper upon accelerated aging tests. **R. Abdul Razak**, R. Othman, M. Barkeshli

10:00 Intermission.

10:15 CELL **378.** Withdrawn.

10:45 CELL **379.** Paper strengthening and desacidification by polyaminoalkylalkoxysilane copolymer networks: A model study. **C. Piovesan**, A. Dupont, O. Fichet, I. Fabre-Francke, B. Lavédrine, H. Chéradame

11:15 CELL **380.** Parylene coatings for cultural heritage paper strengthening. **L. Pei**, M. Pollei, S. Jordan-Mowery, J.W. Baty

11:45 CELL **381.** Paper deacidification using polysaccharide and alkaline nanoparticles. **T. Mohan**, L. Amornkitbamrung, R. Kargl, S. Hribernik, K. Stana-Kleinschek, V. Ribitsch

Section B

Colorado Convention Center
Room 404

Research on Renewable Materials: US and EU Perspectives

Development and Implementation of Bioeconomy Strategies/Initiatives for Collaborative Research and Innovation

P. R. Navard, *Organizer*
P. E. Fardim, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 CELL **382.** European Union policy and initiatives for developing the bioeconomy sector. **P.R. Navard**

8:35 CELL **383.** Renewable materials research in the U.S. Forest Service: A perspective. **W.L. Nieh**

9:05 Intermission.

9:20 CELL **384.** Biobased industries initiative: Realizing the European bioeconomy potential. P. van Leeuwen, **P.R. Navard**

9:50 CELL **385.** Biomass raw materials-related issues on bioeconomy strategies, research and development, and industrial implementation. **D. Da Silva Perez**

10:20 CELL **386.** Network with COST Action FP1205: Innovative applications of regenerated wood cellulose fibers. **Å. Östlund, D. Jones**

10:50 CELL **387.** Horizon 2020: EU research and innovation program. **K. Stana-Kleinschek**

Section D

Colorado Convention Center
Room 406

Renewable Resources for Materials and Energy: Recent Research and Developments in Ibero-America

Applications

M. L. Auad, O. El Seoud, D. Petri, O. J. Rojas, *Organizers*
J. Campos-Teran, *Organizer, Presiding*
E. Torres, *Presiding*

8:00 CELL **388.** Preparation and characterization of antimicrobial cellulose beads. **D. Petri**, L.S. Blachechen, P.E. Fardim

8:25 CELL **389.** Secondary liposomes stabilized by the electrostatic deposition of chitosan-tannin composites as potential delivery systems for proteins. **S. Madrigal-Carballo**, J. Araya-Matey, E. Alfaro-Viquez, D. Esquivel-Alvarado, C.G. Krueger, J.D. Reed

8:50 CELL **390.** Chitosan-Collagen hybrid 3D-scaffolds as potential biomaterials for tissue engineering. P. Cubero-Mora, E. Alfaro-Viquez, D. Esquivel-Alvarado, M. Esquivel-Alfaro, **S. Madrigal-Carballo**

9:15 CELL **391.** Effect of fiber orientation in bacterial cellulose scaffold on cellular response: Adhesion, proliferation, differentiation of equine mesenchymal stem cells. **R.S. Benson**

9:40 Intermission.

9:55 CELL **392.** Tannin-chitosan composite nanoparticles as alternatives to antibiotics. **C.G. Krueger**, E. Alfaro-viquez, S. Madrigal-Carballo, J.D. Reed

10:20 CELL **393.** Bacterial cellulose research experience between Colombia, Finland, and the US. C. Castro Herazo, R. Zuluaga Gallego, J. Arboleda, H. Orelma, L.O. Morales, P. Gañán, **O.J. Rojas**

10:45 CELL **394.** Improved thermal stability of polylactic acid (PLA) film using β-cyclodextrin inclusion complex with PLA. **K. Rodriguez**, Y. Kim, Y. Byun

11:10 CELL **395.** Biotechnological valorization of waste sludge in a food industry: Design and evaluation process at lab scale. **J.M. Naranjo**, W. Osorio viana, A. Merchan, L. Gomez

11:35 CELL **396.** Functionalization of bacterial nanocellulose membranes with *Triticum vulgare* for wound dressing applications. M. Osorio Delgado, I. Oriz, J. Velásquez-Cock, R. Zuluaga Gallego, O.J. Rojas, M.S. Peresin, P. Gañán, **C. Castro Herazo**

12:00 Concluding Remarks.

Section E

Colorado Convention Center
Room 407

Cellulose Dissolution: New Solvents and Mechanisms

Ionic Liquids

N. Abidi, E. L. Quitevis, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 CELL **397.** NMR spectroscopy, relaxometry, diffusion, and rheological studies of cellulose in the ionic liquid 1-butyl-3-methylimidazolium chloride. **M.E. Ries**, T. Budtova, A. Radhi

8:35 CELL **398.** Dissolution, regeneration, and characterization of cellulose and cellulose/chitin in ionic liquid. **P.T. Wansapura**, N. Abidi, T. Jackson, Y. Hu, E.L. Quitevis

9:05 CELL **399.** Dissolution of cellulose and exfoliation of graphene by aralkylimidazolium-based ionic liquids. E. Gurung, K. Mendoza, G. Tamas, R. Bari, T. Jackson, P.T. Wansapurna, M. Green, N. Abidi, **E.L. Quitevis**

9:35 CELL **400.** Application of two-stage ionic liquid-mediated system for cellulose nanocrystals (CNCs) production. **J. Mao**

10:05 Intermission.

10:20 CELL **401.** Synthesis of ionic liquids for pretreatment of lignocellulosic waste. A. Camacho-Dávila, **V. Martínez-Burciaga**, **G.I. Israel-Orozco**, S. Rubio-Perea, G. González-Sánchez, L. Ballinas-Casarrubias, **L. Villanueva**

10:50 CELL **402.** From paper pulp tp dissolving pulp to textile fibres with ionic liquids using IONCELL-P&F. **A.M. Stepan**

11:20 CELL **403.** Optimization of a low temperature lignocellulosic pretreatment process using ionic liquids. **C. Schall**, S. Vasheghani Farahani

11:50 Concluding Remarks.

Polymeric Biomaterials

Instructive Tissue Engineering Matrices

Sponsored by PMSE, Cosponsored by CELL

THURSDAY AFTERNOON

Section A

Colorado Convention Center
Room 403

Conservation Science of Cellulosic Materials - Recent Developments

Paper Conservation: Transition Metal Ions and Specific Topics

U. Henniges, *Organizer*
A. Potthast, *Organizer, Presiding*

1:30 CELL **404.** Removal of the aqueous washing treatment aid ionic fixative from paper. **J. Roller**

2:00 CELL **405.** Analysis of paper surviving from a tragic scene. **K. Ahn**, T. Zweckmair, A. Schedl, A. Potthast

2:30 CELL **406.** Dyes used by Iranian masters in paper dyeing process based on Persian medieval recipes. **M. Barkeshli**

3:00 Intermission.

3:15 CELL **407.** Damage caused by iron ions or pigments (Prussian blue) during aging of Japanese paper. **K. Kida**, M. Inaba, A. Potthast, N. Hayakawa

3:45 CELL **408.** Stabilization of green copper based pigments. **J. Malešič**, J. Kolar, M. Anders

4:15 CELL **409.** Electron paramagnetic resonance as a probe for metal ions and radicals in paper. **A. Zoleo**, M. Bronzato

4:45 Concluding Remarks.

Section B

Colorado Convention Center
Room 404

Research on Renewable Materials: US and EU Perspectives

Clusters and Networks for Research and Innovation

P. E. Fardim, *Organizer*
P. R. Navard, *Organizer, Presiding*

1:30 CELL **410.** Withdrawn.

2:00 CELL **411.** Biomass supply chain innovation: A case study. **S. Jackson**

2:30 CELL **412.** European Polysaccharide Network of Excellence (EPNOE). **P.E. Fardim**, J. van Dam

3:00 Intermission.

3:15 CELL **413.** Sun Grant Initiative: Bringing a regional focus to a national opportunity. **T.G. Rials**

3:45 CELL **414.** Interregional Scientific/Industrial Centre (BIO)-Polymers-Materials-Technologies for Economy, POLINTEGRA, as a model of cooperation between business and science. **D. Ciechanska**

4:15 CELL **415.** Finnish bioeconomy cluster. **P.E. Fardim**, M. Leskela

4:45 CELL **416.** 4D product: Integration over time is the only way to understand sustainability. **M.E. Jones**

5:15 Concluding Remarks.

CHED

Division of Chemical Education

W. Jones, I. Levy, and A. Marsh, *Program Chairs*

OTHER SYMPOSIA OF INTEREST:

Active Learning in the Undergraduate Analytical Chemistry Curriculum *(see ANYL, Tue)*

Diversifying STEM: Uniting through our Differences for a Brighter Scientific Future *(see CMA, Mon)*

Environmental Chemistry: Pedagogical Models and Practices *(see ENVR, Wed, Thu)*

SOCIAL EVENTS:

High School-College Interface Luncheon *(Tickets Required)*, 12:00 PM, Sun

Division Reception, 5:30 pm, Sun

STRETCH Your Students' Polymer Knowledge - For pre-college educators, 4:30 PM, Mon

SUNDAY MORNING

Section A

Sheraton Denver Downtown Hotel
Silver

High School Program

Cosponsored by SOCED

Financially supported by ACS Education Division

S. B. Mitchell, *Organizer, Presiding*

8:00 Registration.

8:30 Introductory Remarks.

8:40 CHED **1.** Demonstrations guaranteed to get ooohs and ahhhs! How to turn ordinary activities into unforgettable learning experiences. **S. Spangler**

10:10 CHED **2.** Writing across the curriculum: Concept journals as a means to teach the metric system. **S.B. Mitchell**

10:30 Intermission.

10:50 CHED **3.** A few insights into classroom and lab safety. **H.W. Gendreau**

11:10 CHED **4.** Spectroscopy of natural resources. **D. McGraw**

11:30 CHED **5.** Spark student's interest in chemistry with resources from the American Chemical Society. **K.M. Kaleuat**i, M. Gmurczyk

Section B

Sheraton Denver Downtown Hotel
Century

Chemistry Education Research

New and Noteworthy in 2013-2014

D. M. Bunce, M. N. Stains, *Organizers*
S. Pazicni, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 CHED **6.** Replicating peer-led team learning in cyberspace: Research, opportunities, and challenges. **P. Varma-Nelson**, J. Smith, S.B. Wilson, J. Banks, L. Zhu

9:10 CHED **7.** Insights into how students learn from molecular visualizations through the lens of variation theory. **R.M. Kelly**

9:45 Intermission.

10:00 CHED **8.** Looking for links: Examining student responses in creative exercises for evidence of linking chemistry concepts. L. Ye, **S.E. Lewis**

10:35 CHED **9.** Argumentation and participation patterns in general chemistry peer-led sessions. **U. Kulatunga**, **R.S. Moog**, **J.E. Lewis**

11:10 Concluding Remarks.

Section C

Sheraton Denver Downtown Hotel

Spruce

Current Practice and Research Using ACS Exams

T. Holme, *Organizer*

K. L. Murphy, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 CHED **10.** Cultivation of creative thinking ability in the course of Food Engineering Operations. **D. Lin**, M. Luo, B. Pu

8:55 CHED **11.** Seven courses, two exams: Designing the ACS Inorganic Chemistry Exams for a diverse undergraduate curriculum. **B.A. Reisner**

9:15 CHED **12.** ACS examination in organic chemistry at Hampton University. **C.M. Bump**, E.M. Ndip, G.C. Nwokogu, M.K. Waddell

9:35 CHED **13.** Assessment of nontraditional students in organic chemistry. **R.D. Barrows**

9:55 Intermission.

10:10 CHED **14.** Creating the Exams Data Analysis Spreadsheet (EDAS) as a tool to help instructors conduct customizable analyses of student ACS exam data and compare the results to national normative statistics. **A. Brandriet**, T. Holme

10:30 CHED **15.** Use of American Chemical Society examinations as assessment tools. **S.M. Socol**

10:50 CHED **16.** Chemical thinking: Exploring the impact of a new general chemistry curriculum. **V. Talanquer**, J.R. Pollard

11:10 CHED **17.** Exploring the use of the Anchoring Concepts Content Map as a programmatic assessment tool. **C.J. Luxford**, T. Holme

11:30 Concluding Remarks.

Section D

Sheraton Denver Downtown Hotel

Denver

Undergraduate Research Papers

Organic Chemistry

Cosponsored by SOCED

C. V. Gauthier, *Organizer*

J. V. Ruppel, N. L. Snyder, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 CHED **18.** Synthetic investigation and application of a substituted 4,6-dimethylcyclohexene compound. **W.P. Miller**, K. Cetto Bales, S. Franke McDevitt

8:45 CHED **19.** Chemistry for chiral skeletons:Building chiral fragments from enantiopure 1,2-amino alcohols. **J.C. Serrano**, Z.V. Boskovic, S. Ferrara, L. Furst, S.O. Figueroa, D.K. Crews, A. Guerrero, C. Brackeen, S.D. Nelson, S. Dandapani, A.J. Phillips, S.L. Schreiber

8:55 CHED **20.** Evaluation of a new rhamnosidic donor containing a sulfonyl directing group for the formation of beta-rhamnosidic linkages. **E.J. Medici**, E.D. Anderson, N.L. Snyder

9:05 Intermission.

9:15 CHED **21.** Regioselective opening of propenylbenzene oxides via intramolecular N-H activation. **C. Tutwiler,** C.J. Monceaux

9:25 CHED **22.** Novel hydroxyproline methodology involving an auxiliary salicylaldehyde capture followed by imine-induced intramolecular rearrangement to achieve chemoselective ligations at difficult proline site. **G.G. Simpson**, K. Ha, A. Katritzky

9:35 CHED **23.** Why does the acetaldehyde enolate favor reaction at the O atom during gas-phase nucleophilic substitution? Contributions by resonance and inductive effects. **C. Seitz**, J.M. Karty

9:45 Intermission.

9:55 CHED **24.** Investigating the mechanism of cyanoacrylate polymerization in latent fingerprint development. **E.M. Persson**, K. McCarthy, A.S. Dutton

10:05 CHED **25.** Methods towards the synthesis of Stachybotrin D. **W. Teh**, D.C. Bromfield Lee

10:15 CHED **26.** Rapid synthesis of N-(2-hydroxybenzyl)acetamide. **K.A. Dockter**, L.I. Bobyleva, M.M. Bobylev

10:25 CHED **27.** Synthesis of trehalose-based oliogsaccharides for medicinal applications. **E.A. Palumbo**, N.L. Snyder

10:35 Concluding Remarks.

Section E

Sheraton Denver Downtown Hotel

Columbine

From Cornerstone to Capstone: Culminating Experiences in the Undergraduate Chemistry Curriculum that Foster Integration and Application of Foundational Knowledge

K. Kneas, J. A. MacKay, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 CHED **28.** Comprehensive chemistry: An efficient approach. **P. Schettler**

8:55 CHED **29.** Introductory investigation into the substituent effect on regio-selectivity of bromination across vinyl systems: A culmination of undergraduate chemical education. **A.N. Schildkret**, V. Fishback

9:15 CHED **30.** Shippensburg University undergraduate research grant writing experience. **R.L. McCann**, **A. Hurley Predecki**

9:35 Intermission.

9:45 CHED **31.** Senior capstone experiences at Stevenson University: Everybody's doing it. **T.M. Mason**

10:05 CHED **32.** Ups and downs of a two-semester independent research project. **J. MacNeil**

10:25 CHED **33.** Chemistry and biochemistry capstone course at Messiah College: A holistic interdisciplinary approach. **R.W. Schaeffer**

10:45 CHED **34.** Electrifying the capstone chemistry experience. **S. Chamberlin**, N.C. Kallan

Section F

Sheraton Denver Downtown Hotel

Gold

NMR Spectroscopy in the Undergraduate Curriculum

Applications

Financially supported by Bruker; JEOL; Thermo Fisher Scientific; Anasazi Instruments

L. J. Anna, D. P. Soulsby, A. S. Wallner, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 CHED **35.** Measurement of phosphates in soft drinks: A general chemistry experiment using NMR. **L.J. Medhurst**, F. Shahnaz, N. Ramnarine, G. Paniconi

8:55 CHED **36.** Free-radical chlorination of alkanes in the undergraduate organic chemistry laboratory: Application of ^{1}H and TOCSY NMR experiments to the analysis of reaction products. **D.P. Soulsby**

9:15 CHED **37.** Withdrawn.

9:35 Intermission.

9:45 CHED **38.** Unequivocal assignment for all PMR and CMR signals of unknown butyl and pentyl acetate esters from Fischer esterification using 2D NMR experiments. **F.J. Matthews**

10:05 CHED **39.** Real-time classroom comparison of structures and NMR spectra using Jmol/JSpecView and nmrdb. **R.M. Hanson**, R.J. Lancashire, L. Patiny

10:25 CHED **40.** Students using esters to construct for themselves the concepts of chemical shift correlation and spin-spin coupling. K.T. Smith, **C.S. Hamann**

10:45 Intermission.

10:55 CHED **41.** Measuring structural and electronic effects on keto-enol equilibrium in 1,3-dicarbonyl compounds. **S.C. Young**, K.T. Smith, J.W. DeBlasio, C.S. Hamann

11:15 CHED **42.** NMR-based activity assays to characterize enzymes in the biochemistry laboratory and in undergraduate research. **B.J. Stockman**

11:35 Concluding Remarks.

Undergraduate Symposium

Sponsored by AGFD, Cosponsored by CHED

SUNDAY AFTERNOON

Section A

Sheraton Denver Downtown Hotel

Silver

High School Program

Cosponsored by SOCED

Financially supported by ACS Education Division

S. B. Mitchell, *Organizer, Presiding*

12:00 Luncheon.

1:00 CHED **43. Award Address** (James Bryant Conant Award in High School Chemistry Teaching sponsored by Thermo Fisher Scientific). Through generations X, Y and Z, learning never ends. **J.L. Ball**

1:40 CHED **44.** ChemSource, the NGSS, and the particle nature of matter: How to develop classroom-ready templates. **P. Smith**, M. Orna

2:00 CHED **45.** Engaging chemistry resources from the Journal of Chemical Education and ChemEd X>. **D. Cullen**

3:00 Intermission.

3:20 CHED **46.** Think safety = work safely. **E.M. Howson**

3:40 CHED **47.** Using Popular Science Magazine articles to improve students' critical thinking and scientific literacy. **M. Gmurczyk**, P. Pages

4:00 CHED **48.** How effective is lecturing in a high school chemistry class? **D.M. Bunce**

4:20 Concluding Remarks.

Section B

Sheraton Denver Downtown Hotel

Century

Chemistry Education Research

K-12 and Professional Development

J. Barbera, N. P. Grove, *Organizers*

D. G. Herrington, *Presiding*

1:30 Opening Remarks.

1:35 CHED **49.** Using the ACAST to characterize high school chemistry teachers' data-driven inquiry practices. **J. Harshman**, E.J. Yezierski

1:55 CHED **50.** Uncovering high school students' chemistry self-concept with cluster analysis. **S.E. Nielsen**, E.J. Yezierski

2:15 CHED **51.** Tool trouble: Challenges with using self-report data to evaluate long-term chemistry teacher professional development. **S.F. Bancroft**, D.G. Herrington, E.J. Yezierski

2:35 CHED **52.** Target Inquiry at Miami University (TIMU): Uncovering novel relationships among affective and cognitive measures of high school chemistry students. **J.H. Carmel**, **J.T. Harshman**, E.J. Yezierski

2:55 CHED **53.** Efficacy of the connected chemistry curriculum. **S. Ryan**, M. Stieff

3:15 Intermission.

3:30 CHED **54.** STEM Modules: A multifaceted approach to enhancing science learning and perceptions in middle school classrooms. E.J. Andrews, T. Robinson, D. Banks, A.L. Curry, **M.L. Curry**

3:50 CHED **55.** Technology integration in the undergraduate chemistry classroom. **T.L. Vickrey**, B. Riesen, M. Abebe, D. Golick, M.N. Stains

4:10 CHED **56.** Building a teaching profile: Using a modified COPUS observation protocol to easily and reliably measure reformed instructional practice. M.N. Stains, **T.J. Lund**

4:30 CHED **57.** Training faculty with the Teaching Dimensions Observation Protocol (TDOP): Process and pitfalls. **M.L. Grunert**, C. Henderson, A. Beach

4:50 Concluding Remarks.

Section C

Sheraton Denver Downtown Hotel

Spruce

Department, University, and National Models for Faculty Development to Support Adoption of Evidence-Based Teaching

Cosponsored by INOR, ORGN and PRES

R. Waterman, *Organizer, Presiding*

1:30 CHED **58.** Creating a coherent STEM gateway for teaching and learning at Michigan State University: An AAU STEM initiative project. **M. Cooper**

1:50 CHED **59.** Starting at the source: Foundational views about teaching influence adoption of learner-centered teaching practices. **C. Rener**

2:10 CHED **60.** Inclusive excellence in the classroom. **R. Hernandez**

2:30 CHED **61.** VIPEr faculty development workshops: Cutting edge content development and sharing pedagogical best practices. **H.J. Eppley**, **A.R. Johnson**, A.K. Bentley, E.R. Jamieson, C. Nataro, J.R. Raker, B.A. Reisner, S.R. Smith, J.L. Stewart, L.A. Watson, **N. Williams**

2:50 CHED **62.** Cottrell Scholars Collaborative New Faculty Workshop program: Helping new faculty adopt effective approaches from day one. **A.L. Feig**, L.A. Baker, P. Beuning, L.M. Columbus, C.J. Douglas, R. Hernandez, M.N. Stains, R. Waterman, J.L. Wesemann

3:10 Intermission.

3:15 CHED **63.** Steering the ship from the front – how can deans change the culture to support evidence-based learning. **P.K. Dorhout**

3:35 CHED **64.** Responding to barriers to and drivers for faculty adoption of evidence-based instructional practices. **S.E. Shadle**, S. Ritter, P. Pyke, A. Marker, T. Roark, A. Moll

3:55 CHED **65.** Development of a structured support fellowship for faculty innovation in teaching. **R. Frey**

4:15 CHED **66.** Mentoring junior faculty: Pedagogy is only important if you keep the job where you use it. **L. McElwee-White**

4:35 CHED **67.** Long-term impacts of the Cottrell Scholars Collaborative New Faculty Workshop. **M.N. Stains**, M. Pilarz, D. Chakraverty, R. Waterman, A.L. Feig, J.L. Wesemann

4:55 CHED **68.** ISSUES: Investigating student success using evidence-based strategies. **K.R. Cousins**

Section D

Sheraton Denver Downtown Hotel

Denver

Undergraduate Research Papers

Analytical and Environmental Chemistry

Cosponsored by SOCED

C. V. Gauthier, N. L. Snyder, *Organizers*

J. V. Ruppel, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CHED **69.** Green extraction of lycopene from tomato (*Lycopersicon esculentum*) using 2-methyltetrahydrofuran. **M.C. Enright**, J. Noseworthy

1:45 CHED **70.** Improved protein digestion for the mass-spectrometric detection of cysteine palmitoylation. **M. Torres-Caban**, N. Gould, H. Ischiropoulos

1:55 CHED **71.** Degradation of estrogen: An NMR study. **K. Davis**, K. Cossey

2:05 CHED **72.** Analysis of application of interpolation techniques to ultraviolet-visible spectroscopy of critical vesicle concentration. **G.P. Nguyen**, S.E. Maurer

2:15 Intermission.

2:25 CHED **73.** Determining the degradation of an antioxidant, lycopene. **K. Foerster**, K. Cossey

2:35 CHED **74.** Application of ionic liquids in forensic chemistry. **M. Jones**, R.E. Del Sesto

‡ *Cooperative Cosponsorship*

2:45 CHED **75.** Analysis of sol-gel processing as a controlled release method for fragrance molecules of essential oils. **K. Ehret**, C.H. Lisse

2:55 Concluding Remarks.

Section E

Sheraton Denver Downtown Hotel
Columbine

From Cornerstone to Capstone: Culminating Experiences in the Undergraduate Chemistry Curriculum that Foster Integration and Application of Foundational Knowledge

K. Kneas, J. A. MacKay, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 CHED **76.** Integration in upper-division instructional chemistry laboratories at Regis University. **S. Mahapatro**

1:55 CHED **77.** Integrated lab: The first year of a laboratory course integrating the sub-disciplines of chemistry and open-ended research experiences. **J.G. Rowley**, D.M. Hitt, D. Gretch, C. Pharr, C.A. Thomas

2:15 CHED **78.** Integrated Laboratory at Guilford College: An authentic research experience for chemistry majors. **G.H. Webster**, R.M. Whitnell, A.G. Glenn

2:35 Intermission.

2:45 CHED **79.** Elizabethtown College chemistry and biochemistry capstone experience. **T.E. Hagan**, **K. Kneas**, **J.A. MacKay**

3:05 CHED **80.** University curriculum meets departmental capstone: Integrating a novel seminar and research capstone into a liberal arts curriculum. **T.W. Johnson**

3:25 Discussion.

3:45 CHED **81.** Transitioning students to four year schools via an introduction to scientific research course. **J. MacArthur**

4:05 CHED **82.** Development of a pre-professional program at a rural community college. **J.L. Hayes**, S. Burchett

4:25 CHED **83.** Advancing chemistry education in two-year college programs through self-assessment. **C.L. Velez**, **H. Sklenicka**

Section F

Sheraton Denver Downtown Hotel
Gold

NMR Spectroscopy in the Undergraduate Curriculum

Pedagogy

Financially supported by Bruker; JEOL; Thermo Fisher Scientific; Anasazi Instruments

L. J. Anna, D. P. Soulsby, A. S. Wallner, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 CHED **84.** NMR in first year chemistry. **J. Alexander**, J. Ashmore, **A. Baker**, S. Chadwick

1:55 CHED **85.** Implementation of NMR spectroscopy into the undergraduate experience at The College of New Jersey. **A.R. O'Connor**, **S.E. Sen**

2:15 CHED **86.** New "spin" on integrating NMR spectroscopy into an undergraduate curriculum. **E.J. McIntee**, K.J. Graham, C.P. Schaller, T.N. Jones

2:35 Intermission.

2:45 CHED **87.** More systematic approach to learning NMR spectroscopy. **C. Gabel**, **M.J. Magrini**, **S.S. Gordon**, J. Salazar, A.N. Gamble, **N. Kuehl**, D. Rourke, S. Norris

3:05 CHED **88.** Using spectra from undergraduate projects to improve higher order cognition. **S.M. Schelble**, K. Elkins

3:25 CHED **89.** ^{13}C should precede ^{1}H NMR in teaching organic chemistry. **D.D. Clarke**, R. Orazi

3:45 Intermission.

3:55 CHED **90.** Incorporation of benchtop NMR spectroscopy into undergraduate laboratories: An active-learning approach. **S.D. Riegel**

4:15 CHED **91.** Providing access to a million NMR spectra via the web. **A.J. Williams**, D. Lowe, C. Coba, P. Corbett, A. Pshenichnov, V. Tkachenko

4:35 Concluding Remarks.

Graduate Student Symposium

Sponsored by AGFD, Cosponsored by CHED

SUNDAY EVENING

Section A

Colorado Convention Center
Hall D

General Posters

I. Black, *Organizer*

7:00 - 9:00

CHED **92.** Impact of chemical demonstrations on student interest and learning in science. H. Salazar, **A. Moore**, D.G. Watson

CHED **93.** Brewing alcoholic beverages as a means of incorporating writing instruction into an existing junior-level laboratory capstone course. **K.A. Brown**, **J.D. Mimbs**, C.S. Seney, D.R. Goode, D.E. Moore, A.M. Kiefer

CHED **94.** Enhancing research for students and new faculty at undergraduate institutions. **M.E. Railing**, J. Fuller, E. Sylvester, J. Coffield

CHED **95.** Scientific connections: Development of a chemistry of art course for non-majors. **S.E. Hubbard**

CHED **96.** On the production of Chinese Purple in the art studio and chemistry laboratory. **J.D. Thoburn**, M.M. Thoburn

CHED **97.** Under the Dome: Student-designed evidence-based inquiry to understand and predict climate change outcomes. **S.A. Stewart-James**, **J. Sutter**

CHED **98.** The chemistry of Thomas Edison. **R.H. Wallace**

CHED **99.** Application of mathematical concepts to teaching and learning of chemistry. **P.K. Yuen**, C.D. Lau

CHED **100.** FUTURE program: Ensuring that underserved populations become the scientific and civic leaders of tomorrow. **A.J. Reig**, **J. Pellegrino**

CHED **101.** Expansion of the Science Resource Center. **S. Richards**, P.J. Iles, L.D. Giddings, M. Alvarez, N.R. Bastian, R.V. Valcarce

CHED **102.** With the scientific research advantages in the discipline, the construction level of chemical characteristic specialty is enhanced. **Z. Jiang**, Z. Yao, H. Yue, Z. Wang, C. Li, L. Zhao, M. An

CHED **103.** Cultivation of chemical engineering talents innovation ability based on the scientific research project trainin. **H. Yue**, Z. Wang, J. Li, Y. Wang, Z. Yao, D. Liu, Z. Jiang

CHED **104.** The 2016 Biennial Conference on Chemical Education. **R.W. Schwenz**, M.L. Miller, J.M. Smist

CHED **105.** "I want to be the inquiry guy!" How research experiences for teachers transform beliefs about teaching science as inquiry. S.F. Bancroft, D.G. Herrington, **M.M. Edwards**, C.J. Schairer

CHED **106.** Using Special English as a tool to engage students in chemistry lecture. **D.J. Swartling**

CHED **107.** Design, development, and delivery of the Nevada GEAR UP STEM Summer Institute. **S. Nealy**, K. Carroll, H. Skaza, E. Marti, E. Gandhi, M. Dulger, D. Gerrity, T. Olson, P. Schrader, M. Orgill

CHED **108.** PROPEL Center at Colorado State University-Pueblo: The effect of a STEM tutoring center on academic excellence. **C. Barnett**, T. Marshall

CHED **109.** Revision of chemical professional undergraduate training scheme guided by "Excellence engineers education program". **Z. Yao**, Z. Wang, C. Li, L. Zhao, M. An, Z. Jiang, H. Yue

CHED **110.** High school students' perceptions and performances on predict-observe-explain tasks in chemistry laboratory. **P. Vadapally**, **J.P. Suits**

CHED **111.** "Building Your Science Toolkit:" Encouraging young female undergraduates to pursue science through laboratory experiences and interactive, tiered mentoring. **C. Normand**, **D. Kumarjiguda**, J. Canfield

CHED **112.** Leveraging REU programs to attract talents in STEM fields: A comparison of outcomes of a discipline-based education research and a molecular science REU program. **A.F. Knedeisen**, **D. Xue**, M.N. Stains

CHED **113.** Balancing "wow" and "satisifying standards" with hands-on activities and critical thinking: Developing middle school science modules. **M.S. Reeves**, C. Bradford, A. Bufford, D. Chappell, G. Griffin, B. Hart, L. Jackson

CHED **114.** Test-based learning with online vs. paper tests. **A. Prisacari**, T. Holme

CHED **115.** When teaching chemistry and text messaging do work together in a classroom. **J. Zhang**

CHED **116.** Younger Chemistry Education Scholars (YCES) committee: Who we are and what we do. M. Anzovino, T.J. Bussey, J.H. Carmel, K.R. Galloway, J. Harshman, K.J. Linenberger, E.B. Moore, J. Reed, **S. Ryan**

CHED **117.** Frequent assessment: Does it make a difference in student learning? **A. Wallace**

CHED **118.** New chemistry advanced placement (AP) test: Hands-on inquiry based experiment workshops. **R. Grunglasse**, **C. Harrilal**, **N.N. Pierre**, **S. Rolle**, A. Riego, M. Exposito, M. Delgado

CHED **119.** Using missing data methods to address the problem of incomplete national normative datasets at the ACS Examinations Institute. **A. Brandriet**, T. Holme

CHED **120.** Incorporation and evaluation of science practices in multiple-choice items. **J.J. Reed**, T.A. Holme

CHED **121.** Importance of demo shows in the community. **J.T. Tomko**, E.P. Kippenhan

CHED **122.** Fostering student success: Advanced topics and research at a community college. **T. Bledsoe**, S. Hinote, M. Murphy, L.D. Burke

CHED **123.** Community outreach at Pima College East Campus: Summer research for high school teachers and high school students. **T. Bledsoe**, **G. Zreda**, A. Frey, D. Donegan, M. Murphy, L.D. Burke

CHED **124.** Introduction of powder X-ray diffraction in K-12 education. **R. Boniak**, **C. Patel**

CHED **125.** Investigating organic chemistry students' ideas about nucleophiles, electrophiles, and reaction mechanisms. **M.E. Anzovino**, S. Bretz

CHED **126.** Developing an interdisciplinary medicinal plant research program that engages agriculture, biology, and chemistry undergraduate students across the curriculum. **W.E. Collier**, M.A. Abdalla, C. Bradford, G. Griffin, D. Mortley, A. Russell

CHED **127.** Connecting organic chemistry and biochemistry. **W. Powell**, K. Aghoram, K.A. Hinton

CHED **128.** Video instruction in organic chemistry: Student perceptions and preferences. **K.B. Fields**

CHED **129.** Climate change outreach demonstrations. **P. Hills-Rieck**, B. Chandler

CHED **130.** Using an online assessment tool to gain insight to students' usage of representations in chemistry. **J. Polifka**, T. Holme

CHED **131.** Practical component to a biochemistry lab final exam. **K.R. Willian**

CHED **132.** Investigating cellular steady state as a threshold concept in biochemistry. **T. Morgan**, J.E. Lewis, J.A. Loertscher, V.M. Thorsell

CHED **133.** Water quality education. **B.R. Bricker**, J.M. Weinkauf, **M.W. Fultz**

CHED **134.** Development of a self-efficacy survey instrument designed to gauge the relationship between completion of AP chemistry and comfort level in first-semester general chemistry. **M.A. Erdmann**, L. Freeman, J. March

CHED **135.** Impact analysis of prerequisite incorporation toward student success in freshman-level college chemistry courses. F.M. Yarberry, **S. Cornish**

CHED **136.** Manual dexterity: assessing its role in the chemistry laboratory. **I.L. Brown**, S.D. Wiediger

CHED **137.** Analysis of meaningful learning in the General Chemistry laboratory. **K.R. Galloway**, S. Bretz

CHED **138.** Teaching chemistry at a technical college through practical field work using performance based instruction: The Milwaukee River Project. **S.A. Schlipp**

CHED **139.** Fearless investigators: Teaching science through experimental design. **R.E. Grote**, P.J. Wendel

CHED **140.** Flipping general chemistry via a highly structured teaching pedagogy: Initial conclusions. **C. Uvarov**, **R. Gamage**, G. Allen

CHED **141.** Using first-day assessments to determine math readiness for general chemistry. **C.M. Chant**, D.S. Heroux

CHED **142.** Use of eye fixation sequence analysis to identify common cognitive processes among students solving conceptual stoichiometry problems. **J. Baluyut**

CHED **143.** CLP: A collaborative learning program in chemistry with benefits for both students and facilitators. **B.A. Davis**, M.A. Fisher, M. Raab

CHED **144.** Development of a service-learning introductory chemistry course for culinary arts students. **A. Wallace**

CHED **145.** Transparency and electronic assessment. **E.M. Epp**

CHED **146.** Constructing a consensus definition of conceptual understanding in chemistry from empirical data provided by instructors. **C.J. Luxford**, T. Holme

CHED **147.** Water quality comparison of city facilities and residences in North Miami, Florida. **N.N. Pierre**, **S. Rolle**, **C. Harrilal**, K. Sanchez, A. Riego, **L. Dean**, **J. Johnson**, **A. Laroche**, **Q. Lockhart**, M. Exposito

CHED **148.** Lewis Misconstruction: An investigation into student's Lewis structure drawings. **N.L. Burrows**

CHED **149.** Describing and characterizing the affective domain in middle and high school science students. **S.F. Bancroft**, **J.H. Carmel**, **J. Harshman**, E.J. Yezierski, D.G. Herrington

CHED **150.** Introducing computational chemistry: A hands-on spreadsheet approach. **P.E. Hoerner**, J. Beck

CHED **151.** Conformational analysis discovery activity using 3D potential energy surface models. **F.A. Carroll**, D.N. Blauch

CHED **152.** Mathcad exploration of Fourier transforms found in physical and analytical chemistry courses. **T.C. Miller**, J.N. Richardson, **J. Kegerreis**

CHED **153.** Mustard: Tiny seed — unlimited possibilities. **I.E. Popova**, M.J. Morra

CHED **154.** Impact of supplemental video prelab material for a biochemistry lab practical on student overall preparedness. **T.M. Whealon**, S.D. Wiediger

CHED **155.** Quantitative analysis of glucose and kinetic study of glucose oxidase for use in an introductory quantitative analysis laboratory. **T.C. Miller**, E.E. Frieben, T. Frielle, **J.N. Richardson**

CHED **156.** Exploration of formaldehyde in apparel fabric using experimental and theoretical infrared and UV–visible spectroscopy. K.A. Leets, K.B. Bramble, **G.D. Gibbs**, L. Tribe

CHED **157.** Measuring silver nanoparticle concentration by inductively coupled plasma optical emission spectroscopy: A laboratory experiment for chemistry and engineering students. **S.W. Brittle**, J.D. Baker, K.M. Dorney, T. Ebrahimian, J.M. Dagher, I.E. Pavel Sizemore, S.R. Higgins

CHED **158.** Comparison of modes of delivery for safety information in an undergraduate laboratory. **A.M. Powe**, A. Jamhawi, O. Ersin

CHED **159.** Microwave-assisted dye synthesis: A more efficient approach for an undergraduate laboratory. **A.B. Ormond**

CHED **160.** Quantifying and recycling precious metals from printed circuit boards: An undergraduate laboratory. **S. Fields**, **C. Rector**, K.J. Sorauf

CHED **161.** Use of the three levels of representation to introduce the concept of buffers. **Z. Medina Torres**, E.L. Ortiz-Nieves, J. Padilla, J. Ortiz

CHED **162.** Periodic Table goes live. **E.J. Andrews**, T. Robinson, A.L. Curry, M.L. Curry

CHED **163.** Concrete solar cells? An investigation into an alternative form of alternative energy. **B. Ackley**, J. Bianchini, J.C. Warner

CHED **164.** Quantum dot sensitized solar cell for the undergraduate laboratory curriculum. **T.M. Ticich**, B.L. Oliva-Chatelain, A.R. Barron

CHED **165.** Integrated upper-division chemistry laboratory: synthesis and characterization of vandyl *bis*- acetylacetonoate complex. **S. Mahapatro**, C. Rector, G. Morgan, A.L. Stuckmeyer

CHED **166.** Separations of acetaminophen and caffeine by high temperature high-performance liquid chromatography. **A. Gizzi**, J.V. Arena

CHED **167.** ^{1}H NMR Analysis of the Methylation of Oleic Acid Catalyzed by Tin (II) Bromide in the Presence of a Cosolvent. **N. Singh**

CHED **168.** Determination of organic and inorganic priority pollutants in herbal teas and coffee. **R. Gray**, R. Richter

CHED **169.** Organic chemistry laboratory sequence alternating experiments with guided inquiry exercises. **S.C. Young**, K.L. Colabroy, M.R. Baar

CHED **170.** Using 3D printing to model steric interactions. **C. Diaz-Allen**, P.A. Sibbald

CHED **171.** Simple technique for students to assign hydrogen atom resonances in heterocyclic ligand metal complexes. **D.P. Rillema**, H. Nguyen

CHED **172.** Integration of green chemistry topics into the traditional organic chemistry experiments. **S.P. Lorimor**

CHED **173.** Boiling point, azeotrope: A simple discovery-based experiment for organic laboratory course. **M.A. Rubin**, M. Rubina

CHED **174.** How to PDB: a class exercise for professional Pharmacy Med Chem. **N.R. Natale**, H.D. Beall

CHED **175.** Novel instructional undergraduate organic chemistry laboratory experiment exploring substitution patterns of various allylic halides. **T.M. Trygstad**, **N.W. Dykes**, **A. Radakovic**, **P.T. Chazovachii**, E.W. Lake, M.M. Hite, J.C. Hicks

CHED **176.** Intermolecular forces: An organic laboratory experiment. S. Candiello, **R.B. Lettan II**

CHED **177.** Isolation and identification of natural products in dried turmeric in undergraduate research. **G.R. Khalsa**, A.J. Pohlod

CHED **178.** Multistep drug synthesis in the sophomore organic lab: Synthesizing *R*-rasagiline, a popular Parkinson's drug. **N. Aguilar**, **B.J. Garcia**, S. David

CHED **179.** Education through an inquiry based environment in the physical chemistry laboratory: The thermodynamic of an electrochemical cell. **C.M. Torres Diaz**, **D.D. Alequin**, R. Arce, A. Colom

CHED **180.** Synthesis and characterization of tricarbocyanine dyes for use in physical chemistry laboratory. **G.R. VandeZande**, A.L. Marsh

CHED **181.** Discovering pressure-volume-temperature phase relationships with 3D models. **D.R. Striplin**, F.A. Carroll, D.N. Blauch

CHED **182.** Portable X-ray fluorescence spectrometry in the undergraduate chemistry curriculum at MWSU. **S.L. Hiley**

CHED **183.** Preparation of samples for introducing undergraduate students to electron paramagnetic resonance. **A. Hanks**, B.E. Sturgeon

CHED **184.** Quantitative determination of kidney cancer biomarkers in urine by liquid chromatography tandem mass spectrometry. S. Gamagedara, **L.M. Nguyen**

CHED **185.** Research and practice of the mode of training research capacity through scientific innovation. **D. Lin**, W. Qin, B. Pu

CHED **186.** Discussion on characteristic specialty construction and cultivating college students' technological innovation ability. **D. Lin**, B. Pu, C. Li

CHED **187.** Development of a hybrid course in sustainable energy. **A. Kahl**

CHED **188.** Using theoretical chemistry to explain S_N2, E2, S_N1 versus E1 mechanism for undergraduate organic chemistry. **A.S. Dutton**, M.L. Dutton

MONDAY MORNING

Section A

Sheraton Denver Downtown Hotel

Gold

ACS Award for Achievement in Research for the Teaching and Learning of Chemistry: Symposium in Honor of Vickie M. Williamson

Cosponsored by WCC

Financially supported by Pearson Publishing

M. R. Abraham, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 CHED **189.** Origins. **M.R. Abraham**

8:55 CHED **190.** Visualization and the learning cycle: A great partnership. **J.I. Gelder**

9:15 CHED **191.** Six years in: Surviving and thriving at a SLAC. **K.R. McCann**

9:35 CHED **192.** Molecular visualizations through the lens of research and practice. **R.M. Kelly**

9:55 Intermission.

10:10 CHED **193.** Visualizations in the chemistry classroom: A visual learner's perspective. **M.J. Sanger**

10:30 CHED **194.** Developing and validating a measure of linked concepts for general chemistry. **S.E. Lewis**

10:50 CHED **195.** Innovation diffusion in a single case: Adoption and re-invention of visualization research findings to improve applied research, instruction, and teacher professional development in chemistry. **E.J. Yezierski**

Section B

Sheraton Denver Downtown Hotel

Century

Experiments for Physical Chemistry Laboratory

Spectroscopy & Thermodynamics

A. Grushow, S. S. Hunnicutt, R. M. Whitnell, *Organizers*

F. J. Creegan, *Presiding*

8:30 Introductory Remarks.

8:35 CHED **196.** Redesigning the hydrogen spectrum experiment for guided inquiry. **C. Salter**, C.M. Teague

8:55 CHED **197.** Using the spectrum of HCl as a model building exercise. **A. Grushow**

9:15 CHED **198.** Incorporation of single-molecule FRET measurements into an undergraduate Physical Biochemistry Laboratory course. **J. Knight**, D. Giardina, A.J. Bonham, M.K. Maron

9:35 Intermission.

9:45 CHED **199.** Guided-inquiry approach for relating the fluorescence spectrum of the pyrene excimer to its thermodynamic properties. **A.R. Noble**

10:05 CHED **200.** Constructing a binary phase diagram for aqueous salts. **R.R. Michelsen**

10:25 CHED **201.** POGIL physical chemistry lab experiment: the vapor pressure of liquid. **B.D. Gilbert**, M.A. Everest, D.E. Gardner

10:45 Intermission.

10:55 CHED **202.** Using food additives to enchance traditional bomb calorimetry experiments. **J.B. Dudek**

11:15 CHED **203.** Are the molecules that make a solution red big or small? A POGIL-PCL recasting of the cyanine dye experiment. **S.S. Hunnicutt**, R.M. Whitnell

11:35 CHED **204.** Guided inquiry solid-liquid phase diagram experiment. **S.S. Hunnicutt**, R.M. Whitnell, A. Grushow

11:55 Concluding Remarks.

Section C

Sheraton Denver Downtown Hotel

Spruce

Integrating Chemistry and Polymer Science Research into the Classroom

Cosponsored by PMSE and POLY

S. E. Morgan, *Organizer*

K. A. Cavicchi, *Organizer, Presiding*

K. Wingo, *Presiding*

8:30 CHED **205.** Developing polymer and chemistry research lessons for the high school classroom – NSF GK-12 at The University of Southern Mississippi. **K. Wingo**, S.S. Herron, S.E. Morgan

8:50 CHED **206.** Integration of polymer research into a lab-based polymer chemistry class at a small, primarily undergraduate institution. **B. McFarland**

9:10 CHED **207.** Aerospace composites and the scientific method: Supporting high school classroom curriculum with real-world applications. **A.S. Frazee**, B.F. Stringfellow, J.S. Wiggins

9:30 CHED **208.** Discovering chemicals through solid-phase microextraction gas chromatography/mass spectroscopy. **C. Rosu**, C. David, R. Cueto, L. Veillon, R. Laine, E. Reichmanis, P.S. Russo

9:50 CHED **209.** Introducing the effect of additives on hydrogel properties. **D.N. Amato**, K. Holmes, D.L. Patton

10:10 CHED **210.** Integrating polymer labs into the NGSS high school chemistry classroom. **M.T. Baker**

10:30 Intermission.

10:45 CHED **211.** Using polymer properties to illustrate and explain concepts in introductory chemistry. **D.E. Bergbreiter**

11:05 CHED **212.** Polymers in biomedicine and hydrophobic surfaces: Two RET experiences at the University of Akron. **D. Hess**, D. Moore, G. Cheng, N. Zacharia, K.A. Cavicchi

11:25 CHED **213.** Research Experience for Teachers program at The University of Akron. **K.A. Cavicchi**

11:45 CHED **214.** Transferring teacher research on wastewater wetlands into effective classroom activities. **A. Glimme**

12:05 CHED **215.** Withdrawn.

12:25 CHED **216.** Make it and break it: Employing a plant starch bio plastics experiment in the high school classroom for addressing engineering education standards. **J.E. Wissinger**, A. Johnson, C. Ahrenstorff

12:45 CHED **217.** Activities in polymer optical physics for STEM education enrichment in the K-12 environment. **A. Fogel**, J. Brownlow, S.E. Morgan

1:05 CHED **218.** Preparation and evaluation of antimicrobial films. **E.D. Matthews**

Section D

Sheraton Denver Downtown Hotel

Denver

Undergraduate Research Papers

Computational, Physical and Inorganic Chemistry

Cosponsored by SOCED

J. V. Ruppel, N. L. Snyder, *Organizers*

C. V. Gauthier, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 CHED **219.** Computational study of disubstituted ammonia borane derivatives for hydrogen storage. **T.E. West**, A.S. Dutton

8:45 CHED **220.** Determining the activation energy of a series of spectroscopic imines. **C. Yeager**, J.B. Dudek

8:55 CHED **221.** Why do Ala, Ala, Lys tripeptides preferentially rearrange to the Lys-Ala-Ala sequence in the gas phase? **E. Kowalczyk**, J. Poutsma

9:05 CHED **222.** Tandem substitution-cyclization-elimination reaction that can account for the mutagenicity of arylamines without the need of nitrenium ions. **S. Shrestha**, J. Bautista, A.G. Leach, A.S. Dutton

9:15 Intermission.

9:25 CHED **223.** Novel ligands for metal oxides colloid stabilization. **A.S. LaBeaud**, C. Mitchell, R. Komati, G.Z. Goloverda, V.L. Kolesnichenko

9:35 CHED **224.** Development of a new method for graphene oxide thin-film growth. **M. Berens**, B.J. Winters

9:45 CHED **225.** Iron-carbonyl clusters: Catalysts for hydrogen generation. **C.A. Mebi**

9:55 CHED **226.** Withdrawn.

10:05 Intermission.

10:15 CHED **227.** Shaped palladium nanoparticle synthesis on carbon substrates. **S.E. Sanders**, P. Duffy, P.E. Colavita, K.M. Metz

10:25 CHED **228.** Silicate nanoparticles from spray flame synthesis for lithium ion batteries. **E. Maccato**, J. Kovacevic, H. Wiggers, B. Mellis

10:35 CHED **229.** Morphological control of film structure in perovskite solar cells. **C. Jackson**, C. Tassone

10:45 CHED **230.** Laminar-flow reactor study of the pyrolysis of 4-vinylguaiacol. **J. Hoang**, E. Ledesma

10:55 Concluding Remarks.

Section E

Sheraton Denver Downtown Hotel

Columbine

Research at Community Colleges: Strategies for Enhancing Student Transfer & Success

Financially supported by 2YC3

D. M. Sarno, *Organizer*

P. D. Svoronos, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 CHED **231.** Using research as a tool to engage, retain and graduate STEM students at Queensborough Community College. N. Gadura, **P.D. Svoronos**

8:55 CHED **232.** Goal, role, and soul of undergraduate research development at the Community College of Denver. **M. Haefele**, **H. Loshbaugh**

9:15 CHED **233.** Black bear research: A case study in undergraduate research at a community college. **J.J. Van Niel**

9:35 CHED **234.** Undergraduate research at Queensborough Community College: The first step for a successful transfer and eventual post-undergraduate career in STEM careers. **P.D. Svoronos**

10:15 Intermission.

9:55 CHED **235.** Transporting an established undergraduate research program to a community college. **D.J. Schauer**

10:25 CHED **236.** Strategies for funding undergraduate research at the community college. **R.H. Jarman**

10:45 CHED **237.** Research-based and interdisciplinary curriculum design for general chemistry and beyond. **K.S. Owens**, A.J. Murkowski, H. Price, A.M. Johansen

11:05 Intermission.

11:15 CHED **238.** Promoting undergraduate research at community colleges to increase STEM competency and transferability to 4 yr institutions within CUNY. **N.H. Phillip**, **T. Brennan**, P. Meleties, J. Rachlin

11:35 CHED **239.** The STEPS Program — a pathway from Community College to Bachelor's degree and beyond. **R.D. Walker**, T. Williams

11:55 CHED **240.** The Community College Undergraduate Research Initiative: A national collaborative. **P. Powers**

12:15 Discussion.

‡ *Cooperative Cosponsorship*

Section F

Sheraton Denver Downtown Hotel
Silver

Chemistry Education: International and Multi-cultural Perspectives

S. Raje, *Organizer*
S. Sandi-Urena, *Organizer, Presiding*
S. Hansen, *Presiding*

8:30 Introductory Remarks.

8:35 CHED **241.** Chemical education in India: Observations. **L.H. Rickard**

8:55 CHED **242.** General Chemistry study habits and instructional practices across borders. **J. Leitón Chacón**, S. Sandi-Urena, A. Villalta-Cerdas, M. Sestilio, L. Pettygrove

9:15 CHED **243.** Language challenges in teaching and learning General Chemistry. **P.K. Yuen**, C.D. Lau

9:35 CHED **244.** Withdrawn.

MONDAY AFTERNOON

Section A

Colorado Convention Center
Halls C/D

Undergraduate Research Posters

Agricultural and Food Chemistry

Cosponsored by AGFD and SOCED

N. Di Fabio, *Organizer*

12:00 - 2:00

CHED **245.** Improving quality control methods in the brewing industry through analytical characterization of hop alpha acids. **K. Dahya**, J. Moon, M. Brush, R.N. Dansby-Sparks

CHED **246.** Analysis of metal ion absorption compared to pH and conductivity changes in hydroponic growing systems. **T.E. Sheppard**, M.E. Railing

CHED **247.** Archaeochemical analysis: Using chemistry to inform history. **D.A. Regan**, A.A. Hill, D. Hill

CHED **248.** Determination of chlorogenic acid and caffeic acid in fruits with evaluation of pesticide concentrations. J.C. Doverspike, C.A. Radford, **J.E. Owens**

CHED **249.** Modifications of brewing parameters: Analysis of volatiles by SPME-GC-MS and hydrogen sulfide analysis in beer. **L. Benedict**, R. Byrnes, A.C. Ricardi, M.S. Qazi, P.J. Gregorich, D.A. Arris

CHED **250.** Characterization of tissue browning products using attenuated total reflection: Fourier transform infrared spectroscopy. **A. Steele**, J. Walton, S. Chakraborty

CHED **251.** Further defining acylsugar structural diversity within *Petunia axillaris*. **M.C. Enright**, X. Liu, A. Jones

CHED **252.** Determining the effects of processing on antioxidant activity in cilantro, parsley, and rosemary. **L.M. Patel**, K. Daus

CHED **253.** Mapping of oxidation products of tissue browning using 2,4-ditrophenylhydrazine and high performance liquid chromatography. **J. Walton**, A. Steele, S. Chakraborty

CHED **254.** Using trace element signatures to determine cocoa liquor provenance. **R. Khalsa**, S.E. Stitzel, R.E. Sours

CHED **255.** Analysis of e-cigarette flavors with gas chromatography. **T. Massetti**, K. Muller

CHED **256.** Extraction and characterization of anthocyanins from organically grown grains. **N. Strobel**, G.L. Milligan

CHED **257.** Comparison of eastern filbert blight resistance in two hazelnut cultivars. **N. Lee**, M. Hoang, A. Hoffman

CHED **258.** Comparison between two extraction techniques used to isolate antioxidants from the pith and carpellary membrane of pomegranates. **S. Ansari**, K.A. Daus

Section A

Colorado Convention Center
Halls C/D

Undergraduate Research Posters

Analytical Chemistry

Cosponsored by ANYL and SOCED

N. Di Fabio, *Organizer*

12:00 - 2:00

CHED **259.** Analysis of elements in nutritional beef bone broth. **A. Poli**, M.E. Piyasena

CHED **260.** X-ray structure and variable-temperature photoluminescent properties of isostructural lanthanide cyanometallates containing DMSO. **K. Xiang**, J. Hendrich, F.D. White, J.D. Taylor, R. Sykora

CHED **261.** Spectrophotometric determination of ethanol concentration in beer utilizing an enzyme activity assay. **J.A. Schafer**, E. Paine

CHED **262.** Determination of cocaine concentrations in dried bloodstains. **B. Gillease**, G.P. Foy

CHED **263.** Detection and extraction of date rape drugs from hair samples using liquid chromatography - mass spectroscopy. **L. Burns**, G.P. Foy

CHED **264.** Elemental analysis of CdSe/ZnS core/shell quantum dots by AA. **K.M. Stallings**, J.L. Dancler, B.E. Eichler, D.E. Weisshaar

CHED **265.** Analyzing thermal degradation of iso-alpha acids by high performance liquid chromatography (HPLC). **J.M. Goff**, **K.M. OBrien**, T. D'Andrea

CHED **266.** pH Dependent Zn(II) binding behavior of an analog methanobactin peptide. **K.L. Cumpian**, M. Deeconda, R. Ortiz, S.M. Wagoner, L.A. Angel

CHED **267.** New method for improving solar energy conversion: Side selective modification of Photosystem I. **L. Thal**, E.A. Gizzie, G. LeBlanc, D.E. Cliffel, G. Jennings

CHED **268.** Quantitative analysis of hydrogen peroxide using crude peroxidase extract from cucumber peel. **L.E. Totten**, S. Kradtap

CHED **269.** Determination of bisphenol A in thermal receipt paper water samples and lake water samples using fluorescence spectrophotometry. **B. Chitwood**, S. Hubbard

CHED **270.** Withdrawn.

CHED **271.** Determination of bisphenol-A (BPA) in canned goods from Arkansas markets using fluorescence spectrophotometry. **R. Pruett**, S. Hubbard

CHED **272.** Rapid identification of designer drugs with NMR spectroscopy. **F. Fowler**, L. Huang

CHED **273.** Optimization of silver shell and silica core nanoparticles as SERS active substrate. **A.G. Telcy**, S. Han, X. Li

CHED **274.** Synthesis, characterization, and catalysis of halogen and nitro substituted Schiff-base organometallic complexes towards the copolymerization of CO_2 and epoxides. **R.L. Ayscue**, N.P. Deifel

CHED **275.** Preparation of hydrophobic thermally polymerized sol-gel monolithic columns for reversed-phase liquid chromatography using "single-pot" approach. **R. Hernandez**, L. Narciso Meirelles, F. Svec, **Z. Zajickova**

CHED **276.** Garnet classification and provenance using laser-induced breakdown spectroscopy (LIBS). **P.A. Defnet**, R.R. Hark, M. Wise, R.S. Harmon

CHED **277.** HPLC method development for caffeine analysis with *Chlorella vulgaris* as a bioremediation agent for aquatic systems. **A.L. Williamson**, S.M. Ethridge, C.A. Miderski

CHED **278.** Laser-enhanced ionization–mass spectrometry for dried blood spot quantification of a biomedically important analyte. **S. Sheffield**, L. Miller, S. Shuttleworth, S. Faber, M. Pamuku, H. Kingston

CHED **279.** Developing paper microfluidic devices to detect drugs of abuse. **J. Bottoms**, L. Wang, B. McCord

CHED **280.** Characterization of patterned anti-fouling xerogel coatings. **Z. Jones**, J. Destino, F.V. Bright

CHED **281.** Investigation of chemical interferences in vehicle arson accelerant identification. **L. Humphrey**, D.G. Klarup

CHED **282.** Identifying more efficient methods for rare earth isobar separations. **C. Meyer**, L. Harvey

CHED **283.** Using fast-scan cyclic voltammetry to quantify serotonin release in Huntington's disease model mice. **S. Fantin**, R. Gehringer, S. Kaplan, M.A. Johnson

CHED **284.** Elemental analysis of enamel and dentin in healthy, carious, and periodontal diseased permanent human teeth using inductively coupled plasma mass spectrometry (ICP-MS). **R. Reed**, M.B. Jacobs

CHED **285.** Extraction and concentration of caffeine from artificial saliva for GC/MS analysis. **J. Mayhew**, B. Zabka, B. Nespor, S. Cole-Harding, N. Winburn

CHED **286.** Determination of fluoride levels in mouthwash and tap water samples. **E.N. Henshaw**, R. Fietkau

CHED **287.** Quantitative determination of methionine sulfoximine by liquid chromatography tandem mass spectrometry. **W. Gilbraith**, S. Gamagedara

CHED **288.** NMR Investigation of the effect of pH on aggregation, counterion binding, and amide proton exchange in amino-acid-based surfactants. **C. Lewis**, A. Wall, E. Billiot, F.H. Billiot, K.F. Morris

CHED **289.** Effect of pH on isocynate amino acid based surfactants. **D. Georgiadis**, F.H. Billiot, C. Lewis, E. Billiot, K.F. Morris

CHED **290.** Surface immobilization of AMPs using click chemistry. **M. Baria**, Y. Li, Z. Chen

CHED **291.** Analysis of nitrate content in vegetables using ion chromatography. **C. Griffin**, M.M. Ivey

CHED **292.** Using regression analysis to determine the mechanism of solvent reactions. **M. Durrant**, M.J. D'Souza

CHED **293.** Apparatus for ultratrace detection of arsenic in drinking water by hydride generation gas chromatography with photoionization detection. **W.R. Borgeson**, S.H. Frisbie, J.N. Driscoll

CHED **294.** Expanding and improving direct-analysis capabilities in mass spectrometry. **S. Michalak**, J.T. Shelley

CHED **295.** Investigation of β-blocker association with a chiral molecular micelle by means of molecular dynamics simulations. **C. Hoffman**, E. Billiot, F.H. Billiot, Y. Fang, K. Morris

CHED **296.** Investigation of the mechanism of chiral recognition by molecular micelles with molecular dynamics simulations. **S. Zack**, E. Billiot, F.H. Billiot, Y. Fang, K. Morris

CHED **297.** Examination of silica sol-gels and aerogels containing silver nanoparticles and 4-mercaptobenzoic acid using surface-enhanced Raman spectroscopy. **T. Corrado**, E.J. O. Atkinson, B.D. Gilbert

CHED **298.** Chromatographic analysis of bee propolis. **K. Symczak**, S.J. Pace, E.E. Mojica

CHED **299.** Studies on the interactions of four nanoceramics (metal oxides) with serum albumin and hemoglobin proteins by spectroscopic techniques. **E. Nguyen**, P.M. Hanson, T.J. Batte, E.E. Mojica

CHED **300.** Trace element analysis of commercially produced red wines and beers. **M.J. Raub**, N.S. Olson, N.J. Ronkainen

CHED **301.** Comparing graphene oxide electrochemically reduced from aqueous and non-aqueous solutions for the purpose of serving as an electrocatalyst support material. **I.B. Agbere**, J.A. Bennett

CHED **302.** Dependence of surface roughness on electropolish time on 316L stainless steel. **E. Hammerstrom**, K.E. Rohly

CHED **303.** Mass spectrometry imaging of the *Torpedo californica* electric organ using MALDI-FT-ICR MS. **A. McDonnell**, E. Schenk, M. Harlow, F. Fernandez-Lima

CHED **304.** Study towards the selective digestion of glyphosate in surface water. **A.F. Bauer**, **A.K. Perry**, A.R. Roerdink

CHED **305.** Method development towards quantifying marijuana consumption using sewage based drug epidemiology: Preliminary results for Treatment Plant #2. **M.C. Pellman**, H. Fryhle, D.A. Burgard

CHED **306.** *C*-arylation methods to a library of covalent modifiers. **A. Diepenbrock**, A. Cassity, N. Asad, P.R. Hanson

CHED **307.** Variance of caffeine in different brews of coffee. **T.L. Self**, K. Cossey

CHED **308.** Method development towards quantifying marijuana consumption using sewage based drug epidemiology: Preliminary results for Treatment Plant #1. **H. Fryhle**, M.C. Pellman, D.A. Burgard

CHED **309.** Study of the impact of ionization conditions on ion formation in electrospray mass spectrometry. **T.J. Hulyk**, S. Norris, K.H. Bennett

CHED **310.** Optimization of the voltammetric analysis of heavy metals. **J. Stapleton**, A.F. Bange

CHED **311.** Synthesis of variable size nanoprisms for application in signal enhancement using Raman spectroscopy. **T.M. Keller**, M.V. Schiza

CHED **312.** Optical evaluation of fluorescent nanoparticles embedded into silica aerogel hosts. **T. Lightner**, J.N. Richardson

CHED **313.** Direct and indirect detection of FMN and FAD released upon target binding. **C.A. Dunlock**, A.G. Gee, S. Sitaula, M.F. Ali

CHED **314.** Preparation of FAD conjugates to signal target binding events. **J. Grennell**, S. Sitaula, A.G. Gee, M.F. Ali

CHED **315.** Synthesis and photophysical and photochemical characterization of osmium complexes for luminescence-based sensing. **A. Wagner**, K. Kneas, J.A. Rood

CHED **316.** Effects of cinnamon components on glycogenesis by anion exchange-high performance liquid chromatography coupled to conductimetric detection. **M. Jones**, K.E. Garrison

CHED **317.** Qualitative and quantitative analysis of fluorine containing synthetic cannabinoids. **J. Davidson**, D.P. Predecki, J.N. Richardson

CHED **318.** Study of an alternative method for quantitative Ni(III) determination. **O.N. Blackmore**, K. Belt, R.V. Whiteley

CHED **319.** Analysis of pharmaceuticals in water samples by gas chromatography-mass spectrometry (GC-MS). **K. Altemose**, Y. Mei-Ratliff

CHED **320.** Comparison of solid phase extraction and solid phase microextraction for the quantitative analysis of *trans*-resveratrol in red wine samples by HPLC. **J.J. Wukovits**, **Z.M. Colson**, J.A. Boiani

CHED **321.** Automated reaction monitoring using liquid chromatography-mass spectrometry. **D.J. Alton**, M.M. Smalley, S.A. Kurtovic, K.C. Lapworth, K.R. Evans

CHED **322.** GC-MS characterization of cell culture media: Optimizing sample preparation using automation and design of experiments (DOE). **L.M. Housel**, C.M. Ingersoll

CHED **323.** Evaluating graphene oxide electrochemically reduced on Pt-black as a support for H_2S detection. **R. Custer**, J.A. Bennett

CHED **324.** Method of collection and detection for airbourne organo-arsenic compounds. **K.M. Clark**, B.M. Hopkins

CHED **325.** Selection of protein-binding DNA aptamers for bacterial detection. **J.M. Clements**, A.M. Bluhm, M. Blatz, J. Nava, S. Evans, A.G. Cavinato

CHED **326.** Development of a DNA biosensor for rapid detection of *Renibacterium salmoninarum*. **T.N. Keohokalole-Look**, **B.L. Mandella**, A.M. Olivo, A.G. Cavinato

CHED **327.** Analysis and quantification of D-aspartic acid in marine bivalve mollusks. **R. Gutierrez**, A. Delascagigas, T. Comnick, E. Rodriguez, G. Fisher

CHED **328.** Triarylmethane and xanthene dye synthesis and characterization of their photophysical properties. **S.E. White**, A.B. Ormond

CHED **329.** Analysis of analgesics in the Quittapahilla Creek watershed. **K. McCardle**, O.A. Moe

CHED **330.** Cross-linker effect on metal ion detection using molecularly imprinted polymers. **D. Baumann**, V. Mai, C. Zanelotti, S.E. Stitzel

CHED **331.** Analysis of trace metals in tattoo inks using Agilent ICP MP-AES. **S. Al-Khalifa**, H.S. Butman, M. Wieler, C.H. Jaworek-Lopes

CHED **332.** Paper-based device for colorimetric detection of malondialdehyde in biological samples. **T.D. Steichen**, A. Fazal

CHED **333.** Optimization of solid phase extraction of petroleum residues implementing green chemistry principles. **R.B. Kamerman**, P.P. Vaughan, A.M. McKenna

CHED **334.** Using solvent parameters for increased precision in chemical shifts. **E.E. Schiller**, W. Carroll

CHED **335.** Lab curriculum development involving the synthesis and characterization of molecularly imprinted polymers in the detection of aspirin. **J.P. Cohen**, D.G. Sykes

CHED **336.** Quantitative analysis of alcohol using nuclear magnetic resonance. **R. Hill**, C. Nicholson

CHED **337.** Conformational kinetics study of microperoxidase-11 using TIMS-MS and molecular dynamics. **C. Harrilal**, F. Fernandez-Lima

CHED **338.** Surface modification of photopolymerized sol-gel monoliths using thiol-ene click chemistry. **T. Sabol**, Z. Rodriguez, G. Soto, D. Britsch, D.M. Gharbharan, F. Svec, Z. Zajickova

CHED **339.** Solid phase extraction (SPE) of urine in postmortem toxicology testing. **V. Davidson**, D. Baker, R. DeRienz

CHED **340.** Obtaining electricity from solar energy utilizing household products. **R. Senter**, E.D. Stemp, A. Calderon, D. Romero

CHED **341.** Stabilities of mephedrone in biological and non-biological matrices. **H.L. Ciallella**, **S.L. Oddi**, K.S. Scott

CHED **342.** Development of paper analytical devices for the detection of substandard azithromycin and erythromycin. **E.P. Aldrich**, T.L. Barstis

CHED **343.** Raman probes as a rapid identification and detection tool for *E.coli* in fresh parsley. **A. Sotomayor-Albino**, A.N. Soler, C.R. Ruiz-Martinez, M.A. De Jesus

CHED **344.** Withdrawn.

CHED **345.** Studying the binding interactions of the chemokines CXCL12 and CXCL14 to heparin and heparan sulfate using affinity capillary electrophoresis. **A. Schrader**, A.K. Korir

CHED **346.** Best spinach that Popeye ever ate. **K. Weishaar**, J. Potratz

CHED **347.** Cyclic voltammetry of *tris*-dithiocarbamates in room temperature ionic liquids. **J. Becca**, A. Eisenhart, J. Coffield

CHED **348.** Development of analytical methods for detection of pharmaceutical pollution of surface water in Georgia using purge-n-trap GC/MS. **K. Hachat**, N. Potter, C.H. Lisse

CHED **349.** Withdrawn.

CHED **350.** Investigation of toxic metals in over-the-counter eye shadow makeup. **J. Mendez**, R. Huschka

CHED **351.** Assessing the reproducibility and applicability of a miniature gas chromatograph. **M. Akinlaja**, R.J. Noll

CHED **352.** Synthesis of 1-butyl-3-methylimidizolium hexafluorophosphate: Investigation of its use as an electrochemical solvent for electroanalytical studies of metal dithiocarbamate complexes. **A. Eisenhart**, J. Coffield

CHED **353.** Influence of the *cis/trans* ratio of hop iso-alpha-acids on beer bitterness. **M. Baginski**, B. Fleshman, D.L. Donohoue

CHED **354.** Separation of cations for waste reduction. **C. Cookenmaster**, M. Claus

CHED **355.** Identification of volatile organic compounds present in cigarette smoke via purge-n-trap coupled with GC/MS. **P. Skersick**, E. Smith, C.H. Lisse

Section A

Colorado Convention Center

Halls C/D

Undergraduate Research Posters

Biochemistry

Cosponsored by BIOL and SOCED

N. Di Fabio, *Organizer*

12:00 - 2:00

CHED **356.** In vivo expression of antimicrobial peptides in *Escherichia coli*. **S.A. White**, N.S. Muthunayake, **C.S. Chow**

CHED **357.** Role of copper in the oxidative stress response of *Chlamydomonas reinhardtii* to heat shock. **M. Brann**, O. Marcu

CHED **358.** Effect of antidiabetic agents on the *in vitro* glycation of bovine serum albumin. **A.T. Shuck**, **E.C. Daniels**, **R.L. Hein**, **A.M. Overgard**, **M.E. Lee**

CHED **359.** Ion-pair reverse-phase liquid chromatography analysis for separating and quantifying RNA generated via in vitro transcription reactions. **M. Bestwick**, **H. Wienkers**

CHED **360.** Inhibition of the bacterial fatty acid biosynthetic enzyme FabI by secondary metabolites isolated from *Artemisia californica*. **P.M. Joyner**, **S. Bryant**

CHED **361.** Increased growth and mutagenesis in bacteria exposed to titanium dioxide nanoparticles. **V.F. Smith**, **V. Mukherjee**

CHED **362.** Investigation of the effects of titanium dioxide nanoparticles on phospholipid bilayers using differential scanning calorimetry. **R. Gall**, **V.F. Smith**

CHED **363.** Adsorption of snake venom by activated charcoal. **S. Sivakumar**, **R.A. Kopper**

CHED **364.** Variation of protein components in successive regenerations of individual coralsnake venom. **P. Spradley**, **R.A. Kopper**

CHED **365.** Metal ion cofactor requirements of phosphomonoesterase. **V. Ventrano**, **R.A. Kopper**

CHED **366.** Inhibition of lecithin-cholesterol acyltransferase by reactive aldehydes in electronic cigarettes. **P. Hanna**, R.**E. Rigsby**

CHED **367.** Phylogenetic analysis of the upstream region of the arcanolysin gene from smooth and rough biotypes of *Arcanobacterium haemolyticum*. **D.L. Ross**, H.S. Ruther, **D. McGee**

CHED **368.** Identification and characterization of a membrane-associated esterase from *Proprionibacterium acnes*. **R. Chapin**, **B. Harville**

CHED **369.** Characterization of a *Tannerella forsythia* collagenase by SDS-PAGE and fluorescent spectroscopy. **B.J. Sanders**, **B. Harville**

CHED **370.** Porphyrin derivatives and photodynamic therapy effects on triple negative breast cancer. **S. Rogers**, **J.E. Bradshaw**, **T.E. Hayes**

CHED **371.** Expression of recombinant intimin and translocated intimin receptor proteins in *E.coli* cells. **K. Page**, **C. Sobraske**, **L. OBrien**

CHED **372.** Influence of the second-sphere coordination on the nitrite reductase activity of globins. **A. Rodland**, J. Gowen, **M.I. Galinato**

CHED **373.** Optimization of fragment inhibitors for the class D β-lactamase OXA-24. **R.C. Hoogmoed**, **R.A. Powers**

CHED **374.** Fox-4 cephamycinase: Analysis of structure and function. **B. Biju**, M. Noel, **E.C. Mundorff**, R. Toro, V. Malashkevich, S. Almo, J. Aguilan, E. Nieves, K. Papp-Wallace, F. Prati, E. Caselli, J. Frere, G. Bou, R. Bonomo, S.T. Lefurgy

CHED **375.** Denaturation resistance of polygalacturonase obtained from coffee mucilage. **J.M. Henning**, G.R. Oppenlander, A.F. Rilett, M.L. Zuteck, E.A. Gay, **M. Caspers**

CHED **376.** Hydrogen deuterium exchage used to study the interface of *Plasmodium falciparum* glutathione reductase and the antimalarial drug methylene blue. **S. Lim**, **H. Prieto**

CHED **377.** Role of cytochrome c and its effects on the programmed cell death pathway of *P. falciparum* using yeast as a model organism. **E. Orozco**, **H. Prieto**

CHED **378.** Expression and purification of DPAP-1, a malaria protease, and its role in the putative apoptosis pathway of the parasite. **A. Bains**, **H. Prieto**

CHED **379.** Yeast cell survival in different concentrations of canavanine. **P. Angkanaworakul**, J. Iverson, **T.T. Saxowsky**

CHED **380.** Characterization of the non-native 1,2-naphthoquinone in vivo incorporation into the A_1 site in PS I complexes of *Synechocystis* sp PCC 6803. **E. Gosselin**, **T.W. Johnson**

CHED **381.** Characterization of highly reducing anthraquinones in the A_1 site of PS I complexes of Synechocystis sp. PCC 6803. **P. Kerns**, **T.W. Johnson**

CHED **382.** Effects of sphingosine 1-phosphate at the blood brain barrier. **A.C. Love**, S. Spampinato, **A. Cotleur**, **R. Ransohoff**

CHED **383.** Characterization of a putative haloalkane dehalogenase from *Saccharomonosporea azurea*. **E. Zhou**, **E.C. Mundorff**

CHED **384.** Expression and purification of farnesyl diphosphate synthase from *Thermoplasma volcanium*. **C. Banos**, B. Horrigan, **J. Himmelberger**

CHED **385.** Mutagenesis of a TfdA-like B. pertussis enzyme. **N. Pierce**

CHED **386.** Quantifying *Escherichia coli* in recreational freshwater of the Saginaw Bay Watershed using Colilert and quantitative PCR. **A. Lukowski**, **T. Sivy**

CHED **387.** Development of an LC-MS/MS-based assay for the quantification of trehalose. **P.M. Kretschmer**, A.J. Rouff, M.K. O'Brien, L.A. MacManus-Spencer, **M.G. Paulick**

CHED **388.** Quantitative analysis of hydrocortisone levels in human saliva due to the effects of positive and negative stressors. **S. Riley**, **H.S. Greenberg**, M.B. Hargrove, **R.L. McCann**

CHED **389.** Determination of the signaling pathway leading to tight junction disassembly in diabetic retinopathy. **S. Prettner**, **R.L. McCann**

CHED **390.** Modified ELISA to determine levels of TTX and its links to the life history of the eastern newt, *Notophthlmus viridescens*. **H. Winter**, P. Delis, **R.L. McCann**

CHED **391.** Toxicity of imidazolium room temperature ionic liquids towards biofilms. **L. Sanders**, **E.G. Ennis**

CHED **392.** Toward inhibitors of cystathionine β-synthase (CBS): Examination of both the transsulfuration and hydrogen sulfide evolution reactions. **L.M. Szczesniak**, M.L. Beio, C.D. McCune, W. Shen, **D.B. Berkowitz**

CHED **393.** Conformational variability of MTHFR characterized by hydrogen-deuterium exchange and mass spectrometry. **S.S. Webster**, A. Stahly, E.E. Trimmer, **E.M. Marzluff**

CHED **394.** Spectroscopic properties of the GFP chromophore containing substituted phenylalanine derivatives in place of tyrosine. **J.D. Stevens**, J. Tharp, A. Tuley, **W. Liu**

CHED **395.** Investigation of IPTG and its products of oxidation in the induction of protein biosynthesis. **M.M. Schmauch**, M.Y. Kasmani, **J.M. Chalker**

CHED **396.** Lipid dynamics of cardiolipin/DMPC and cardiolipin/DOPC in nanodiscs. **K. Stipe**, H. Steele

CHED **397.** Biochemistry in the cosmetic industry: The effectiveness of synthetic and natural preservatives. **A.M. Wilburn**, J.T. Peace

CHED **398.** Binding kinetics and transition of structural components of RNA polymerase. **M. Mecha**, M. Poulos, R. Sreenivasan, T. Record

CHED **399.** Amyloid-perturbing dyes inhibit adhesion of *Cryptosporidium parvum* to the human ileocecal adenocarcinoma HCT-8 cell line. **D.R. Lee**, C.X. Chan

CHED **400.** Relationship between redox potential and light production in the mucus of the marine tubeworm *Chaetopterus sp*. **F.X. Migliolo**, D. Deheyn

CHED **401.** Identification of acid/base residues important to the mechanism of ThiI. **T. Brondhaver**, E.G. Mueller

CHED **402.** General method for analysis of RNA structures by deoxyribozyme sensors. **R. Karadeema**, D. Kolpashchikov

CHED **403.** Designing peptide-coated gold nanoparticles for the bottom-up assembly of amyloid nanocompartments. A. Sementilli, **J. Smith-Carpenter**, D.G. Lynn

CHED **404.** Chemical characterization of novel bacterial LOV-domain photoreceptors. **K. El-Arab**, B.D. Zoltowski

CHED **405.** Initial steps toward antimicrobial photodynamic textiles. **S.L. Stanley**, R. Ghiladi

CHED **406.** Species differences in detoxification rates. **L. James**, L. Browning, C. Dadabay, J. Forbey

CHED **407.** Effects of dia2 degradation on checkpoint recovery in *Saccharomyces cerevisiae*. **C.C. Torres Cabán**, D. Koepp

CHED **408.** Computational and experimental approaches to investigate substrate binding of the enzyme OGA. **K.A. Brown**, K. Cotto, R. OKeefe, G. Crawford

CHED **409.** Characterization of xanthine dehydrogenase regulator protein of *Ralstonia solanacearum*, a tomato infecting bacterium. **D.T. Johnson**, S. Sivapragasam, A. Grove

CHED **410.** Dissociation constant (p*Ka*), pH and related thermodynamic functions of TRIS buffer from 5 to 55°C. **T.R. Wehmeyer**, R.N. Roy, L. Roy, L.S. Tebbe

CHED **411.** Application of the Pitzer Formalism for the aqueous solution of HCl + KCl, HCl + NiC_{a2}, HCl + $PrCl_3$, and HCl + $ThCl_4$ at 25 °C. K. Hundley, **L. Roy**, R.N. Roy

CHED **412.** Carbon nanotube separation beyond size-selective protein hydrogels. J. Rowland, **K.C. Tvrdy**

CHED **413.** Combining metabolic inhibitors to preferentially target cancers with deregulated p27. **K.B. Chancellor**, A. Alarbi, N. Santa-Pinter, J. Sabo, R. Sheaff

CHED **414.** Analogs of cisplatin: 4,4'-disubstituted-2,2'-bipyridine complexes of Pt(II) dichloride. **L. Cobani**, B.L. Bennett

CHED **415.** Identifying biocompatible redox mediators for electrochemical imaging of *Dictyostelium discoideum*. **C. Chira**, A. Maselli, R.J. Lesuer

CHED **416.** Detection and Identification of biochemical molecules secreted by *Entamoeba* varieties for taxa discrimination based on aggregative behavior. **S. McDonough**, J.A. Leitao, A. Espinosa

Technical program information known at press time. The official technical program for the 249th ACS National Meeting is available at: www.acs.org/denver2015

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CHED **417.** Effect of retinoid receptor agonists on K562 cellular adhesion, proliferation, and α5β1 integrin cell surface expression. **R. Phomakay**, M.D. Kelley

CHED **418.** Thiophene N-substituted tetrahydro pyridinium salts as functionally selective muscarinic partial agonists. J.F. Boulos, **P.N. Nwokoye**

CHED **419.** Lactate dehydrogenase: A study of kinetics and inhibition. **C. Chandler**, N. Beres

CHED **420.** Effect of catalase overexpression on ethanol-induced hepatic mitochondrial DNA damage in mice. **S. Watkins**, A.A. Caro

CHED **421.** Effect of oral chronic ethanol administration on hepatic mitochondrial biogenesis in mice. **T. Spradley**, A.A. Caro

CHED **422.** Effect of ethanol and catalase overexpression on hepatic mitochondrial DNA content in mice. **S. Fobare**, A.A. Caro

CHED **423.** Effect of catalase overexpression on ethanol-induced oxidative stress in mice. **C. Dunn**, A.A. Caro

CHED **424.** N-acetylcysteine inhibits the upregulation of mitochondrial biogenesis genes in livers from rats fed ethanol chronically. **M. Bell**, A.A. Caro

CHED **425.** Effect of chronic ethanol administration on hepatic genomic (nuclear and mitochondrial) DNA integrity in mice. **A. Stuppy**, A.A. Caro

CHED **426.** Effect of polycystin-2 disruption on osmotic response of renal epithelial cells. **R. Comer**, B.J. Siroky, B.P. Dixon

CHED **427.** Effect of transglutaminase on the deregulation of the p27 protein. **R. Patel**, L. Zhang, A. Greene, W. Crawford, R. Sheaff

CHED **428.** Analysis of p53 protein in hepatocellular carcinomas using 2D and 3D culture models. **J.M. Pomo**, R. Taylor, J. Wu, R.R. Gullapalli

CHED **429.** Turning off the lights: A novel luciferase inhibitor. **D. Stranford**, J.C. Dicesare, R. Sheaff

CHED **430.** Isolation of bioactive compounds from novel actinomyces strains. **W. Johnston**, M. Fakhr, S. Marasini, R. Sheaff

CHED **431.** Molecular docking studies of novel flavonoid derivatives as dual binding site acetylcholinesterase inhibitors. **L. Gainey**, B. Lor, O.M. Newman, C. Mills

CHED **432.** Standard buffer POPSO for use in the physiological pH range. **K. Hundley**, R.N. Roy, L. Roy

CHED **433.** Mechanistic and kinetic studies of a new ROS-activated compound. **E.D. Pullen**, E. Merino

CHED **434.** Dietary sodium suppresses digestive efficiency: Role of the renin-angiotensin system. **F. Morales-Santiago**, J.L. Grobe

CHED **435.** Pattern analysis of abnormal blood producing low velocity spatter. **C.A. Weiss**, G.P. Foy

CHED **436.** Alteration of the specificity of putrescine oxidase by mutations to the active site. **L. Woodcock**, K. Colvert

CHED **437.** Identification of sulfopeptides as HIV entry inhibitors through phage display. **G.M. Roman**, T. Ju, J. Guo, W. Niu

CHED **438.** Screening peptidomimetic ligands against patient-specific chronic lymphocytic leukemia monoclonal antibodies. A.L. Hackler, **S. Simanski**, M. Sarkar, T.J. Kodadek

CHED **439.** Oxidation of cytochrome C by guanine radicals. M. Safaeipour, M. Bekarian, **M. Sanchez**, J. Juaregui, S. Castillo

CHED **440.** Effect of glutathione on DNA-protein crosslinking caused by guanine oxidation. **M. Safaeipour**, **M. Bekarian**, **M. Sanchez**, **S. Castillo**, **J. Juaregui**, E.D. Stemp

CHED **441.** Expression and purification of homocysteine methyltransferase *Sam4* recombinant in *Escherichia coli*. **L.J. Negron**, W. Qu, Z.S. Zhou

CHED **442.** Analysis of the antibody binding of MUC1 peptides and substituted peptides by STD NMR. **A.R. Lynch**, T. Yang

CHED **443.** Investigation of the aqueous chemistry in the elimination of glutathione from the glutathione-3-methyleneoxindole conjugate: A potential therapeutic agent. **K. Bukis**, E.J. Brush

CHED **444.** Thermostabilization of water soluble variants of the human β_2 adrenergic receptor. **P. Kurtzweil**, A. Kikonyogo, A.L. Parrill-Baker

CHED **445.** Evaluation of off-target effects through double-stranded RNA interference in *C.elegans*. **S.M. Litz**, T.A. Sugrue, T. Dwyer

CHED **446.** Designing an undergraduate lab procedure for the synthesis of [R,S]-Boc-Phenylglycyltryptophan methyl ester. **T.J. Smith**, D.A. Wing

CHED **447.** Arabidopsis MMD-like genes and their roles in chromosome biology during male reproduction. **M.M. Shroder**, C.A. Makaroff

CHED **448.** Molecular recognition of diatomic gases in *Rhodopseudomonas Palustris* Cytochrome *c'*. **J.P. Bard**, **S.S. Safaie**, **Z. Nilsson**, C.R. Andrew

CHED **449.** Natural antisense RNA plays a role in *Arabidopsis thaliana* growth and development. **A.A. Simoni**, C.A. Makaroff

CHED **450.** Reaction of strained alkynes with cysteine proteases. **M.M. Tierney**, G.H. Jones, J.M. Chalker

CHED **451.** Platinum(II) complexes with sulfur-containing peptide building blocks for use in RNA binding studies. **N. Hardin**, C.S. Chow

CHED **452.** Role of H57 in synchronizing ammonia transfer within E. coli CTP synthetase. **M.R. Abbott**, J.L. Johnson

CHED **453.** Kinetics of the reaction of 6-aminohexanoic acid with chlorine(I): Evidence for a role for dichlorine monoxide. **Z.A. Cockrell**, G.H. Purser

CHED **454.** Isolation of corticosterone and its effect on personality in convict cichlids (*Amatitlania nigrofasciata*). **C. Marshall**, **N. Ali**, R. Fox

CHED **455.** Effect of brewed coffee from various sources on the formation of amyloid-beta fibrils in vitro. **R.J. Tokarski**, M.A. Fisher

CHED **456.** Identification of bovine pregnancy markers in urine samples. **R. Lalmansingh**, A. Rafalowski, N.M. Wachter, M. DeCastro

CHED **457.** Interaction of anthrax toxin protective antigen protein with model cell membranes at the air-water interface. **J. Jarosz**, N. Meyer, A. Serfis, J. Bann, S. Mamillapalli

CHED **458.** In silico studies of MMP-1. D. Pusztai, **E. Healy**

CHED **459.** Investigation of the apoptotic biochemical mechanism of ajulemic acid in Ewing's sarcoma cell lines. **J. Ubeda**, L. Hensley, M.D. Perry

CHED **460.** Enhancing the bioavailability of RAGE inhibitors: Toward new anti-Alzheimer's therapeutics. **T. Dwyer**, **M. Randolph**, **M. Ross**, B.L. Miller

CHED **461.** Effects of apolipoprotein E on M2 microglia. **B. Bieger**, H. Ferguson, S. Rose, R. Frye, S. Barger

CHED **462.** Use of enhanced chemically defined media to improve uptake of L-telluromethionine by *Escherichia coli* DL41(DE3). **V. Sublett**, B. Cooper, J.O. Boles

CHED **463.** Role of apoptosis in modulating effects of 2-aminoanthracene in pancreatic tissue of Sprague Dawley rat dams. **J.W. Jay**, E. Venable, E.W. Howerth, W.E. Gato

CHED **464.** Hepatic gene expression in pups exposed to 2-aminoanthracene in utero indicative of susceptibility to metabolic syndrome. **G.W. Barnett**, W. Yau, E.W. Howerth, W.E. Gato

CHED **465.** Aliphatic protein side chain density correlates with phosphate crowding and helical curvature in protein/DNA crystal structures. L.A. Isom, **N. Hunter**, B. Grant

CHED **466.** Protein purification and expression for glycitein complex with rat estrogen receptor beta. **A. Heldt**, G.T. Marks

CHED **467.** 4T1 Murine breast cancer cell cytotoxins in *Rumex crispus* (Yellow Dock). **A.M. Rivera**, S.C. Kelly, J.R. Kenneson, R.T. McCutcheon, T.E. McElwain, D.W. Capps, A.J. Reinhart, G.O. Gray

CHED **468.** Investigation of a HAD phosphatase from *Mycobacterium tuberculosis*. **C. Barnier**, A. Roberts

CHED **469.** Establishing RNAi in *Tribolium castaneum* at MSU Denver. **C.M. Lowrance**, E. Ragan

CHED **470.** Measuring the stability of iso-1-cytochrome *c* variants using heme spectra. **S. Eikenberry**, A. Wold, M. Cherney

CHED **471.** Effect of 2,3,7,8-tetrachlorodibenzo-*p*-dioxin (TCDD) on estrogen receptor beta and aryl hydrocarbon receptor using RT-qPCR. **M. Kinney**, G.T. Marks

CHED **472.** Investigating the mechanism of furfural inhibition in *E. coli*. **K.D. Hannie**, **S.D. Johnson**, M. Holle, A. Sostarecz, L. Moore

CHED **473.** Bacterial screening in search of novel pharmaceuticals. **A. Jorski**, O. Oyewole, K. Lacey, M. Fakhr, R. Sheaff

CHED **474.** Fluorination of DNA aptamers through "Click Chemistry" synthesis. **J. Dotson**, J.C. Easdon

CHED **475.** Evaluating the expression levels of putative biomarkers in a panel of pancreatic cancer cell lines by qPCR. **A. Smith**, N. Goonesekere, K. Dhanwada

CHED **476.** Probing the identity of the distal heme ligand in Cys80 variants of iso-1-cytochrome *c*. **A. Wold**, S. Eikenberry, M. Cherney

CHED **477.** Investigation of macromolecular crowding on ferredoxin and ferredoxin-NADP$^+$ reductase kinetics. **D. Bautista**, S. Owen, D.W. Seybert

CHED **478.** RNA phosphoramidite monomer synthesis: An examination of phosphite selectivity improvement. **E.E. Yancey**, **K.F. Harvey**, **S.D. Holt**, V.K. Dunlap

CHED **479.** Detection of catecholamines using a paper-based microfluidic device. **C. Smith**, M.A. Fisher

CHED **480.** Analysis for genetic polymorphism of eastern Pacific bluefin and yellowfin tuna with microsatellite sequence PCR primers developed for Atlantic and western Pacific bluefin and western Pacific yellowfin tuna. **S. Wagner**, M.E. Pugh

CHED **481.** Purification and expression of modified calmodulin protein (N-Cam.Y). D. Weiss, **C. Chant**, C. Ricciardi, M. Smith, D.E. Bourne

CHED **482.** Purification and characterization of *Bdellovibrio* derived α-glucosidase, malA. **A. Simpson**, J.E. Hanson, M. Martin, J. Grinstead, P. Smith, C. Isabella

CHED **483.** Effects of floodplain silt on plant cell biochemistry. **A.N. Anderson**, D.M. Anderson, A. Marry

CHED **484.** Potential effects of betulinic acid on the formation of the calmodulin/CaMKKII complex. **R. Woloshun**, M.A. Fisher

CHED **485.** 2,3,7,8-Tetrachlorodibenzo-p-dioxin (TCDD) induces cell death in human granulosa cells. **C.J. Venes**, G.T. Marks

CHED **486.** Identification of genes involved in RQ_9 biosynthesis in *C. elegans* using RNAi knockdowns. **H. Xun**, J. Shepherd

CHED **487.** Investigation of *Nocardioides sp.* metabolic, structural, biochemical properties, and its potential role in the sulfur cycle. **K. Lachmayr**, E. Oduaran

CHED **488.** Investigation of the interference of extracted cinnamon components on the glucose oxidase-peroxidase test. **A. Diepenbrock**, C. Breaux

CHED **489.** Screening an enaminone library for histone deacetylase inhibitors. **B. DeMier**, N. Koduri, S.R. Hussaini, R. Sheaff

CHED **490.** Improved model to predict the free energy contribution of dinucleotide bulges to RNA duplex stability. **J.C. Tomcho**, M. Tillman, B. Znosko

CHED **491.** Challenges in visualizing RecA-DNA interaction in chemiluminescent electrophoretic mobility shift assays. **J.R. Kenneson**, R.L. Moore

CHED **492.** Analysis of rhodoquinone production in knockout strain candidates in *Rhodospirillum rubrum*. **B. Titus**, J. Shepherd

CHED **493.** Rhodium(II) metallopeptides as a structural platform for selective Abl tyrosine kinase inhibition. **M.J. Wheadon**, S. Knudsen, J. Ohata, F. Vohidov, Z.T. Ball

CHED **494.** Investigation of the change in expression of neuropeptides with gluten free based diets. **C.R. Fencil**, B.A. Davis

CHED **495.** Role of aspartic acid 101 in *E. coli* alkaline phosphatase architectural activity and stability. S. Chamberlin, **A. Moauro**, J.K. Brown, K. Wallerius

CHED **496.** Increasing the activity of E. coli alkaline phosphatase through a structurally destabilizing mutation. **S. Chamberlin**, **O. Kilbarger**, B.J. Anderson, D.A. Than

CHED **497.** Why taking your vitamins is essential: The importance of architecture in metabolite sensing by the B_{12} riboswitch. **S. Chamberlin**, **L.D. Kramer**, C. Hofmeister, D. Cutshall, O. Kilbarger, H. Kim, H. Benasutti

CHED **498.** Peptides designed to target G-quadruplexes for transcriptional and translational regulation. **S.K. Patel**, A.L. Stewart

CHED **499.** Biobased composites produced from collagen and vegetable oil polymers. **R.L. Lewis**, A.L. Stewart

CHED **500.** Peptides designed as mimics of NF-κB for transcriptional regulation. **J. Page**, A.L. Stewart

CHED **501.** Analyzing exonuclease-induced hyperchromicity by UV spectroscopy: An undergraduate biochemistry laboratory. **C. Ricciardi**, D. Weiss, C. Chant

CHED **502.** Characterizing the aggregates of a mutant Alpha 1-Antitrypsin protein associated with Alpha 1-Antitrypsin Deficiency. **M. White**, M.A. Fisher, O. Long

CHED **503.** Analysis of lipid membrane content in dynamic environments. **A. Chamberland**, S.E. Maurer

CHED **504.** Investigation of bi-substrate enzyme kinetics for the introductory biochemistry lab. **K. Scinto**, K. White, B.J. Alper

CHED **505.** Determining the function of Coq4 in *S. cerevisiae* coenzyme Q_6 biosynthesis via biochemical and genetic screening of Coq4 suppressors. **C.R. Colgan**, **N.R. Olivieri**, T.P. Nguyen

CHED **506.** Effects of deletion of the Rru_A3004 gene on rhodoquinone biosynthesis in *Rhodospirillum rubrum*. **M.R. Kuenzi**, J. Shepherd

CHED **507.** Characterization of a human orphan G-protein coupled receptor, GP133. **T.C. Miller**, T. Frielle

CHED **508.** Prefractionation of natural product extracts provides a value added resource for high-throughput anticancer screening applications. **B. Beall**, **A. Musick**, K. Gustafson

CHED **509.** Engineering of metalloenzymes with stacked metalloporphyrin dimers. **M. Getachew Zewde**, J. Kleingardner

CHED **510.** Pedagogical innovation: Using 3D printer technology in an undergraduate biochemistry course. **K. Janousek**, C. Mills

CHED **511.** Characterizing HIV-specific CD4 T cell targeting and proliferation among HIV controllers. **D. Walter**, **B. Walker**, **S. Ranasinghe**

CHED **512.** Characterization of the haloalkane dehalogenase, DccA. **L.E. Carlucci**, **E.C. Mundorff**

CHED **513.** Determination of aggregation equilibrium of fatty acid vesicles using gas chromatography with flame ionization detection. **L. Aakjar**, **S.E. Maurer**

CHED **514.** Designing small molecule autoinducers for investigation into the binding pocket of *LasR*. **D.J. Kenney**, **E.S. Garcia Sega**

CHED **515.** Acute and chronic effects of somatostatin on fast and slow calcium oscillations in the pancreatic β-cell. **K. Harms**, B. Thompson, E. Glynn, **L. Satin**

CHED **516.** Effects of creatine supplementation on serum testosterone response in *Mus musculus*. **C. Gill**, **D. Martin**

CHED **517.** Construction of a *Burkholderia cenocepacia*-specific gene replacement vector. **T.A. Demers**, **K.M. Specht**

CHED **518.** Electron transfer reactions of cytochrome c oxidase: Isolation, characterization, and ligand binding studies. **S. Rodriguez**, K.J. Farrell, **S. Mahapatro**

CHED **519.** Detection of melatonin and cortisol in hair. **M.R. Ferguson**, A. Alarbi, **W. Potter**

CHED **520.** Purification of components from *Inula hilinium* (elecampane) which are cytotoxic to the 4T1 murine breast cancer cell line. **S.C. Kelly**, T.E. McElwain, A.M. Rivera, J.R. Kenneson, R.T. McCutcheon, **G.O. Gray**, **A.J. Reinhart**

CHED **521.** Discovery of a potential Middle East respiratory syndrome (MERS) PLpro inhibitor for the development of anti-MERS-CoV drugs. **S. Loperena-Medina**, Y.M. Baez-Santos, **A.D. Mesecar**

CHED **522.** Inhibition of Y-family DNA polymerases. **E. Zlibut**, N.M. Antczak, **P. Beuning**

CHED **523.** Purification and characterization of wild type nickel uptake regulator (NUR) from *Streptomyces coelicolor*. **D.J. Peppers**, **N.E. Grossoehme**

CHED **524.** Inhibition of formation of blood clots by tetrapeptide inhibitors acet-LSPR-amide and acet-ISPR-amide. **A. Lacerte**, **T.A. Trumbo Bell**

CHED **525.** Probing the substrate specificity of lysine deacetylases using mutagenesis. **K.A. Nichols**, T.B. Toro, D.S. Garrett, **T.J. Watt**

CHED **526.** Two systems for modulating back electron transfer between guanine radicals and 2-aminopurine in duplex DNA. **P. Garcia**, **D. Galindo**, **S. Cruz**

CHED **527.** Conformational analysis of cyclic disulfides and selenenyl sulfides in peptide redox motifs. **D.B. Pollard**, S. Rozovsky, **C.A. Bayse**

CHED **528.** DNA binding and selectivity of dapsone derivatives. **C. Blake**, C.E. Stephens, **K.L. Buchmueller**

CHED **529.** Using acute promyelocytic leukemic cells to test for receptor binding of ajulemic acid. **B. Monk**, A. Eubanks, **L. Hensley**

CHED **530.** Observing the folding behavior of bi1 group II intron. **K.L. Weber**, **J. Potratz**

CHED **531.** Development of small molecules as potential RNA-binding molecules. **J. Lewis**, **E.G. Sega**

CHED **532.** Characterization of the disulfide crosslinking in lysyl oxidase. **M. Ali**, **K.M. Lopez**

CHED **533.** Use of solubility tags to characterize lysyl oxidase. **A. Hussain**, **K.M. Lopez**

CHED **534.** Cooperativity of TU100 and ascorbic acid in the production of reactive oxygen species. **P.C. Borden**, J. Whelan, **R. Sheaff**

CHED **535.** Supramolecular guanine-rich quadruplexes and their transfection into mammalian cells. **E. Eklund**, T.C. Marsh

CHED **536.** Detecting DNA-protein crosslinking in DNA with 2-aminopurine via fluorescence polarization. **H. Brueck**, **S. Cruz**, M. Marquez

Technical program information known at press time. The official technical program for the 249th ACS National Meeting is available at: www.acs.org/denver2015

CHED **537.** Function of laforin in glycogen metabolism and lafora disease. M.U. Raththagala, K. Brewer, **K.D. Auger**, **B.D. Turner**, C. Vander Kooi, M.S. Gentry

CHED **538.** Analysis of antibacterial components of honey. **L. White**, J. Pruneski

Section A

Colorado Convention Center
Halls C/D

Undergraduate Research Posters

Biotechnology

Cosponsored by BIOT and SOCED

N. Di Fabio, *Organizer*

12:00 - 2:00

CHED **539.** Encapsulation of superparamagnetic nanoparticles in mPEG-PLGA micelles for targeted drug delivery. **H.M. Legaspi**, M. Flores, Y. Ba

CHED **540.** Exploring simple pattern transfer using microcontact printing. **Y. Freeman**, D. Shenault, V. Goss

CHED **541.** Identification of previously unsequenced viruses from wild-caught mosquitoes by metagenomic sequencing. **T.M. Biser**, K.G. Frey, C.L. Redden, J.J. Anderson, J.C. Andersen, K.L. Schully, R.Z. Cer, V.P. Mokashi, K.A. Bishop-Lilly

CHED **542.** Modified coarse-grained DNA model and its application to surface density effects on decamer hybridization. **W.C. Scamman**, J.M. Stubbs

CHED **543.** Proof-of-concept for rapid point-of-care LFCC detection of serum cancer biomarkers. **J. Mencke**, C. Cox, **K.J. Voorhees**

CHED **544.** Sensor circuit for streamlining *E. coli* cell phase determination. **D. Stork**, K.A. Haushalter

CHED **545.** Development of a cellular probe based on a synthetic receptor. **C. Young**, B. Vinciguerra, L.D. Isaacs, A.R. Urbach

CHED **546.** Characterization of a cucurbit[7]uril-rhodamine conjugate as a chemical sensor. **S. Vivatson**, B. Vinciguerra, L.D. Isaacs, A.R. Urbach

CHED **547.** D-Lactic acid biosynthesis from corn stover using engineered *Lactobacillus plantarum*. **E.L. Demel**, Y. Zhang, P.V. Vadlani

CHED **548.** Engineering light-gated, transmembrane proteins for use in hybrid systems. **S.J. von Hoyningen-Huene**, V. VanDelinder, **G.D. Bachand**

CHED **549.** Measuring amyloidogenic protein interaction with lipid membranes via colorimetric assay. **E. LaManna**, E.A. Yates

Section A

Colorado Convention Center
Halls C/D

Undergraduate Research Posters

Chemical Education

Cosponsored by SOCED

N. Di Fabio, *Organizer*

12:00 - 2:00

CHED **550.** Gold(I) complexes of benzene-1,3,5-tricarboxamide ligands for Conia-Ene Catalysis. **J.B. Gordon**, M. Raynal, L. Bouteiller

CHED **551.** Greener synthesis of electroluminescent compounds. **N. Rosenfeld**, J. Bennett

CHED **552.** Development of a simple, qualitative tyrosinase inhibition assay for organic chemistry laboratory. **E. Stopler**, J. Bennett

CHED **553.** Greener synthesis of thiosemicarbazones. **D. Dragotta**, K. Flessa, J. Bennett

CHED **554.** Synthesis of C-glycosides as potential antihyperglycemic agents. **C. Tucker**, J.L. Chaytor

CHED **555.** Charaterization of self-assembled monolayers on zinc selenide. **S. Zwart**, A.R. Noble

CHED **556.** Reduction of infectious biofilms on the native oxide surface of titanium. **N. Bruneel**

CHED **557.** Development in undergraduate organic chemistry laboratory curriculum. **E. Mueller**, R. Starr, O. Michels

CHED **558.** Extraction and functional assay of cloned thymopentin 5. **R. Greenstein**, K.S. George Parsons

CHED **559.** Modification of FTY720 for use as a prodrug for cancer therapy. **K.C. Cotto**, B.E. Young, C.M. Watanabe

CHED **560.** Auto-oscillatory/excitable boundary and complex dynamics in the Belousov-Zhabotinsky reaction. **D. Prado**, T. LongJohn, J.A. Wepy, E.R. Kast, D. Guralnik, S.G. Sobel, H.M. Hastings

CHED **561.** Ascorbic acid enhances cytotoxicity of a novel naphthoquinone containing a modified anthracycline Ring System. **R. Al-Refai**, S. Shehata, J.C. Dicesare, R. Sheaff

CHED **562.** Site selective Pd-catalyzed intramolecular cyclization of oxygen nucleophiles. **D. Thach**, S.J. Thompson

CHED **563.** Comparison of nutrient deprived cellular behavior in transformed and untransformed cells. **P.J. Gasser**, R. Sheaff

CHED **564.** Photographic evidence of reactions in organic chemistry: The formation of *trans*-diols from cyclohexene and *meta*-chloroperbenzoic acid. **A.O. Diouf**, D. Trana, J.M. Quirke

CHED **565.** Carbonic anhydrase as a model for matrix metalloproteinase inhibition. **D. DeGenova**, R. Venna, R. Patel, A. Plonski, A. Forchonie, W.A. Richert, S. Al-Abdul-Wahid, D.L. Tierney

CHED **566.** Completing a green chemistry laboratory manual for general chemistry. **K. Wood**, S. Henrie

CHED **567.** Utilization of polymeric quaternary ammonium salts-clay composite in triphase catalysis. **A.P. Sneed**, C. Chapple, N. Shabestary

CHED **568.** Efficiency of synthetic pyrazoline derivatives on inhibiting *Entamoeba histolytica* growth as novel treatment against amebiasis. **K. Schindelwig-Franca**, **J. Tashjian**, **H. Kumar**, **S. McDonough**, A. Espinosa, L. Rossi

CHED **569.** Role of *GRK4* in bladder exstrophy-epispadias complex. **M. Ielmini**, N. Wilken, D.J. Lamb, C. Jorgez

CHED **570.** Impact of nanoparticles on bacterial community. J. Ha, **A. Bally**

CHED **571.** Hands-on activity incorporating the threefold representation on the liming reactant concept. **A.M. Gonzalez-Sanchez**, E.L. Ortiz-Nieves, Z. Medina

CHED **572.** Probing the question-order effect on chemistry concept inventories. **M. Undersander**, T.J. Lund, M.N. Stains

CHED **573.** Impact of an intensive workshop on STEM faculty's fidelity of implementation of peer instruction. **K. Rosploch**, M. Pilarz, **M.N. Stains**

CHED **574.** Elimination reaction of tropic acid as a simple example of an E1cb reaction. **D. Li**, E.D. Helms, K. Best

CHED **575.** Chemistry teaching laboratories: What is the point? **A. Neybert**, J. Barbera

CHED **576.** Effect of *Azadirachta indica* tree in the CYP450 system of chinese hamster ovarian cells. **N.I. Negrón**, L. Santos

CHED **577.** Dioxygen activation by mononuclear non-heme iron oxygenases and the corresponding model complexes. **S. Kingston**, L. Cunningham, J.P. Caradonna

CHED **578.** Developing and evaluating a collaborative learning environment in analytical chemistry. **A. Palmer**, K.A. Pettigrew

CHED **579.** Holistic trace analysis: Development of an upper-level chemistry experience. **D. Hughes**, C.D. Hatch

CHED **580.** Paper microfluidic method to quantify taurine in urine samples: A college-level introductory chemistry experiment. **L. Nguyen**, O. Baawuah, S. Gamagedara

CHED **581.** Epoxyeicosatrienoic acid analog mitigates kidney injury in experimental radiation nephropathy. **B. Vo**, A. Khan, J. Neckar, A. Sharma, K. Molter, J. Imig

CHED **582.** Toward a comprehensive integration of calorimetry across the curriculum. **O. Summers**, B. Bruske, H. Sklenicka

CHED **583.** Documenting collective activity in a large scale introductory chemistry class. **J.D. Byers**, C.L. Stanford, R.S. Cole

CHED **584.** Synthesis of highly functionalized nitrogen containing monoadducts via copper catalyzed atom transfer radical addition (ATRA). **J. Martin**, G. Pros, T. Pintauer

CHED **585.** Targeting Glutaminolysis to selectively kill cancer cells with deregulated p27. **J.A. Sabo**, M.R. Ferguson, P.J. Gasser, R. Sheaff

CHED **586.** Impact of cost on chemistry laboratory teaching practices. **R.A. Livermore**, S.B. Boesdorfer

CHED **587.** Developing a redox themed assessment instrument using the three levels of representation. **S. Santos**, A.M. Gonzalez-Sanchez, E.L. Ortiz-Nieves, Z. Medina

CHED **588.** Use of organic base to restore catalytic activity of [Cu(Me_6TREN)Cl][Cl] in Atom Transfer Radical Addition (ATRA) in the presence of ascorbic acid as a reducing agent. **M.C. Wasson**, G. Pros, A. Kaur, T. Pintauer

CHED **589.** Investigation of HOBS methodology in nucleic acid NMR studies. **J.M. McKenna**, J.A. Parkinson

CHED **590.** Enantiomeric interactions of amino-acids adsorbed in zeolites: An investigation, using solid-state NMR, thermogravimetry (TGA) and differential scanning calorimetry (DSC). **L. Topchyan**, **S. Krishnan**, **S. Ira**, **M. Garcia**, **N. Sankari**, M. Ramirez, A. Martinez, D. Cizmeciyan, R. Senter

CHED **591.** Synthesis of pyridone-based ligands for homogenous hydrogenation iron-based catalysts. **H.K. Caddes**, **S.L. Willis**

CHED **592.** Adapting a set of organic chemistry experiments for delayed analysis time. **S.C. Kenea**, N.J. Beyer

CHED **593.** Preparation of NiFe supported catalysts for hydrotreatment. **C. Peterson**, E. Marceau, A. Lamic, G. Laugel

CHED **594.** Near infrared spectroscopy chemical Imaging for the determination of component segregation. T. **Vélez-Burgos**, E. Hernández, R.J. Romañach

CHED **595.** Preparing and screening brominated phenols: An organic laboratory experience. **J. Bietsch**, T. McCoy, A.A. Yeagley

CHED **596.** Applying a greener approach to the Grignard reaction. **A.E. Burgos- Aviles**, I. Montes Gonzalez

CHED **597.** Total synthesis of a calixarene cage. **A. Ferrari**, E. Wade

CHED **598.** Human carbonyl reductase as target for alleviating anthracycline cardiotoxicity: Understanding small molecule binding by human carbonyl reductase. **L. Brown**, H. Charlier

CHED **599.** Comparison of metacognative abilities of introductory chemistry students. **J. Johnson**, A.B. Mahoney, M. Nagel

CHED **600.** Biochemical analysis of G-quadruplex secondary structures in CDK5R2 mRNA and of their role in fragile X syndrome. **C.M. Gaetano**, M. Mihailescu

CHED **601.** Theoretical description of chemical shift anisotropy. **K. Phillips**, R. Iuliucci

CHED **602.** Designing catalytic N-heterocyclic carbene complexes for enantioselective allylic oxidation. **R.J. Morrison**, P.J. Lombardi

CHED **603.** Development of a selection marker for automated genome construction. **E. Aponte**, J. Norville, G.M. Church

CHED **604.** Expression of major hominoid seminal proteins in a mammalian cell culture system. **M. Hockman**, J. Vill, T. Pollock, A. Zielen, M. Jensen-Seaman

CHED **605.** Adsorption of thioethers on Au(111) using scanning tunneling microscopy. **R. Miller**, **A. Whitney**, D. Del Sesto

CHED **606.** Heavy metal isotope analysis of historic skeletal remains using ICP-MS. **C. Klesner**, N. Little, D. Owsley

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CHED **607.** Detection of the *cp4 epsps* gene in maize line NK603 and comparison of related protein structures: An advanced undergraduate experiment. **N. Swope**, P.J. Fryfogle, T. Sivy

CHED **608.** Investigating the synthesis and role in molecule-based-magnets of bis(4-pyridyl) acetylene. **T. West**, A.C. McConnell

CHED **609.** Laboratory course as journal house: An advanced organic chemistry course incorporating writing/reviewing scientific manuscripts and green chemistry. R. Beltman, T.M. Dierker, A.G. Fei, W.K. Fuchs, T.D. Gornall, A.M. Katsimpalis, M.J. Ponkowski, R. Wong, **M.J. Mio**

CHED **610.** Electrocatalytic activity of metal-centered porphyrin thin films. **C. Myers**, W.M. Ames

CHED **611.** Versatile lecture demonstration and laboratory exercise illustrating steric hindrance, electron induction, and catalyst nucleophilicity effects on catalyzed ester hydrolysis. K.R. Smith, D.J. Clague, D.J. Alexander, S.C. Butler, **R.N. Mason**

CHED **612.** Lipid raft TNF-α pathway analysis of cytochrome C with methylparaben and UVB treatment. **R.S. Wood**, R. Stahl, K.S. George Parsons

CHED **613.** Investigation of student understanding in spectroscopy labs. **D.P. Jacinto**, L.T. Tien, D. Rickey, M.A. Teichert

CHED **614.** Novel regulation of p27 by transglutaminase. **A. Greene**, L. Zhang, R. Patel, W. Crawford, R. Sheaff

CHED **615.** Development of histone deacetylase inhibitors. **R. Kidney**, L. Ma, T.D. Do, S. Szabolcs, S.F. Paula

CHED **616.** Progress toward synthesis of a novel trifluoromethyl substituted aurone as a potential cyclooxygenase-2 inhibitor. **J. DePhillips**, M. Polk, C. Mills, A. Zuver

CHED **617.** Modification of the p27 tumor suppressor by the transglutaminase enzyme. **W. Crawford**, L. Zhang, A. Greene, R. Patel, R. Sheaff

CHED **618.** Analysis of organic compounds isolated from particulate matter produced by biodiesel and diesel fuel. **N. Brown**, M. Cavacas, N. Traviss, J.R. Kraly

CHED **619.** Synthetic studies toward *Corynanthe* indole alkaloid derivatives. **S. Petritis**, E.K. Leggans

CHED **620.** Free radical effect on the quantum yield of silicon nanoparticles. **R. Ellison**, C. Radlinger, A. Goforth

CHED **621.** Determining the rate of oxidation of promethazine to its sulfoxide and sulfone in atmospheric O_2 using HPLC-MS and UV-VIS spectrophotometric analysis. C.M. Baker, K.N. Bettridge, I. Webb, G. Guitierres, P. Chaisri, **A.L. Kesler**, S. Bedi, S. Christensen, K. Oakes, S. Bremer, R.V. Valcarce, P.J. Iles, M. Alvarez, L.D. Giddings, N.R. Bastian

CHED **622.** Detection of organic pollutants using EVA with GC-MS and AFM analysis. **T. Schreyer**, C. Carr, A. Timmerman, C. Peak, K.N. Bettridge, I. Webb, M. Vanweerd, R.V. Valcarce, S.T. Lindsey, P.J. Iles, M. Alvarez, N.R. Bastian, L.D. Giddings

CHED **623.** Analysis of University of Utah Fine Arts Museum Egyptian sarcophagus by scanning electron microscopy. **J. Van Wagoner**, R. Haynie, L. Kelly, S.T. Lindsey, S. Bremer, R.V. Valcarce, P.J. Iles, L.D. Giddings, N.R. Bastian, M. Alvarez

CHED **624.** Determining source of discoloration in renaissance fresco using infrared spectrophotometry. **J. Van Wagoner**, R. Haynie, L. Kelly, S. Bremer, S.T. Lindsey, R.V. Valcarce, P.J. Iles, L.D. Giddings, N.R. Bastian, M. Alvarez

CHED **625.** 1,3-Dipolar cycloaddition reaction. **M. Muni**, S.R. Hussaini

CHED **626.** Solvation equilibria of proximally-substituted copper bis-phenanthroline derivatives. **N.A. Arnista**, S.P. Watton

CHED **627.** Aromatization of fragrant monoterpenes via palladium-catalyzed dehydrogenation. **T.S. Hill**, A.M. Hartel

CHED **628.** Optimization of algae-derived biodiesel for use in undergraduate chemistry laboratories. **M.R. Barron**, C.S. Harper, K.L. Braun

CHED **629.** Forensic analysis of commercial color and black inkjet printer inks by micellar electrokinetic chromatography. **C.S. Harper**, K.L. Braun

CHED **630.** Enzymatic reduction of a ketone for a college-level organic chemistry course using alcohol dehydrogenase. **L. Zhao**, P.M. Joyner

CHED **631.** Synthesis of the SRS and SSR isomers of lentiginosine from D-glucopyranoside and D-galactopyranoside. **D.C. Fager**, L.J. Liotta

CHED **632.** Team-based assessment of introductory organic chemistry lecture. **R. Tieu**, J. Soria

CHED **633.** Team-based assessment of a two-semester introductory organic chemistry laboratory course. **V.F. Vartabedian**, J. Soria

CHED **634.** Initial investigation of pyrrolizidine alkaloids in *Pscalium decompositum*. **J. Burklund**, K. Hamann, D. Morales, R.B. Kelley

CHED **635.** Cost effective ion selective electrodes from metal-azo complexes. **W.A. Nanney**, B.L. Belmont

CHED **636.** Burning truth about sunscreens: Zinc oxide nanoparticle growth kinetics. **V. Smith**, P.A. Brletic

CHED **637.** Small angle X-ray scattering (SAXS) of β_2-glycoprotein I suggests an alternative mechanism for antibody interaction in antiphospholipid syndrome. **A. McLaughlin**, N. Pozzi, E. Di Cera

CHED **638.** Dynamics study of the resorcin[4] arene supramolecular assembly. **P.B. Calio**, J. Harvey, W. Thompson

CHED **639.** Synthesis and luminescence studies of rhenium(I) tricarbonyl complexes using LabQuest 2. **N.V. Vecchio**, M.O. Odago

CHED **640.** Attachment inhibition of invasive species. **K. Marcus**, **C. McKellar**, **R. Pearce**, S. Beck, R. Del Sesto

CHED **641.** Writing exam questions that elicit evidence of process skills. **H. Moon**, J.A. Schmidt, R.S. Cole

CHED **642.** Understanding the cognitive load generated by constructing Lewis structures. **A. Coleman**, R. Balok, J.M. Tiettmeyer, T. Gampp, P. Duffy, K. Mazzarone, N.P. Grove

CHED **643.** Synthesis of 2'-phenoxy-4-hydroxyacetophenone. **S. Ortiz-Piccard**, J. Peterson, T. Field, R.S. Givens

CHED **644.** Longitudinal study of the effects of a professional development program on the content knowledge and teaching practices of middle and high school science teachers. **H.A. Hayes**, **J.S. Corrales**, R. Lewis, E.E. Gonzalez, B.D. McCormick, A.R. Chaudhuri

CHED **645.** Southern Utah University general chemistry case study: Identification of curriculum obstacles. **K.B. Weaver**, R. Stewart, S. MacFarlane, A.C. McConnell

CHED **646.** Research on surface modification of zinc oxide nanoparticles and incorporation into fibers. **T. DiPasquale**, J.E. Whitten, D.M. Steeves, J. Soares

CHED **647.** Newly established documentation and imaging system detecting DNA hybridization serves as a potential point of care device to further distinguish genetic susceptibility to diseases. **D.W. Capps**, J.R. Kenneson, R.L. Moore

CHED **648.** Analytical techniques in environmental chemistry: Detection and quantification of common herbicides in surface water. **T. McCall**, E.M. Marzluff

CHED **649.** Determination of mercury levels in living and nonliving systems of southwest Arkansas. **D. Campbell**, J. Lowe, H. Wayland, D. Bateman

CHED **650.** Physiological effects of massage therapy in college students and the elderly. **H.A. Wayland**, C. Dickson, D. Bateman

CHED **651.** Continued study in Facebook™ as a collaborative learning platform for sophomore organic chemistry students. S.F. Hornbuckle, **J. Lawrence**

CHED **652.** Isolation and characteristics of flavonoids from ash tree leaves. **A.M. Gallegos**, **E.E. Wilson**, **M.P. Smith**, **S.T. Mirza**, **A.V. Daspit**, B.A. Clement

CHED **653.** Kinetics of the reduction of nitrobenzene using hydrazine hydrate and cobalt (II) sulfide. **D. Cedillo**, J. Garcia, T. Treviño, J.G. Parsons, J. Gutierrez-Gonzales

CHED **654.** Biophysical analysis of *CDK5R2* DNA secondary structures. **K. Bandi**

CHED **655.** Histone deacetylase (HDAC) inhibitors containing thioamide: Synthesis and biological evaluation. **A.J. Onate**, . Szabolcs, E. Merino, S.F. Paula, L. Ma

CHED **656.** Synthesis of (2R,3S,4S)-2-(hydroxymethyl)pyrrolidine-3,4-diol from α-methyl-D-galactopyranoside. **M.J. Smith**, L.J. Liotta

CHED **657.** Withdrawn.

CHED **658.** Synthesis and characterization of sol-gel monoliths as glucose biosensors. **S. Moore**, C.H. Lisse

CHED **659.** Synthesis and characterization of potential TNR hairpin formation inhibitors. **S. Crowley**, M. Welch

CHED **660.** Effect of pH in sulflactoperoxidase formation. **J. Feng Baez**, B. Ríos-González, J. Lopez Garriga

CHED **661.** Investigating the effects of steric bulk on γ-silyl bridging by varation of the γ-electron-donating and α-substituent. **L. Macary**, J. Hauck, L.J. Tilley

CHED **662.** Synthesis of 9-fluoro-9H-fluoren-1-ol. **D. Memon**, R.E. Rosenberg, R. Ferrill, . Johnson, J. Bier

CHED **663.** Synthesis of polyhydroxylated pyrrolidine from a D-glucose derivative. **A. Harney**, L.J. Liotta

CHED **664.** Synthesis of lentiginosine form D-glucose. **K. McAndrews**, L.J. Liotta

CHED **665.** Computational investigation of the surface tension of supercooled water. **T.R. Rogers**, K. Leong, F. Wang

CHED **666.** DFT analysis of copper-based chemotherapeutics. **T.M. Kolb**, J.S. Anderson, L.A. Tyler

CHED **667.** Peptide sequencing using gas-phase peptide carbocations. **A. Plaviak**, M.J. Van Stipdonk

CHED **668.** Maximizing the extraction efficiency of arsenic in solid matrices followed by graphite furnace atomic absorption spectrometric analysis. **M. Wakeman**, C.D. King

CHED **669.** Curriculum development for BSU's outreach program geared to spark interest in chemistry. **B. Morgan**, C.D. King

CHED **670.** Microwave synthesized succinimides purified by flash chromatography. T.F. Guetzloff, **B. Dudding**, M. Fultz

CHED **671.** Transesterification of hypophosphorous esters: Elucidating the synthetic scheme of phosphorous-based surfactants. S. Deprele, **A.L. Perez**, **N. Neris**, **C. Alvarez**

CHED **672.** Accessing vinyl fluoroalkyl-substituted cyclopropanes from homoallyl mesylates *via* a destabilized cation-mediated electron cascade. **A.E. MacInnis**, L.J. Tilley, N.E. Leadbeater, E.R. Carnaghan, M. Doherty, D.C. Fager, J. Hauck, C.B. Kelly, M.A. Mercadante

CHED **673.** Chemistry laboratory safety: Misconceptions among first- and second-semester general chemistry students. **J. Melvin**, W.E. Schatzberg

CHED **674.** Chemical and biochemical stability of guanine lysine cross-links formed by guanine oxidation. **J. Mincitar**, **D. Esparza**, **N. Tran**, **A. Ramos**

Section A

Colorado Convention Center
Halls C/D

Undergraduate Research Posters

Computational Chemistry

Cosponsored by COMP and SOCED

N. Di Fabio, *Organizer*

12:00 - 2:00

CHED **675.** Comparisons of Synaptotagmin 1 and Synaptotagmin 7 C2A domains in membrane associations by molecular dynamic simulations. **N.L. Chon**, J.A. Henderson, J.D. Knight, H. Lin

CHED **676.** Computational modeling of STAT3 SH2 domain inhibition. **C.T. Williams**, P. Daka, E.E. Csatary, H. Wang, R.C. Page

CHED **677.** Computational modeling of temporary anion states in the field of dipole or quadrupole moment. **E.M. Tharnish**, **L. Williams**, M.F. Falcetta

CHED **678.** Computational modeling of resonant vibrational excitation of CO by electron impact. **L. Williams**, **E.M. Tharnish**, P.E. Linn, M.C. Fair, M.F. Falcetta

CHED **679.** Cyclic voltammetric and computational structure-electrochemistry relationship studies of the reduction of a series of 9,10-anthraquinone derivatives. **N. Fox**, T.W. Johnson

CHED **680.** Effect of unequal strand length on DNA hybridization in a model microarray system via Monte Carlo simulation. **S. Cooper**, J.M. Stubbs

CHED **681.** Journey of 4-HNE: How biochemistry became computational. **A.K. LaPidus**, C.M. Byron

CHED **682.** Predicting the function of structural genomics proteins of unknown function in the crotonase superfamily. **S.R. Little**, C.L. Mills, P.J. Beuning, M.J. Ondrechen

CHED **683.** Conformational sampling of glucose oxidase for bio-fuel cell applications. **E. Gomez**, T. Tran, N. Tran, D. Chakravorty

CHED **684.** Role of glycosylation in protein structure: A bioinformatics-based computational study. **J. Rogers**, S. McHugh, Y. Lin

CHED **685.** Effect of motor protein binding on microtubule depolymerization. **D.G. Witte**, N. Yu, R. Dima

CHED **686.** Solid-state NMR chemical shift peak matching of geometry optimized organic crystals by computational methods. **S. Upadhyay**, M.N. Srnec, J.D. Madura, R. Iuliucci

CHED **687.** Theoretical study of the factors that contribute to the conformational energy of six-membered rings. **M. Abdulsalam**, R. Balilli, R. Baello, C. Brutofsky, S. Suresh, M.L. Kasner, R. Booth

CHED **688.** Computational study of the contributions to the relative stability of the α and β conformers of D-glucopyranose. **R. Balilli**, M. Abdulsalam, R. Baello, R. Booth, S. Suresh, M.L. Kasner

CHED **689.** Solid-phase heats of formation of energetic compounds using computational methods. **D. White**, M. Elioff

CHED **690.** Computational studies of the hyperpolarizability of halogenated saccharins and their anions and salts. **M.B. McDaniel**, D.A. Clabo, Jr.

CHED **691.** Electronic structure calculations of Li_2-II-IV-VI_4 diamond-like semiconductors. **J. Worst**, A.J. Glaid, M.N. Srnec, J.D. Madura, J.A. Aitken, J. MacNeil

CHED **692.** Coarse-grained modeling of reverse micelles. **M. Rea**, A.T. Moser

CHED **693.** Computational study of the visible spectrum of curcumin's protonation states. **P. Braegelmann**, J.D. Alia

CHED **694.** In silico insight into mechanism for the formation of C8 products from the reactions of guanine with substituted aniline. **J. Bautista**, S. Shrestha, A.S. Dutton, A.G. Leach

CHED **695.** Computationally simulating the metabolic enantiospecificity of CYP2C9 using molecular dynamics. **P. Onyuru**, G.P. Miller, M.D. Perry

CHED **696.** Elbow room: How surfactant proportions modify interfacial properties. **J.A. Palumbo**, K.E. Johnson

CHED **697.** Computational docking to analyze substrate metabolism in CYP2E1. **M. Rogers**, G.P. Miller, M.D. Perry

CHED **698.** Computational investigations on ligand isoform selectivity in the liver X receptors. **M. Ndukwe**, **B. Theard**, K. Riley

CHED **699.** Studies of factors affecting the reaction mechanism of formation of the levoglucosan. **L. Aebersold**, T. Daeschlein, J. Henry, B.N. Leja, D. Wang, A. Seitz, J. Song

CHED **700.** Mechanistic insights into the alkylation reactions of quinone methide precursors: Studies towards the realkylation of aged acetylcholinesterase. R.J. Yoder, **T. Blanton**, K. Fitzpatrick, A.J. Franjesevic, S. Higgins, C. Callam, C.M. Hadad

CHED **701.** Unpaired electron density in retinal model compounds. **T. Vaid**, E.D. Glendening

CHED **702.** Computational study on the formation of hexamethylene triperoxide diamine. **A. Sindt**, J.N. Woodford

CHED **703.** ARGOS: A rigid geometry optimizer for supramolecular complexes. **R. Meyerson**, S.E. Wheeler

CHED **704.** Group 13 chiral Lewis acid stereoselective control of enal Diels-Alder reactions. **A.N. Ahmed**, B. Vernier, A. Kelly, J. Rohde, J.D. Evanseck

CHED **705.** Solvation effects in bimolecular Diels Alder cycloaddition of cyclopentadiene: A tool for benchmarking expected errors in more sophisticated Diels Alder reactions. **A. Kelly**, B. Vernier, A.N. Ahmed, J. Rohde, J.D. Evanseck

CHED **706.** Computational modeling of fluorescent probes to understand how lithium treats manic depression. **S. Claridge**, D.L. Nutbrown

CHED **707.** Using the relativistic particle in a box to model conjugated dyes. **B. Barrett**, J.E. Lacy

CHED **708.** Using molecular dynamics to computationally simulate metabolic enantiospecificity of CYP2C9. **N.D. Hall**, G.P. Miller, M.D. Perry

CHED **709.** Folding of meta-poly-phenylene ethynylene. **K. Hefel**, A. Moser

CHED **710.** Further computational investigation on the conformationally-restricted allenyl cope rearrangement of *Syn*-7-allenylnorbornene. **M.A. Lyon**, J.A. Duncan, C.S. Jamieson

CHED **711.** Possible explanation for the formation of trans-Whiskey lactone: A computational approach. **T. Le**, E. Simanek, B.G. Janesko

CHED **712.** Investigation of biological anion effects on phospholipid structure and oxygen diffusion free energy. **T. Ricard**, S.C. Pias

CHED **713.** First principle calculations of optical properties of platinum(II) diimine complexes. **L. Lystrom**, S. Kilina, W. Sun

CHED **714.** Conformational distribution of cysteine and selenocysteine dyads in biological redox processes. **L.M. Froehle**, S. Vyas

The use of any device to capture images (e.g., cameras and camera phones) or sound (e.g., tape and digital recorders) or to stream, upload or rebroadcast speakers or presentations is strictly prohibited at all official ACS meetings and events without express written consent from ACS.

Section A

Colorado Convention Center
Halls C/D

Undergraduate Research Posters

Environmental Chemistry

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N. Di Fabio, *Organizer*

12:00 - 2:00

CHED **715.** Evaluating oil dispersant systems via emulsion stability and optical microscopy. **W. Fagan**, W. Ervin, Y. Zhang, B. Gikonyo, M. Tsianou

CHED **716.** Core shell vs. alloy iron/nickel nanoparticles for water treatment. **M. Voecks**, K. Estoque, L.F. Greenlee

CHED **717.** Orange G dye degredation using iron-nickel nanoparticles: Effect of iron to nickel ratio, concentration and pH. **K. Estoque**, M. Voecks, L.F. Greenlee

CHED **718.** Electrochemical characterization of iron nanoparticle–clay interaction for groundwater remediation. **K. Roberts**, B.A. Balko

CHED **719.** Analysis of mineral content in MWSU parking lot runoff water using PXRF, FAA, and EDTA titration. **J. Mitchell**, S.L. Hiley

CHED **720.** Drugged wildlife: The potential impacts of environmental endocrine disruptors on reproductive development. **M.Y. Kramer**, N.A. McNabb, L.J. Guillette, S. Kohno

CHED **721.** Monitoring the long term effects of fracturing in Western Pennsylavnia, Butler County: How long is long enough? **R.L. McLaughlin**, C. Kriley, N. Rutter

CHED **722.** Development of 2-component surrogate mixtures for alcohol-to-jet fuel. **M.H. Jones**, D.J. Luning Prak

CHED **723.** Analytical identification of polycyclic aromatic hydrocarbons: The bio-monitoring of Cyprus trees in Los Angeles. **A. Kerl**, S. Castillo, Y. Torres, S. Deprèle

CHED **724.** Potential heavy metal water remediation using 5-formylfuran-2-sulfonic acid thiosemicarbazone (DIFANEX) chelating resins. **A.L. Werlein**, A.J. Crook, E.P. Hoy, D.D. Ensor, E.C. Lisic

CHED **725.** Novel method for the extraction of lead ions from bulk water supplies using chelation chemistry. **K.M. Sheetz**, K.A. Mies

CHED **726.** Metal-sequestration from water using a polysulfide synthesized from sulfur and limonene. **A.M. Evans**, M.P. Crockett, J.M. Chalker

CHED **727.** Determination of total mercury in the top three consumed seafood products of the United States. **A.L. Kramer**, C.N. Hill, S. Aloisio

CHED **728.** Reactions of alcohol amines with atmospheric oxidants N_2O_5, H_2O_2 and O_3 analyzed through a Particle-into-Liquid Sampler coupled to dual ion chromatographs. **R. Jauregui**

CHED **729.** Analysis of the open limestone channel at the Swank 13 abandoned coal mine. J. Krug, **R.C. Krupa**, **D. Mosier**, C.J. Weyant, E.P. Zovinka

CHED **730.** Degradation of the layer of calcium carbonate ($CaCO_3$) on the *Pyrodinium bahamense* (dinoflagellates) from bioluminescent lagoons in Puerto Rico. **A. Rodriguez-Velazquez**, K.D. Ortiz, L. Delgado, S. Delgado

CHED **731.** Separation of oil contaminates from oil-in-water emulsions using nylon 6,6 nonwoven fabric filters. **K.A. Murrell**, E.S. Carter, F.D. Hileman, A.E. Ortgega

CHED **732.** Synthesis of water filtration composites for use against microorganisms and heavy metal in water. **M.M. Samson**, K.M. Metz

CHED **733.** Bioremediation of nickel and cobalt by *Bacopa monnieri*. **P.C. Vera-Santiago**, Z. Serrano-Rivera, J. Arbelo-García, M. Ramos-Fontán

CHED **734.** Influence of cation charge density, ionic strength, and pH on NOM particle size distributions in aqueous solution. **H. Argersinger**, G.M. Bowers

CHED **735.** Three years of full scale testing an enhanced bioswale. **N.P. Lesner**, W. Kuzmishin, H. Yang, P. Edmiston

CHED **736.** Catalysis in chromic acid oxidations: A co-oxidation model for the detoxification of hexavalent chromium in water. S. Mahapatro, **A.I. Lujan**

CHED **737.** Studying reactivity and leaving group effects in aryl chloroformate esters. **A. Bilbrough**, **D. Williams**, M.J. D'Souza

CHED **738.** Correlation analyses of solvent reactions of 2-fluoroethyl chloroformate and 2-benzyloxyethyl chloroformate. **V.M. DeBarros**, M.J. D'Souza

CHED **739.** Confirming the use of phenyl chloroformate as an appropriate addition-elimination standard in LFER analyses. **J.K. Deol**, M.J. D'Souza

CHED **740.** Integrons and multiple-antibiotic resistant bacteria in Minnesota surface waters. K.H. Wammer, **E.W. Beck**, C. Haines, T. LaPara

CHED **741.** Viability of ozonation as a water treatment method for the elimination of the antibiotic roxithromycin. **C.H. Fuerste**, D.C. Harmes, D.R. Stoll, K.H. Wammer

CHED **742.** Aqueous photochemistry of altrenogest. **K.C. Anderson**, K.H. Wammer

CHED **743.** Analysis of San Antonio River water for metals using inductively coupled plasma-mass spectrometry. **H.A. Hayes**, **J.S. Corrales**, P.P. Gonzalez, A.R. Chaudhuri, B.D. McCormick, E.E. Gonzalez

CHED **744.** pH profile determination of the cation exchange capacity of heavy metals from estuarine sediment and its correlation with outer shell content of benthic organism *Mercenaria mercenaria*. **J.M. West**, S.K. O'Shea

CHED **745.** Characterization of metal cation binding to pyridine-based compounds in aqueous solution. **J. Moose**, S. Tajc

CHED **746.** Analysis of heavy metal leaching from motor oil into water. **C.R. Stear**, C.L. Fish

CHED **747.** Photochemical reactive oxygen species production by petroleum water accommodated fractions. **A.M. West**, **J. Haney**, P.P. Vaughan

CHED **748.** Did the Bastrop wildfire affect the phosphorus quantity in the soil? **M. Abu-Esba**, H.G. Altmiller

CHED **749.** Cd, Ni, Zn and Cu concentrations in fish muscles collected from sites along the Ashley River. **M. Mirano**, B. Adair

CHED **750.** Algal toxin dynamics in a eutrophic lake and indicators of toxins in raw drinking water. **K. Rude**, C. Weirich, S. Bartlett, M. Seaman, J. Piatt, T. Miller

CHED **751.** Effects of woolly adelgid induced hemlock productivity decline on soil nutrient content. **B. Redder**, J. Balnis, Z. Balogh-Brunstad

CHED **752.** Analysis of heavy metals in *Lutjanus griseus* and *Lutjanus campechanus at* the natural reserve "La Parguera", Puerto Rico. **N.M. Lopez Pena**, R. Tremont

CHED **753.** Detection of precursors to methamphetamine in city sewers lines. **C. Craine**, M.P. Butner, T.H. Boles

CHED **754.** Optimization of fly ash nanogeopolymer and its application in pervious concrete for bioremediation of fecal coliform-containing water. **V. Hwang**, E. Montalvo

CHED **755.** Extracting metal (II) cations from aqueous solution using dipicolinic acid. **M. Porter**, A. Richardson, S.G. Tajc

CHED **756.** Pesticide analysis in Southeast Michigan waters by gas chromatography-mass spectrometry. **C.C. Conrad**, **P.M. Dine**, D.M. Dreffs, B.H. Keith, S. Zoma, T.Y. Zurawski, R. Dutta, K.R. Evans, E.S. Roberts-Kirchhoff

CHED **757.** Study of analyte recovery using headspace solid-phase microextraction. **J. Tillman**, **W. Weckel-Dahman**, F.M. Dunnivant

CHED **758.** Scanning electron microscope analysis of Columbia River, Chesapeake Bay, Lake Hartwell, and Mississippi River sediment suspensions. **X. Yi**, J. Morgan, F.M. Dunnivant

CHED **759.** Quantification of epoxides from their carbamate derivatives: Environmental applications. **G. Amon**, W. McCue, C.M. Strollo

CHED **760.** Detection of amphetamine type substances in sewers using Polar Organic Chemical Integrative Samplers. **M.P. Butner**, C. Craine, T.H. Boles

CHED **761.** *Mercenaria mercenaria* a potential bioindicator of heavy metal releases into Narragansett Bay, RI. **K.D. Audette**, S.K. O'Shea

CHED **762.** Study of the effects of two PPCPs on algal growth. **T. Meece**, T. Knight

CHED **763.** Exploring the interactions between citrate-stabilized silver nanoparticles and humic acid via fluorescence quenching. **L.A. Warning**, B.D. Anderson

CHED **764.** Investigating the formation of thioarsenic species under sulfidic conditions. **J. Loving**, V. Stucker, J.F. Ranville

CHED **765.** Study on UV-Vis spectroscopic characteristics of soil humic substances. **J.L. Ragon**, H. Zhang

CHED **766.** Rhodium catalyzed hydrodehalogenation of fluoroarenes in mild conditions. **A.M. Luke**, A.A. Peterson

CHED **767.** Removal of phosphate from aqueous media by adsorption onto humic acid-coated magnetite. **N. Price**, M. Rashid, K. OShea

CHED **768.** Use of CYCLAM and other tetraamines to probe the mechanism of influence of surfaces on ligand exchange. **S.J. Hinkle**, N.E. Boland

CHED **769.** Studying the reactions of alcohol amines with atmospheric oxidants. **J. Dulla**, R. Jauregui, D.J. Price, K. Purvis-Roberts, D. Cocker

CHED **770.** Effects of "real world" biodiesel and petroleum diesel combustion on PM composition and production of ROS in BEAS-2B cells. **N. Martin**, A. Bosco, T. Pratt, N. Traviss

CHED **771.** Impact of "real world" biodiesel and petroleum diesel combustion on particulate matter composition and oxidative potential. **P. Kelley**, **R. Klaski**, N. Martin, N. Traviss

CHED **772.** Enhancing the chemical mixture methodology: Revising the health code number assignments of hazardous chemicals to account for varying intensities of respiratory irritation. **J. Jablonski**, J. Yao, X. Yu, C. Glantz

CHED **773.** Chemical analysis in the *Eryngium foetidum L.* **N.N. Olmeda**, S.A. Maldonado, R. Tremont

CHED **774.** Static quenching of acridine yellow G and norfloxacin by humic acid. **R. Ferrie**, B.D. Anderson

CHED **775.** Correlation of nitrogen dioxide and ozone gas concentrations between Milwaukee and Chicago. **T. Antoniewicz**, T. Robers, M.D. Schuder

CHED **776.** Extraction of barium from aqueous solution using pyradine based small molecules. **J. Merchant**, S.G. Tajc

CHED **777.** Design and characterization of a pulsed laser cavity ring-down spectrometer for use in the measurement of aerosol optical properties. **J.C. Castillo**, **J.M. Pittman**, L.W. Bevill, K.S. Dooley

CHED **778.** Size characterization and metals analysis of particulate matter generated by candle burning. **L.W. Bevill**, K.S. Dooley

CHED **779.** Quantitative determination of antidepressants in wastewater effluents and biosolids. **J. Brotman**, C. Moffett, K. Shiavone, M.M. Schultz

CHED **780.** Closing the gap on secondary organic aerosol formation: Oligomerization of glyoxal. **L.E. Rusch**, C.M. Strollo

‡ *Cooperative Cosponsorship*

CHED **781.** Submarine groundwater discharge as a potential hidden pathway for eelgrass decline in San Juan county. **E.L. Johnson**, J. Beets, J. Dixon, R.A. Lyons, P. Swarzenski, S. Wyllie-Echeverria

CHED **782.** Arsenic analysis and speciation of water samples from Chihuahua México, by HG-CT-AAS. **V. Medina**, Y. Rodriguez, D. Acosta, L. Ballinas-Casarrubias

CHED **783.** Photodegradation of organic dyes using quantum dots of Cd(Se,S) in aqueous solutions. **G. Rivera Rodriguez**, O. Perales-Perez, F.R. Roman, S. Bailon-Ruiz, L. Alamo-Nole

CHED **784.** Photodegradation of antibiotics in aqueous solutions using quantum dots of Cd(Se,S). **I.N. Leon Feliciano**, O. Perales-Perez, F.R. Roman, S. Bailon-Ruiz, L. Alamo-Nole

CHED **785.** Cadmium phytoremediation of in vitro culture with micro-propagated clones of *Spermacoce assurgens*. **B.L. Vargas Perez**, L. Rodriguez

CHED **786.** Profile of metal bioaccumulation in selected invertebrates from the eastern and western shores of the Susquehanna River near Hummels Wharf Pennsylvania. **A. Pritzlaff**, C.P. Hallen, C. Venn

Section A

Colorado Convention Center
Halls C/D

Undergraduate Research Posters

Geochemistry

Cosponsored by GEOC and SOCED

N. Di Fabio, *Organizer*

12:00 - 2:00

CHED **787.** Selective synthesis of ribose via the formose reaction under prebiotic conditions. **P.S. Donmoyer**, A.L. Marsh

CHED **788.** Impact of methanotrophy on methane gas hydrate dissolution rates. **M. von der Lippe**, R.K. Larsen, L. Lapham

CHED **789.** Formic acid uptake on montmorillonite clay: An FTIR study. **L.A. Hancock**, R.M. Weingold, C.D. Hatch

CHED **790.** Exploring the mechanism for iron uptake by phytoplankton: A biomarker study. **M.J. Christie**, C.D. Hatch

CHED **791.** Water adsorption on montmorillonite clays. **R. Meredith**, C.D. Hatch

CHED **792.** Influence of a metal oxide surface on ligand exchange reactions between strong chelating agents. **J. Conrad**, N.E. Boland

CHED **793.** Influence of pH on ligand exchange rate with phosphonate-containing chelating agents. **M.V. Harned**, T. Nelson, N.E. Boland

CHED **794.** Sediment and water analysis of a glacially formed lake. **K.F. O'Connor**, Z. Balogh-Brunstad

Section A

Colorado Convention Center
Halls C/D

Undergraduate Research Posters

Green Chemistry & Sustainability

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N. Di Fabio, *Organizer*

12:00 - 2:00

CHED **795.** Southeastern Massachusetts student network for biodiesel research and education. **L. Sprague**, B. Ackley, K. Bukis, J. Hooper, I. Korslund, P. Kurriss, K. Roebuck, E.J. Brush

CHED **796.** Series of meso-tetrasubstituted porphyrins synthesized using mechanochemistry. **Q. Su**, T.D. Hamilton

CHED **797.** Entrainment sublimation for purification of mechanochemically-synthesized porphyrins. **V.S. Hoelscher**, T.D. Hamilton

CHED **798.** Effects of halide salt hydrates on isomerization of glucose to fructose. **M. Swannell**, C. Yoo, X. Pan

CHED **799.** Plasticizing sulfur with limonene: A functional material synthesized entirely from industrial waste. **M.P. Crockett**, A.M. Evans, J.M. Chalker

CHED **800.** Malonic acid as a green alternative to formaldehyde in cell fixation. **D. Szlosek**, R. Byrnes, P.M. Doherty, D. Finocchietti, D. Currie

CHED **801.** Oxidation of anthracene catalyzed by a recyclable vanadium(IV) oxide complex using hydrogen peroxide in an aqueous biphasic medium. **S.L. Moran**, C.A. Mebi, A. Bhuiyan

CHED **802.** Vacuum distillation via solar irradiation. **L. Nurmomade**, D.J. Swartling

CHED **803.** Further progress with Claisen condensations via solar irradiation. **S.M. Amin**, D.J. Swartling

CHED **804.** Further progress with Fisher esterification via solar irradiation. **C.R. Buckner**, D.J. Swartling

CHED **805.** Preparation of tetraphenylporphyrins via solar irradiation. **T. Pinto**, D.J. Swartling

CHED **806.** Research to develop a more efficient reflux process for methanol capture in biodiesel synthesis by applying green chemistry principles. **P. Kurriss**, E.J. Brush

CHED **807.** Development of green chemistry metrics to assess improvements to the efficiency in the synthesis of biodiesel from waste vegetable oil. **K. Roebuck**, E.J. Brush

CHED **808.** Applying green chemistry principles in the synthesis of oxindole-3-acetic acid: The initial intermediate in the bromination of indole-3-acetic acid to 3-bromoxindole-3-acetic acid. **M. Steadman**, E.J. Brush

CHED **809.** Synthesis of glucosamine-based single chain nonionic and cationic surfactants. **R. Gonzalez**, C. Coss, R. Palos Pacheco, J.E. Pemberton

CHED **810.** Endo/exo thermal isomerization of a green Diels-Alder adduct. **S. MacColl-Garfinkel**, **M.S. Erickson**

CHED **811.** Design of experiments approach to optimize the yield of 1-(4-vinylbenzyl) thymine. **R. Koelln**, **H. Schalck**, **C. Horgan**, **K. Vickey**, N. Chen, J. Pallozzi, K. McDonough, K. Dupuy, N.E. Lee, R.W. Gurney

CHED **812.** Interactions of partially green double reduced gold nanoparticles with lead. **A. Cruz Torres**, R. Noriega Rivera, B. Mercado Toro, E. Medina, E.J. Ferrer Torres, C. Osorio Cantillo, J.I. Ramirez Domenech

CHED **813.** Green synthesis of silver nanoparticles using extracts from *Leucaena leucocephala (Lam.) de Witt.* leaflets. **J. Delgado Irizarry**, **J. Rodriguez Ortiz**, R. Aleno, E. Medina, C. Osorio Cantillo, E. Ferrer Torres, J.I. Ramirez Domenech

CHED **814.** Cross-linking and surface functionalization of polycarbonate films using thiol-ene click chemistry. I. Blythe, Y. Wang, D.J. Darensbourg

CHED **815.** Chloride retention in biomass with the addition of lime and dolomite. **M.W. Smith**, G.P. Chea, T.A. Hoemberg, J.C. Barbour

CHED **816.** Investigation of thiosemicarbazone ligands in "green" palladium catalyzed Suzuki cross-coupling reactions. **J.R. Hall**, B.J. Anderson

CHED **817.** Discovery of a new copper bismuth oxide material for the conversion of sunlight into a solar fuel. L.R. Sharpe, **J.S. Compton**, C. Peterson, D. Dervishogullari

CHED **818.** Mechanochemical synthesis of biologically relevant porphyrin targets. **D. Cordero**, T.D. Hamilton

CHED **819.** Conversion of ethanol to gasoline over zeolite H-ZSM-5 catalyst. **A. Ali**, Z. Wang, S. Adhikari

CHED **820.** Hydrolysis of fungal chitin utilizing ionic liquids as a solvent and catalyst. **J. Gayton**, C.D. Estefan, E.D. Anderson, M. Faralli, W. Reichert

CHED **821.** Investigation of transesterification of canola oil using basic ion exchange resin. **R. Deal**, G.L. Milligan

CHED **822.** Mechanochemical reactions for green chemical synthesis. **E. Hanna**, G.K. Kaufman

CHED **823.** New metric to evaluate sustainability in the undergraduate organic laboratory course. **B. Saunders**, K. McMahon

CHED **824.** Effects of cation structure on the acidity of Brønsted acid ionic liquids: A computational study. **C.D. Estefan**, J.N. Gayton, M. Faralli, E.D. Anderson, W.M. Reichert, E.A. Salter

CHED **825.** Developing and applying new thin film combinatorial techniques for the discovery of new metal oxide semiconductors for the efficient photoelectrolysis of water. **V.A. Kong**, J.G. Rowley

CHED **826.** Development of carbohydrate-based heterogeneous solid acid catalyst for biodiesel production. **M.L. Jordan**, B.S. Chilukuri, B. Jang

Section A

Colorado Convention Center
Halls C/D

Undergraduate Research Posters

Inorganic Chemistry

Cosponsored by INOR and SOCED

N. Di Fabio, *Organizer*

12:00 - 2:00

CHED **827.** Aminebis(phenolate) complexes of palladium as catalysts for the Suzuki-Miyaura coupling reaction. **A.K. Bowser**, B. Wile

CHED **828.** Alternative to detection: Europium(III)-tetracycline species association with biological molecules. **B.G. Vo**, G. Muller

CHED **829.** Triflimide activation of azaferrocene-boranes for hydroboration of simple alkenes. **D.I. Szymanik**, T.J. Brunker

CHED **830.** Liquid sorption studies of Co^{II}-4,4′-bipyridine 1D chains and 2D square grid MOFs. **K.C. Carlson**, C.L. Weeks

CHED **831.** Synthesis and characterization of 1-D ladder crystals grown in methanol. **T.D. Petersen**, N.G. Weissenfluh, C.L. Weeks

CHED **832.** Reaction of copper(II) chloride dihydrate with formamide. **A.G. Nicholson**, G.L. Seebach

CHED **833.** Synthesis and investigation of novel thiosemicarbazone ligands and their metal complexes. **K.A. O'Rourke**, B.J. Anderson

CHED **834.** Synthesis and characterization of a larger neutral macrocycle for transition and lanthanide(III) metal complexes. **A.J. Sprecher**, A.J. Jircitano

CHED **835.** Synthesis, characterization, and electrochemical properties of tris(3-isopropylpyrazolyl)borate nickel complexes. **V. Doll**, N. Piro, W.S. Kassel, W.G. Dougherty

CHED **836.** Synthesis, characterization, and electrochemical properties of tris(3-*tert*-butylpyrazolyl)borate copper complexes. **O. Beale**, N. Piro, W.S. Kassel, W.G. Dougherty

CHED **837.** Synthesis, characterization, and ion-binding studies of $Ru(bpy)_3^{2+}$ macrocycle host complexes. **T. Carroll**, M. Harris

CHED **838.** Complexation reactions of cerium (III) and cerium (IV) salts with amides. **T.L. Amburn**, G.L. Seebach

CHED **839.** Synthesis and characterization of copper-thiosemicarbazone complexes: Interaction with DNA and anti-oxidant behavior. **K.R. Webb**, B.C. Helbert, F.A. Beckford

CHED **840.** Curcuminoids as ligands in zinc and vanadium complexes: Synthesis and biophysical reactivity. **B. Helbert**, S. Smith, K.R. Webb, F.A. Beckford

CHED **841.** New ethylene cross-bridged and side-bridged tetraazamacrocycles featuring acid and amide pendant arms and their transition metal complexes for oxidation catalysis. **M. Gorbet**, **M.B. Allen**, **A.D. Shircliff**, G. Yin, T.J. Hubin

CHED **842.** 1,7-Dimethyl-1,4,7,10-tetraazacyclododecane complexes of Mn, Fe, Co, Ni, Cu, and Zn: Synthesis and characterization. **M.A. Ayala**, **A. Walker**, T.J. Hubin

CHED **843.** Electrochemical stability of ruthenium-arene complexes. **M.T. Piedmonte**, S.M. Young, W.J. Vining

CHED **844.** Ion selective redox chemistry of a rhenium (I) complex using cyclic voltammetry. **N. Rambhujun**, S.M. Young, W.J. Vining

CHED **845.** Synthesis, NMR characterization, and x-ray crystal structure of quinoline-2-carboxaldehyde tert-butyl thiosemicarbazone: The [Pd(QCA-tBTSC) Cl] complex and MIC studies. **J. Chen**, J.D. Conner, N.P. Riggsbee, E.C. Lisic

CHED **846.** Comparison of a series of 2-acetylpyridine-thiosemicarbazone Cu(II) and Pd(II) metal complexes. **B.C. McGill**, R.E. Scott, E.C. Lisic

CHED **847.** Investigating bispyrrolidine based chiral C_2-symmetric tetradentate ligand. **J. Kaplan**, H. Reed, J.M. Keane

CHED **848.** Quantitative determination of silver inhibition of halide accelerated aluminum corrosion. **K.D. Lopez**, **H. Gill**, S.G. Sobel

CHED **849.** Metal – organic assemblies of meso– tetrasubstituted porphyrins. **M. Basden**, M. Knol, T.D. Hamilton

CHED **850.** Iodination and MWI cyanation of *closo*-dodecaborate(2-) and *closo*-1,2-dicarbadodecaborate. **H.R. Midget**, M.A. Juhasz

CHED **851.** Investigations of the halogenation, radiohalogenation, and functionalization of CB9 carborane clusters. **C.R. Vorauer**, M.A. Juhasz, D.S. Wilbur

CHED **852.** Synthesis of new gold-isocyanide and acyclic diaminocarbene complexes for catalysis. **J. Coronado**, A.A. Ruch, V. Nesterov, L.M. Slaughter

CHED **853.** Copper-catalyzed triazole synthesis in the presence of halides. **M.D. Womble**, R.M. Moorman, M.B. Collier, B.H. Frohock, J. Chalker

CHED **854.** Mercury concentration in washed and unwashed leaves of differing plant species. D.W. Lehmpuhl, **K.A. Wager**, L.M. Bartolo

CHED **855.** Designing novel electrodes of 3D porous V2O5:PANI films by colloidal particle lithography. **J.A. Zavala**, C.J. Chalker, A. Parija, H. An, J.L. Lutkenhaus, J.D. Batteas

CHED **856.** Cobalt catalyzed cyclotrimerization of alkynes using a microwave reactor. **J. Legere**, E. Hawrelak

CHED **857.** Modulating the electrochemical properties of iron-carbonyl clusters using thiolate ligands. **A.L. Haley**, L.S. McDaniel, L.N. Broadbent, C.H. Hinkle, S.T. Heckman, J.L. Randall, **S.L. Moran**, **C.A. Mebi**

CHED **858.** Adsorbtion studies and immobilization of metal complexes on supports: Solid-state NMR and catalysis. **J. Benzie**, K.J. Cluff, J. Bluemel

CHED **859.** Chemical pressure effects on $Ga_{2-x}Fe_xO_3$ magnetoelectric ceramic structure. **E. Velasquez**, C. Lefevre, F. Roulland, A. Demchenko, N. Viart

CHED **860.** Synthesis and characterization of a novel hydrozone thiophene ligand. **A. Angeledes**, W.A. Weigand

CHED **861.** Synthesis and magnetic characterization of lanthanide 12-metallacrown-4 complexes. **C. Daly**, C.M. Zaleski

CHED **862.** Corrosion testing of anti-corrosion coatings by Scanning Electrochemical Microscopy (SECM). **C. Lee**, M.C. Calhoun, R.L. Calhoun

CHED **863.** DNA binding studies of [Rh(tacn)(dppz)$(H_2O)]^{3+}$: A new metallointercalator with a modifiable coordination site. **I.M. Williams**, H.L. Hancock, S.C. Haefner

CHED **864.** Speciation of europium(III)-tetracycline species. **A. Huy**, K. Deol, G. Muller

CHED **865.** Toward the development of luminescent metal organic frameworks for use as sensors. **M. Peiffer**, K. Kneas, J.A. Rood

CHED **866.** Interaction of DNA with [Cu(phen)(4-amino-pteridino(6,7-f)phenanthroline)$](PF_6)_2$, a potent DNA cleavage agent. **A. Lopez**, G.H. Rawji

CHED **867.** Investigation of DNA binding and photocleavage properties of [Zn(4-amino-pteridino(6,7-f)phenanthroline)(triflate)$_2$]. **P. Wong**, G.H. Rawji

CHED **868.** Ligand exchange of an enzyme-mimic Schiff-base copper(II) complex: A kinetic study. **S. Colling**, J.J. Stace

CHED **869.** Synthesis of enzyme-mimic copper(II) Schiff-base complexes. **S. Williams**, J.J. Stace

CHED **870.** Synthesis and reactivity of a enzyme-mimic nickel(II) complex. **D.M. Beagan**, J.J. Stace

CHED **871.** Development of sulfhydryl-functionalized silica particles for use in diffusive gradient in thin-films passive samplers. **D. Manley**, A. Pham, H. Hsu-Kim

CHED **872.** Capturing carbon dioxide with metal-organic frameworks. **N. Oostendorp**, E. Maslowsky

CHED **873.** Preparation of SnO_2 substrate for sensitized solar cells. **Q. Yang**, L.A. King, M. Kern, B.A. Parkinson

CHED **874.** Synthesis of novel green inorganic catalysts. **N. Wolford**, E. Rajaseelan, S.A. Roberts

CHED **875.** Studies of cytotoxicity and cellular internalization of small-molecule conjugates of metal oxide nanoparticles in tumor cells. **A. Henry**, P. Promdet, C. Blumenfeld, R.A. Moats, R.H. Grubbs, H.B. Gray, K. Sorasaenee

CHED **876.** Investigating a hybrid organosilyl class of Dawson-Wells polyoxometalates through Langmuir-Blodgett. **J. Perryman**, E.J. Atkinson, R.C. Chambers

CHED **877.** Synthesis of a novel green chemical catalyst. **P. Bekere**, E. Rajaseelan, S.A. Roberts

CHED **878.** Synthesis and catalytic properties of a novel triazole based N-heterocyclic Iridium carbene complex. **E. Dalbey**, S.A. Roberts, E. Rajaseelan

CHED **879.** Characterization of metal dithiocarbamate complexes derived from amino acids. **G. Azzarello**, E. Sylvester

CHED **880.** Corrosion of aluminum by aqueous $CuCl_2$: An SEM-EDS study. **A. Brodovskaya**, S.G. Sobel, G.L. Polak, M. Akhtar

CHED **881.** Microwave-promoted synthesis of heavily iodinated 10- and 12-vertex boron clusters. **G.R. Matheson**, M.A. Juhasz, P.S. Chang

CHED **882.** Novel synthesis and catalytic properties of triazole-based N-heterocyclic carbene complexes of rhodium and iridium. **W.J. Maximuck**, E. Rajaseelan, S.A. Roberts

CHED **883.** Heteroleptic salicylaldiminate magnesium amides: Solid-state and solution characterization. **S.M. Tretter**, A.M. Landis, J.A. Rood

CHED **884.** Synthesis and characterization of ground and excited state properties of a new ruthenium(II) polypyridine complex. **A.T. Vu**, R.N. Garner

CHED **885.** Time-based investigation of the vapochromic response of platinum(II) complexes. **K.A. Mengle**, M. Abdolmaleki, M. Riasi, W.B. Connick

CHED **886.** Synthesis of Co-complexes with pentadentate ligands for catalytic hydrogen evolution. **T. Tall**, M. Vennampalli, M. Zhang, X. Zhao

CHED **887.** Exploration of coordination chemistry with arsenazo III, DTPA and metal complexes using NMR and UV-VIS. **C. Winking**, C. Breaux

CHED **888.** Coordination chemistry of divalent group 12 thiocyanate complexes containing phthalazine. **T.J. Paca**, P.M. Secondo, R. Baughman

CHED **889.** Coordination chemistry of divalent group 12 thiocyanate complexes containing quinazoline. **C. Martello**, P.M. Secondo, R. Baughman

CHED **890.** Coordination chemistry of divalent group 12 thiocyanate complexes containing 2-amino-5-cyanopyridine. **A. Shoroye**, P.M. Secondo, R. Baughman

CHED **891.** Imidazolium salts as reaction media for preparation of metal halide cluster networks. **S.K. Gnewuch**, D.H. Johnston

CHED **892.** Catalytic oxidation of primary alcohols by transition-metal-TRIPHOX complexes. **E. Lamping**, C.M. Davis

CHED **893.** NKU organometallic research: Examining new synthetic strategies that functionalize fullerene and coronene for organometallic supramolecular systems. **C. Beneker**, K.A. Walters

CHED **894.** NKU Spectroscopic Research: Studies on polymers and their subunits that incorporate fullerenes and transition metal chromophores. **S. Siemer**, K.A. Walters

CHED **895.** NKU Polymer Research: Synthesis of polymers and their subunits that incorporate fullerenes and transition metal chromophores. **J. Callihan**, K.A. Walters

CHED **896.** NKU solar cell research: Fullerene-transition metal sensitized solar cells — construction and efficiency studies. **H. Hearn**, K.A. Walters

CHED **897.** NKU organometallic research: Simplified synthetic strategies for fullerene-bipyridine ligands used in organometallic complexes for solar cell dyes. **J. Horn**, K.A. Walters

CHED **898.** Dye inclusion on the {101} face of KDP crystals. **L. Strange**, J.R. Williams

CHED **899.** New N-heterocyclic carbene (NHC) silver fluorides facilitate dihydrogen activation to form a silver hydride cluster where sterically demanding NHC ligands increase stability and rate of hydrogen activation. **J. Nguyen**, B. Tate, J.P. Sadighi

CHED **900.** Synthesis and catalytic activity of tin (IV) halides functionalized with bidentate phosphine ligands. **M. Leverich**, R.W. Hartmann

CHED **901.** Effect of ZnO morphology on the photodegradation of malachite green oxalate. **S.C. Bryant**, K.O. Laughlin, J.D. Harris

CHED **902.** Synthesis, characterization, and reactivity of ruthenium(II) complexes involving *p*-cymene and hexamethylbenzene ligands. **A.D. Riner**, J.P. Lee

CHED **903.** Synthesis and characterization of cyclopentadienyl- and pentamethylcyclopentadienyl-Co(III) mixed sandwich compounds containing either tridentate nitrogen, sulfur, or carbon donor ligands. **T.P. Latendresse**, J.P. Lee

CHED **904.** Electronic properties and composition of $GaAs_{1-x}P_x$ grown by close-spaced vapor transport. **A. Davis**, A. Greenaway, S.W. Boettcher

CHED **905.** Synthesis and characterization of transition metal clusters/polymers supported by pyridylamide ligands. **M. Pauly**, L. Yang

CHED **906.** Synthesis and bacterial activity studies of acetylacetonate metal complexes. **N.P. Riggsbee**, A.L. Koch, A.J. Crook

CHED **907.** Stabilization of catalytic tin species with phosphine ligands. **J.H. Murray**, R.W. Hartmann

CHED **908.** Towards the synthesis of a water-souluble β-brominated cobalt(II) porphyrin. **J. Williams**, K.C. McGill

CHED **909.** Synthesis of a novel water soluble porphyrin-chalcone complex. **R.E. Tucker**, J.C. Bradshaw, J.E. Bradshaw

CHED **910.** Electronic structure and electrochemical elucidation of human serum albumin–heme complex. **G.O. Tomoiaga**, E.M. Luteran, K.S. Kang, R.S. Fogle, M.I. Galinato, J.A. Bennett

CHED **911.** Contrasting the biomimetic reactions of NO_x with Fe (III) porphyrins and Fe (IV) corroles. **S.M. Russo**, S.K. O'Shea

CHED **912.** Synthesis of a nickel(II) chloride chemosensor. **M. Allegrezza**, J. Fautch

CHED **913.** Exchange between Fe(III) and Ni(II) dithiocarbamates in solution. **N.M. Barker**, J. Coffield, N.V. Duffy

CHED **914.** Novel halometallates incorporating 2, 2'-biimidazole. **E.L. Sears**, J.G. Kelley, L. Peterson, Jr., M.D. Smith

CHED **915.** Synthesis and high resolution powder diffraction pattern refinement of novel rare-earth substituted pyrochlores. **J.D. Aldridge**, D.A. Polvani

CHED **916.** Synthesis and characterization of di-2-pyridyl ketone oxime complexes with transition and lanthanide metals. **K. Knopf**, B.L. Westcott

CHED **917.** Synthesis and spectroscopic analysis of spin-crossover cobalt complexes. **H. Zecca**, H. Kim, A.C. Bowman

CHED **918.** N-heterocyclic carbene ligands as supports for Cp*Co(I) fragments. **J.M. Andjaba**, C.A. Bradley

CHED **919.** Developing a copper-catalyzed asymmetric reduction of 2*H*-azirines. **D.K. Yi**, T.J. Mathews, J. Unger

CHED **920.** Investigation of the mechanism of arene perfluoroalkylation by iron perfluoroalkyl reagents. **R.S. Thompson**, J.D. Lawrence

CHED **921.** SNC-Rh(I) pincer complexes bearing thioether and *N*-heterocyclic carbene donors: Catalytic activity in transfer hydrogenation. P.L. Osburn, **T. Grimes**

CHED **922.** Utilization of pyrazole based copper complexes in atom transfer radical addition (ATRA) and atom transfer radical cyclization (ATRC). **E. Perez**, G. Pros, T. Pintauer

CHED **923.** Iminophosphorane reagents for synthesis of electrically diverse diimine and N-heterocyclic carbene ligands. **A.M. Hodge**, C.A. Bradley

CHED **924.** Comparative structural studies of A_2BTeO_6 (A = Ca, Sr, or Ba; B = Ca or Cd) double perovskites. **A. Flores**, H. Albert, A. Stiner, T. Mansur, P. Barnes, A. Fry

CHED **925.** Design, synthesis, and characterization of zinc dithiolato/dithione (donor/acceptor) and vanadium dithione complexes. **S.C. Ratvasky**, M.J. Van Stipdonk, B. Mogesa, P. Basu

CHED **926.** Bis(oxazolinylphenyl)amines complexes. **A.J. Rupprecht**, J.K. Vohs

CHED **927.** Synthesis metal-organic frameworks containing Mn-SALEN active sites and their catalytic properties. **B. Chicoine**, M. Mathews, W. Schumacher, L.G. Beauvais

CHED **928.** Formation of mixed monolayers on TiO_2 and Ti-6Al-4V using carboxylic and phosphonic acids. **A. Dalal**, N.A. Reger, E.S. Gawalt

CHED **929.** Influence of annealing conditions on electrical properties in calcium cobalt oxide misfit layered compounds. **D. Lofdahl**, G. Whinery, C. Heideman

CHED **930.** Synthesis and characterization of symmetric and asymmetric bimetallic ruthenium(II) complexes. **M.T. Mongelli**, **J. Pozo**, P. Menta, L. Zierten

CHED **931.** Modification of MOF-5 hydrostability for peptide adsorption studies. **M. Nivison**, Z. Mensinger

CHED **932.** Investigating aurophilic interactions: Synthesis, structural, and photoluminescent properties of lanthanide cyanometallates containing 1,10-phenanthroline. **J.M. Hendrich**, R. Sykora, J.D. Taylor, F.D. White, K. Xiang

CHED **933.** Functionalization of the *rho*-ZMOF framework with fluorescent probes. **A. Kalbach**, J. Miksovska

CHED **934.** Synthesis and reactions of a tris-(tributylamine)triborate cation. **S. Bertrand**, **C. OKeefe**, G.M. Edvenson

CHED **935.** Reaction of 1-{2-[diphenylboryl] benzyl}-2,2,6,6-tetramethylpiperdine with hydrogen. **K. Gurung**, **T.K. Bader**, G.M. Edvenson

CHED **936.** Synthesis of mononuclear ruthenium complexes containing a tetradentate bipyridine dicarboxylic acid equatorial ligand and two N-heterocyclic carbene axial ligands. **E.E. Kukura**, J.K. Vohs

CHED **937.** Characterizing novel Mg alkoxide compounds as potential precursor electrolytes for next-generation batteries. **C. Nist-Lund**, J. Herb, C.B. Arnold

CHED **938.** Withdrawn.

Section A

Colorado Convention Center
Halls C/D

Undergraduate Research Posters

International Research Experience for Undergraduates

N. Di Fabio, *Organizer*

12:00 - 2:00

CHED **939.** Analysis of selective oligonucleotide release from photothermally active hollow gold nanospheres using surface enhanced Raman scattering. **D.G. Mackanic**, D. Graham, S. Mabbott

CHED **940.** Examining bridged oligothiophenes as small-molecule semiconductors in organic photovoltaic devices. **L.R. Savagian**, N. Findlay, A. Kanibolotsky, P. Skabara

CHED **941.** Synthesis and characterization of CdSe quantum dots via low temperature thermolysis of a single organometallic precursor. **C.M. Gentle**, S. Famiani, L. Tarpani, L. Latterini

CHED **942.** Stabilization of light-harvesting complexes from *Rhodopseudomonas acidophila* in dipeptide gels. **E.K. Reagan**, N. Javid, S.K. Nalluri, R. Ulijn

CHED **943.** S_2O_3 treated cuprous oxide electrochemical reactivity with carbon dioxide. **G. Panetti**, A.D. Handoko, B. Siang Yeo

CHED **944.** Synthesis and characterization of divalent ligands with photoswitching capabilities. **L. Hristov**, A. Senf, S. Hecht

CHED **945.** Optimization of ferroelectric behavior in lead-strontium-titanate (PST) ceramic thin films. **G. Ruehl**, M. Benkler, T. Hanemann

CHED **946.** Synthesis and characterization of light-responsive hybrid polymer thin films. **D. Brauer**, N. Wagner, P. Theato

CHED **947.** Synthesis and exploration of spiropyran-containing poly-(3-hexylthiophene) oligomers. **A. Kim**, M. Schulz, A. Staubitz

CHED **948.** Growth of carboxylated UiO-66 metal-organic framework crystals for CO_2 capture. **S.J. Faucher**, D. Zhao, Z. Hu

CHED **949.** Development of a sustainable and efficient protocol for palladium-catalyzed Sonogashira cross-coupling reactions. **M. McLaughlin**, G. Strappaveccia, M. Gruttadauria, L. Vaccaro

CHED **950.** Investigation of temperature dependent electrochemical CO_2 reduction on copper by gas chromatography including formic acid detection via derivatization. **B. Ferguson**, J. Grote, K. Mayrhofer

CHED **951.** Modification of ultrafiltration membranes for improved purification of nanoparticle dispersions. **T.J. Myers**, M. Ulbricht

CHED **952.** Development in poly-thiophene and poly-benzotriazole block copolymer for use in polymer solar cell. **T. Range**, C. Ping Sen, S. Valiyaveettil

CHED **953.** Experimental studies of shutdown procedures for water-gas shift catalysts in high temperature polymer electrolyte fuel cell systems. **K. Fong**, D. Krekel

CHED **954.** Organoiridium catalyst as a functional mimic of both oxygen evolving complex and hydrogenase. **S. Barnett**

CHED **955.** Threshold implementation and testing in local coupled cluster doubles theory (PNO-LCCD). **J. Ford**, M. Schwilk, H. Werner

Section A

Colorado Convention Center
Halls C/D

Undergraduate Research Posters

Medicinal Chemistry

Cosponsored by MEDI and SOCED

N. Di Fabio, *Organizer*

12:00 - 2:00

CHED **956.** Identification and synthesis of novel cyclin-dependent kinase inhibitors. **N.A. Pham**, P. Tram, T.K. Nguyen, R.L. Schroeder, S. Jennings, T. Vu, H.E. McFerrin, J. Sridhar

‡ *Cooperative Cosponsorship*

CHED **957.** Using isothermal titration calorimetry (ITC), circular dichroism (CD) and DNA unwinding studies to investigate the DNA binding properties of abietane diterpenes natural products. **G.S. Gullickson**, **B.S. Kasper**, R.E. McKnight

CHED **958.** Study of antitumor effects of quercetin and amine or methoxy polysubstituted derivatives on metastatic and non-metastatic mouse cells. **J. Winkelbauer**, D. Rzewnicki, A. Abel, C. Kriley, T. Homan, D. Ray

CHED **959.** Prevention and disruption of bacterial biofilms. **A. Newsham**, D. Warner, R.E. Del Sesto

CHED **960.** Transition metal complex dual CXCR4/CCR5 antagonists. **D.J. Davilla**, D. Schols, S.J. Archibald, T.J. Hubin

CHED **961.** New thiazolecarboxaldehyde thiosemicarbazone ligands: NMR structure studies and complexation with Cu(II) to form [Cu(TZCA-ETSC)Cl] and with Pd(II) to form [Pd(TZCA-ETSC)Cl]. **S.D. Simpson**, J.D. Conner, N.P. Riggsbee, E.C. Lisic

CHED **962.** New 2-acetyl-6-bromopyridine thiosemicarbazone ligands: NMR and complexation with Cu(II) to form [Cu(ABrPy-TSC)Cl] compounds. **T.B. Milligan**, B.C. McGill, L. Hatmaker, E.C. Lisic

CHED **963.** Comparison of a series of 2-acetyl-6-methoxypyridine (AMOPY) thiosemicarbazone metal complexes. **M.K. Monroe**, A.M. Barnes, B.C. McGill, R.E. Scott, E.C. Lisic

CHED **964.** New terpenoids from the Caribbean gorgonian *Pseudopterogorgia acerosa*. **P.D. Scesa**, L.M. West

CHED **965.** Antibacterial activity of 4-alkyl and 4-arylbutenolides. **W. Heartsill**, J. Stevenson, A. Damron, N. Estes II, J.M. Hutchison

CHED **966.** Insulin-specific inhibition of insulin-degrading enzyme using a synthetic receptor. **C. Young**, L. Logsdon, A.R. Urbach

CHED **967.** Manganese-52: cyclotron production and PET/MR imaging. **R. Gross**, A.L. Wooten, B. Lewis, P. Woodard, S. Lapi

CHED **968.** 4-methylimidazole effect on extrinsic tooth discoloration: A computational model of the Maillard reaction. L. Tribe, **M. Yacoub**

CHED **969.** Computational model for tooth discoloration with sunset yellow treated with H_2O_2. **A. Naeem**, L. Tribe

CHED **970.** Synthesis of a highly fluorescent aminopyronin calcium sensor. **A.T. Bayasi**, Z. Woydziak, N. Nayigihugu

CHED **971.** Evaluation of organogel nanoparticles as a means of drug delivery. **C.L. Spartz**, F. Brouillet, J. Garrigues, S. Franceschi, E. Perez

CHED **972.** Progress toward synthesis of photomodulated SIRT1 activators. **T. Scheckelhoff**, C.N. Streu

CHED **973.** Cytotoxicity and cell cycle studies of *trans*-diiodophosphine Pt (II) complexes. **S.M. Dennis**, A. Medrano, A. Alvarez-Valdés, J. Perles, A. Quiroga, T. McGregor Mason

CHED **974.** Identification, synthesis, and biological activity of galloyl nhibitors of human low molecular weight protein tyrosine phosphatase. **S. Klinker**, E.J. McIntee, H.V. Jakubowski

CHED **975.** Progress toward synthesizing transition metal complexes to mimic complex natural products. **N. Smith**, S. Knecht, J.R. Olexa, C.N. Streu

CHED **976.** Selective nitration of Hsp90 by peroxyntrite in the presence of ALS-linked mutant SOD. **J. Titus**, K. Thomas, C.N. Dennys, A.G. Estevez, M.C. Franco

CHED **977.** Antimicrobial effect of improved antibiotics combined with Ni and semi-green Ag nanoparticles in *Klebsiella pneumoniae*. **K. Rodriguez Graciani**, R. Aleno, M.A. Miranda Belandria, **J. Delgado Irizarry**, E. Medina, **L. Diaz**, E.J. Ferrer Torres, J.I. Ramirez Domenech

CHED **978.** Natural product discovery through bioassay methods on *Ilex decidua*. **O. Clem**, M.J. Campbell

CHED **979.** Design and synthesis of a new $mGluR_5$ modulator. **L. Kalfayan**, **D. Kawamba**, K.J. Friedrich

CHED **980.** Investigation of a synthetic approach to new substituted 1,2,3-triazoles. **A. Murdock**, S. Alias, K.J. Friedrich

CHED **981.** Search for an ideal selective estrogen receptor modulator (SERM). **N. Till**, R.G. Yahn, R. LaLonde

CHED **982.** Investigating pancreatic anticancer activity of spiroxin A derivatives. **H. Zhang**, K. Kartub, R. Zhou, A.C. Webb, D. Carrico-Moniz

CHED **983.** Effect of cell culture components on the preferential cytotoxicity of isoprenylated coumarin derivatives. **H. Zhang**, R. Zhou, M. Jun, A. Bacay, A.C. Webb, D. Carrico-Moniz

CHED **984.** Design of tautomerically ambiguous cytosine-based nucleosides as potential anti-HIV agents. **C.A. Elkin**, Z.T. Ford, V.K. Dunlap

CHED **985.** Using rational drug design toward the synthesis of novel flavonoid derivatives as acetylcholinesterase inhibitors for the treatment of Alzheimer's disease. **J. Minnick**, A. Kranzlein, O.M. Newman, C. Mills

CHED **986.** Molecular modeling and docking studies of peptide macrocycles as potent inhibitors of the 20S proteasome. **D.L. Wilson**, M.G. Götz

CHED **987.** Design and synthesis of sphingolipid derivatives. **A. Chatters**, M. Foroozesh, L. Lovings, J. Liu

CHED **988.** Design, synthesis, and evaluation of a novel hydroxamic acid series for treatment of human African trypanosomiasis. **J. Rutledge**, K. Kim, G. Parfenov, A.B. Dounay

CHED **989.** Synthesis of coumarin derivatives as potential inhibitors of human cytochrome P450 enzymes. **P. Pham**, J. Liu, M. Foroozesh, L. Lovings

CHED **990.** Design and synthesis of coumarin propargyl ethers as potential cytochrome P450 inhibitors. **S. Bellow**, J. Liu, L. Lovings, M. Foroozesh

CHED **991.** Design and synthesis of flavone propargyl ethers as potential inhibitors of human cytochrome P450 1A1 and 1A2 enzymes. **L. Mensah**, L. Lovings, J. Liu, M. Foroozesh

CHED **992.** Synthesis of beta-lactam analogs of belactosin A. N.K. Dunlap, **N. Shokur**, J. Byrd, **A.L. Pathiranage**

CHED **993.** Synthesis of new toll-like receptors 2 (TLR2) ligands for pancreatic cancer imaging. **N.M. Haq**, M. Doligalski, A.S. Huynh, J. Vagner, D.L. Morse, M.L. McLaughlin

CHED **994.** Synthesis of novel heterocyclic naphthoquinone imines and evaluation of their biological activity. **A. Delawder**, D. Dopp, K. Liles, S. Elisha, M. Manpadi

CHED **995.** Ketoconazole activates CYP3A4-mediated metabolism of letrozole. **S. Black**, J.M. Chan, J. Harrelson

CHED **996.** Determination of inhibitor specificity for low molecular weight protein tyrosine phosphatase isoforms A and B. **E. Sinner**, H.V. Jakubowski, E.J. McIntee

CHED **997.** Potential antiviral effects of phenazine derivatives on the La Crosse virus. **Z. Carpenter**, C.J. Monceaux

CHED **998.** Quantification of longevity of aminopyronin in *E. coli*. **N. Vita**, A.T. Bayasi, N. Nayigihugu, Z. Woydziak

CHED **999.** Developing controlled-release chloroquine. **K. Davis**, K.E. Rohly

CHED **1000.** Cyclic sulfinimidamides prospective use as non-GAT1 inhibitors. **S. Knudsen**, C.J. Monceaux

CHED **1001.** Synthesis of 2-(2-sulfonamidopheny)lbenzothiazole and 2-(2-sulfonamidophenyl)benzimidazole as potential inhibitors of anthrax lethal factor and other zinc metalloenzymes. M.J. Rouffet, **C. Kay**

CHED **1002.** Triflic acid mediated thiophenyl sulfonylation of arenes and subsequent antimicrobial activity determination of thiophenyl aryl sulfones. **C. Foley**, J.R. Mckee, B. Peethambaran

CHED **1003.** Oxadiazoles as biofilm and bacterial growth inhibitors. **K. Childers**, **A. Weber**, A. Zanella, R.E. Grote

CHED **1004.** Synthesis of multitarget ligands for the treatment of Alzheimer's disease. **V. Anto**, D. Fish

CHED **1005.** Withdrawn.

CHED **1006.** Saccharin and its carbohydrate-conjugate shows promise for isoform selective inhibition of carbonic anhydrase IX: A lead approach to anti-cancer drug development. **J.M. Driscoll**, B.P. Mahon, G.M. Rankin, S. Poulsen, C.T. Supuran, R. McKenna

CHED **1007.** Using essential oils to combat the threat of multidrug resistant bacteria. **Z.T. Rahman**, J. Mack

CHED **1008.** Optimization of thiadiazole small molecule inhibitor of the hippo signaling pathway to reduce pro-EMT cancerous cell growth. **N.A. Werwie**, S. Strellec, A. Rebbaa, R. Lettan

CHED **1009.** Targeting sphingosine kinase 2: Converting highly selective substrates into inhibitors. **R. Dyer**, T.K. Dawson, Y. Kharel, K. Lynch, T.L. Macdonald

CHED **1010.** Novel anticancer drugs on the basis of diversely functionalized N-containing heterocycles. **K. Zingler**, L. Frolova, S. Rogelj

CHED **1011.** Diastereoselectivity in an exhaustive bromination of anthracenyl-isoxazoles. **M.J. Campbell**, M.J. Weaver, N.R. Natale

CHED **1012.** Preparation and photolysis of non-glucosinolates. **E.M. Voigt**, E.H. Pauley, J.R. Mays

Section A

Colorado Convention Center
Halls C/D

Undergraduate Research Posters

Nanochemistry

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N. Di Fabio, *Organizer*

12:00 - 2:00

CHED **1013.** Activity and selectivity of PVP-capped palladium nanocatalysts immobilized on silica microspheres for the hydrogenation of phenol. **J.E. Kauffman**, N.D. Muench, A.L. Marsh

CHED **1014.** Luminescent gold nanoparticles-based fluorescence and dynamic light scattering dual-modality sensor for copper (II) detection. A**.J. Fatino**, C. Zhou

CHED **1015.** Nanostructured metal oxides with tunable Lewis base sites for the conversion of L-α-phosphatidylcholine to biodiesel. **K.I. Tooke**, D.S. Heroux

CHED **1016.** Characterizing the partitioning of hydrophobic solutes into the surfactant bilayer on gold nanorods. **I.M. DiMucci**, L.B. Thompson

CHED **1017.** Investigating the interactions between gold nanoparticles and *L. catebeianus* and *L. sylvaticus*. **L.L. Lee**, L.B. Thompson, P. Fong, K. Andresen

CHED **1018.** Low temperature, size-selective fluorescence spectroscopy of PbSe quantum dots. **I. Corcione**, J. Peterson, W. Stephans, M. Ruggiero

CHED **1019.** Templated gold nanorod arrays for improved plasmonic biosensing. **S.L. Melnyk**, I.R. Bruzas, L.B. Sagle

CHED **1020.** Developing a silica-coated nanovehicle for targeted cancer therapy. **Z. Liao**, N.H. Kolodny, N.T. Flynn, A.C. Webb

CHED **1021.** Synthesis of activated palladium nanoparticles (PdNPs) on carbon microspheres (CMs) for use as a hydrogenation catalyst. **J.P. Pender**, S.E. Sanders, M.R. Dix, P.E. Colavita, K.M. Metz

CHED **1022.** Self assembly and ordering at the nanomaterial liquid crystal interface. **D. Hofmann**, S. Crotty, A. Sharma, Y. Gao, T. Hegmann, E. Hegmann

CHED **1023.** Investigating the integrity of novel nanovehicles for targeting pancreatic cancer. **S.N. Musetti**, A.W. Cheema, N.T. Flynn, A.C. Webb, N.H. Kolodny

CHED **1024.** UV spectrophotometric titration of graphene oxide with ascorbic acid to follow reduced graphene oxide formation. **E. Olson**, G.J. Mancini-Samuelson

CHED **1025.** Nanosized organometallic building block synthesis for the formation of a polyoxometalate-based framework. **M. Lund**, W.A. Neiwert

CHED **1026.** Organic dyes improving the efficiency of dye-sensitized solar cells. **J.L. Gesell**, C. Kelley, S. Geiger, E.A. Nalley

CHED **1027.** Activation and stabilization of electrodeposited p-Cu_2O with underpotentially deposited Ni. **K. DeHority**, G. Clause, A. Fillinger

CHED **1028.** Synthesis of silver gallium sulfide nanoparticles. **M. Kessler**, S. Hughes

CHED **1029.** Tailoring cadmium selenide nanocrystals with mixed ligand systems. **C. Bloom**, A.S. Tysoe, D. Jackson, **J.D. Kehlbeck**, M.E. Hagerman

CHED **1030.** Surfaced enhanced infrared absorption on optimized copper nanostructures. **W.A. Henry**, D.A. Perry

CHED **1031.** Noble metal-TiO_2 and noble metal-ZnO nanocomposites for improved photocatalysis. **J.C. Franco**, P.Z. Ray, R.M. Prevost, M.A. Tarr

CHED **1032.** Comparative interactions of gold and silver nanoparticles and lead in the rates of germination and root elongation of radish plants. **R. Noriega Rivera**, **B. Mercado Toro**, A. Cruz Torres, E. Medina, C. Osorio Cantillo, E. Ferrer Torres, J.I. Ramirez Domenech

CHED **1033.** Functionalization of indole-3-acetic acid with gold nanoparticles synthesized through a double reduction reaction using leaflets' extracts of *Leucaena leucocephala* (Lam.) de Witt. **G. Maldonado Velez**, E. Medina, C. Osorio Cantillo, E. Ferrer Torres, J.I. Ramirez Domenech

CHED **1034.** Synthesis of small, ligand-stabilized copper nanoparticles as building blocks for electroreduction catalysts. **A. DiAscro**, S.L. Young, J.E. Hutchison

CHED **1035.** Probing nanosize-dependent oligomerization by using fluorescence dynamics of fluorescein amyloid beta 1-40 peptides. **C. Catalfamo**, H. Chen, M. Spencer, E. D'Ambrosio, K. Yokoyama

CHED **1036.** Influence of pore size on cobalt loaded mesoporous materials for oxidation catalysis. **E. Murchie**, D.S. Heroux

CHED **1037.** Comparative study of the application of nanostructured materials to fingermarks impressions. **M. Feliciano** Sanchez, Y. Lugo, W.J. Rivera Martinez, E. Medina, J.I. Ramirez Domenech, C. Osorio Cantillo, E.J. Ferrer Torres

CHED **1038.** Comparative study and characterization of MgO, ZnO and CuO nanoparticles using amino acids as capping agents. **A. Lopez**, R. Aleno, M.A. Miranda Belandria, E. Medina, C. Osorio Cantillo, J.I. Ramirez Domenech, E.J. Ferrer Torres

CHED **1039.** Functionalization and characterization of bimetallic silver-gold nanoparticles with antibiotics. **M.A. Miranda Belandria**, M. Feliciano Sanchez, P. Rivera Pomales, E. Medina, J.I. Ramirez Domenech, C. Osorio Cantillo, E.J. Ferrer Torres

CHED **1040.** Preparation of metalloporphyrin nanoparticles. **J. Seidel**, L.K. Lee

CHED **1041.** Synthetic methods of CTS and CZTS nanocrystals. **R.R. Bohling**, **B.J. Gerold**, M.M. Davis, T.M. Pappenfus

CHED **1042.** Thin films of gold nanoparticles: Temporal stability and mechanisms of degradation. **J. Xu**, N.T. Flynn

CHED **1043.** Synthesizing dendrimer-ligand conjugates for peptide mediated cellular delivery systems. **C.R. Pace III**, J. Manono, S.C. Dimaggio

CHED **1044.** Diazonium-derived nitrobenzene layers on nanoporous gold. **C.L. Chevalier**, E.C. Landis

CHED **1045.** Stability of alkane-thiol monolayers on nanoporous gold surfaces. **R.B. Chevalier**, D. Patel, E.C. Landis

CHED **1046.** Zinc oxide and zinc sulfide nanoparticles for DNA detection: Synthesis, functionalization, characterization, and applications. **B. Etz**, S. ORiley, S.M. Basu

CHED **1047.** Nano size, pH, and temperature dependence of interfacial self-assembly of α-synuclein peptide. **L. Morrow**, M. Yuan, K. Chung, K. Yokoyama

CHED **1048.** Solvent interactions in vegetable oil solutions of C_{60} fullerene. **L.D. Bienski**, **R.N. Callahan**, **J.A. Galvan**, **K.A. Morris**, **M. Wirianto**

CHED **1049.** Ambient and UHV STM studies of metal surface restructuring by amino acids. **A.L. Lee**, H.R. Morgan, J.A. Phillips, L.E. Jackson, E.V. Iski

CHED **1050.** Probing the interactions of polyethylene glycol-coated magnetic nanoparticles with human hemoglobin. **J.L. Bowers**, Z. Liu, A. Fazal

CHED **1051.** Solution-processed templated organic semiconductor nanowires. **E. Avery**, A. Haruk, J. Mativetsky

CHED **1052.** Toxic heavy metal removal via a recyclable gold nanoparticle complex. **O. Hull**, R. Huschka

CHED **1053.** Nanostructured polymer lithography for photovoltaic applications. **A.J. Christy**, N.L. McKibben, **J.D. Harris**, D. Estrada, J.S. McNatt

CHED **1054.** Impact of poly(ethylene glycol) molecular weight and degree of conjugation on the thermodynamics of DNA complexation and colloidal stability of polyethylenimine-graft-poly(ethylene glycol) copolymers. **R.J. Smith**, R. Beck, L. Prevette

CHED **1055.** Deposition of gold nanoparticles on silicon via a galvanic displacement using a block copolymer technique. **R. Sronce**, D. Dávila Pineda, C. Hierold

CHED **1056.** Double shell CdSe/ZnSe/ZnS nanoparticle spectral shifts before and after a manganese dopant is introduced. **A.N. Dobracki**, S.J. Gravelle, J.K. Vohs

CHED **1057.** Structural and electronic properties of endohedral and exohedral derivatives of C_{20} and C_{24} fullerenes; TM@C_{20}, TM-C_{20}, TM@C_{24}, and TM-C_{24} (TM = Group 11 & 12 metals): Density-functional theory investigations. **M. Gonzalez**, K.A. Beran

CHED **1058.** Withdrawn.

CHED **1059.** Inkjet-printed multisensor arrays on flexible substrates. **H. Mitchell**, A. Wanekaya

CHED **1060.** Direct growth of alpha-Fe_2O_3 by vapor deposition on stainless steel as anode for Li-ion battery. **D. Phan**, A. Dangerfield, A. Navulla, L. Meda

CHED **1061.** Chemical vapor deposition of cubic NiO nanoplates on stainless steel substrates as anode for lithium-ion battery. **C. Arnold**, A. Navulla, L. Meda

CHED **1062.** Cyclic voltammetry study on the origin of excess capacity on ruthenium oxide. L. Meda, A. Navulla, **L. Douglas**, J. Adkins

CHED **1063.** Synthesis of MnO nanoparticles and their electrochemical properties. **L. Leban III**, M. Jones, A. Navulla, L. Meda

CHED **1064.** Vapor phase synthesis of cubic CoO nanocrystals as anode in lithium ion battery. **B. Tate**, A. Navulla, L. Meda

CHED **1065.** Energetic effects of metal nanoparticle fuel additives on the combustion of ethanol. **C. Potter**, P.W. Barnes

CHED **1066.** Fluorescence quenching in organic and inorganic solutions using gold nanoparticles. **A. King**, H.G. Altmiller

Technical program information known at press time. The official technical program for the 249th ACS National Meeting is available at: www.acs.org/denver2015

CHED **1067.** Cheap and cost effective synthesis of metal (gold, silver)/reduced graphene oxide nanocomposites for antibacterial applications: A comparative study. **S.A. Alazzam**, **E.H. Alsharaeh**

CHED **1068.** Enhanced visible light driven photocatalytic degradation of organic dyes and antibacterial properties of iron oxide/RGO nanocomposites. **M. Alturki**, E.H. Alsharaeh

CHED **1069.** Synthesis, characterization, and antibacterial activity of reduced holey graphene. A.S. Al Saud, **S.A. Alazzam**, E.H. Alsharaeh, Y. Aldawsari

CHED **1070.** Facile synthesis of reduced graphene oxide layer supported cobalt nanoparticles and their antibacterial activity against E. coli. Y. Mussa, **M. Alturki**, E.H. Alsharaeh

CHED **1071.** Tuning the forces between conjugated nanoparticles. **G. Satishchandran**, D. Venkataraman

Section A

Colorado Convention Center

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Undergraduate Research Posters

Organic Chemistry

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N. Di Fabio, *Organizer*

12:00 - 2:00

CHED **1072.** Investigation of the ability of dibenzyl sulfoxide and triphenylphosphine oxide to form cocrystals with carboxylic acids and phenols. **C. Kemppainen**, D. Adsmond

CHED **1073.** Complete synthesis of analogs of a tuberculosis medication, ethambutol, with known intermediates, diethyl ethylmalonate and diethyl phenylmalonate. **K.C. Haney**, D.S. Masterson, D. Rosado

CHED **1074.** Investigation of the ability of sulfisomidine to form cocrystals with carboxylic acids. **S.H. Douglas**, D. Adsmond

CHED **1075.** Synthesis of novel bactericidal aminoglycosides. **A. Elleman**, A. Felten, J. Weibel, P. Pale

CHED **1076.** Palladium-catalyzed coupling of *O*-benzylbenzimidoyl iodides and boronic acids. **B. Sharma Poudel**, **S.K. Ayer**, Z. Li, K.H. Shaughnessy, T.S. Snowden, D.D. Dolliver

CHED **1077.** Palladium-catalyzed Songashira coupling reaction between diaryl telluride and alkyes. **J. Diaz**, J. Jin, S. Zhang, C. Ailneni

CHED **1078.** Investigation of the non-covalent binding between benzo-crown ethers and bis(trifluoromethyl)dibenzylammonium ion. **K.A. Carter**, S.L. Blosser, L. Webber, D. Nguyen, P.A. Bonvallet

CHED **1079.** Tethered quionolide ligands for stereoselective lactide polymerization. **E. Draper**, M. Haaf, Z. Jones

CHED **1080.** Diversifying covalent organic framework designs through nonreversible linkages and non-planar aromatic monomers. **R.L. Snyder**, A. Alsbaiee, X. Zhang, M. Haaf, W. Dichtel

CHED **1081.** Studies on Suzuki and Hiyama coupling of halopyridines with bromoacetates. A.M. Walls, C. Linne, **R.W. Fitch**

CHED **1082.** Design and synthesis of multifunctional peptoid-NSAID conjugates. **B. Auvil**, K.L. Molchany, C. Young, A. Schell, S.C. Young

CHED **1083.** Desilylation and deuterium enrichment of ethynyl substituted pyridines. **B.S. Gelinas**, J.A. Jaye, E.H. Fort

CHED **1084.** Synthesis of 3,4-bis(2-acetoxybenzoyl)-1,2,5-oxadiazole-2-oxide. **S. Aggarwal**, N.M. Wachter

CHED **1085.** Investigating the stereochemistry of 2-pyridinecarboxaldehyde in aldol reactions. **S. Morich**, N.M. Wachter

CHED **1086.** Impact of cyclopentadienone substitution on the activity of (cyclopentadienone)iron tricarbonyl catalysts. **D.J. Ruff**, K.P. Fodale, T.W. Funk

CHED **1087.** Towards the synthesis of a photocleavable linker for GlcNAc-ligated protein purification. **K.R. Mrugalski**, R.I. Meador, T.W. Funk

CHED **1088.** Synthesis of diepoxy- and triepoxy c-ring analogs of triptolide: An antileukemic, male contraceptive and an anti-inflammatory diterpenoid triepoxide. **C. Fussell**, **S. Jiva**, **G.E. Rudd**

CHED **1089.** Synthesis of HIV-1 capsid protein inhibitors based on SAR analysis. **Z. Whitescarver**, J. Brown, T. Jarvis, A.K. Schrock, **M.T. Huggins**, M.F. Summers

CHED **1090.** Factors affecting the product distribution of substitution and elimination reactions: An experiment for an undergraduate organic lab. **K.N. Hipp**, R.V. Macri

CHED **1091.** Synthesis of phthalocyanine photosensitizers for potential use in photodynamic therapy. **E. Baker**, K.P. Schultz

CHED **1092.** Potassium detection using crown ethers. **M. McConville**, K.P. Schultz

CHED **1093.** New methyl-imidazolecarboxaldehyde thiosemicarbazones ligands: NMR structural studies and complexation with Pd^{2+} to form [Pd(MIZCA-TSC)Cl] compounds. **R.E. Scott**, B.C. McGill, N.P. Riggsbee, W.F. Carroll, E.C. Lisic

CHED **1094.** Utility of C2 substituted imidazolium room temperature ionic liquids in basic reaction media. **M.K. Gard**, E.G. Ennis

CHED **1095.** Synthesis of dicalix[4]arenes with methylene-bridge flexible linkers. **R.S. Rabb**, J.L. Fantini

CHED **1096.** Synthesis and reactions of a 2-oxocalix[4]arene. **I.M. Delahunty**, J.L. Fantini

CHED **1097.** Synthesis of calix[4]arenes with a triaryl- or tetraarylalkene group at the 2-position. **N.J. Tran**, J.L. Fantini

CHED **1098.** Synthesis of rhodium(III) azuliporphyrins. **L.M. Stateman**, T.D. Lash

CHED **1099.** Study of the substituent effects on the anti-oxidant potential of anthocyanidins: A computational investigation. **T.L. Seto**, B.W. Gung

CHED **1100.** Mechanistic aspects of the photocatalytic peroxidation of squalene on TiO_2. M.E. Byrd, M.L. Kaak, **J.A. Ganske**

CHED **1101.** Separation of alpha and beta sodium glucoheptonate. **E.M. Lewoczko**

CHED **1102.** Progress toward the synthesis of (S)-curvularin. M.W. Fultz, **T. Slater**

CHED **1103.** Synthesis of capsaicin analogs. **T. Slater**, E. Higginbotham, M.W. Fultz

CHED **1104.** Energies and conformational preferences of perfluoronated ⍰-furanoses. **A.A. Hunt**, J.S. Rhoad

CHED **1105.** Synthesis and purification of aspernigrin A analogs. **L.M. Martin**, **P.G. Roth**, A.M. Reeve

CHED **1106.** Efforts toward synthesis of isoindolinone core of muironolide A. **C.A. Olson**, **B.L. Thompson**, C. Shaner, T.A. Mitchell

CHED **1107.** Sequence-specific, nanomolar peptide recognition via the folding and inclusion of neighboring sidechains in cucurbit[8]uril. **D. Leach**, B. Blaylock, L. Smith, O. Ali, A.R. Urbach

CHED **1108.** On the reaction of strained alkynes with cysteine thiolates. **G.H. Jones**, M.M. Tierney, J. Chalker

CHED **1109.** Synthesis of dimethoxyindole-based eumelanin and indigo analogs. **W. Ryu**, **J.C. Quirke**, **J.M. Belitsky**

CHED **1110.** Investigation of [5+2] oxidopyrylium cycloadditions. **C.R. Zwick**, J.A. Simanis, T.A. Mitchell, J.R. Goodell, C.M. Law

CHED **1111.** Halide inhibition of the copper-catalyzed azide-alkyne cycloaddition: An NMR analysis. **B.H. Frohock**, R.M. Moorman, M.B. Collier, M.D. Womble, J.M. Chalker

CHED **1112.** Exploring the rearranagement of complex benzylic trichloroacetimidates to benzylic trichloroacetamides. **R.J. Gilbert**, A. Adhikari, J.D. Chisholm

CHED **1113.** Quantitative assessment of the effect of reaction variables on racemization of alpha-amino acids during amide bond formation. **A. Ott**, D. Castagna, C. Jamieson, A.J. Watson

CHED **1114.** Prelimanary assesment of volatile organic compounds (VOCs) in indoor parking facilities in the greater Houston area. **R.B. Reed**, S. Tarver, B. Wilson

CHED **1115.** Progress toward the total synthesis of hemerocallisamines. **D. Bruce**, B. Maki

CHED **1116.** Synthesis of antioxidants: Modified arginine derivatives. M. Ohoueu, **M. Perea**, **K. Molinar**, B. Maki

CHED **1117.** Continued efforts toward the total synthesis of solomonamide B. **L. Calvo**, J. Hazlerig, S.C. Butler

CHED **1118.** Utilization of monohalogenated alkyl halides in copper-catalyzed atom transfer radical addition (ATRA) at elevated temperature. **A.B. Jansto**, T. Pintauer

CHED **1119.** Determination of products formed by the photolysis of 2,4,6-trinitrotoluene in seawater. **E.A. Rios**, D.W. OSullivan, D.J. Luning Prak

CHED **1120.** Oximes derivatives from ferrocenyl chalcone as potential antibacterial agents. **N.E. Caldero-Rodriguez**, I. Montes Gonzalez

CHED **1121.** Improving the efficiency of fluorescein diether cytochrome P450 substrates. **A.J. Milto**, **J. Norley**, R.A. Cloyd, L. Wysocki

CHED **1122.** Designing an efficient and practical polarity assay for xanthene dyes. **J.S. Santana**, **J.C. Miller**, L. Wysocki

CHED **1123.** New frontiers in organizing crystals by molecular shape. **M. Schutzbach**, K.A. Wheeler

CHED **1124.** Nucleophilic [4+4] cyclodimerization of cyclopropenylmethanol derivatives to 4,9-disubstituted-2,7-dioxatricyclodecanes. **T. Bennin**, A. Edwards, M.A. Rubin

CHED **1125.** Synthesis of precursors of aromatic diamidines: Bisnitriles and hydroximalimine with ether and amide as linkers. **R. Luciano**, S. Colón, A. Batista

CHED **1126.** Synthesis, characterization, and kinetic application of tris-(2-aminoethyl) amine (TREN) ligand derivatives. **J. Connell**, K.D. Oshin

CHED **1127.** Library synthesis of novel Xanthoglow fluorophores. **J.I. Garcia**, Z. Woydziak

CHED **1128.** S_NAr reactions utilizing iterative decomposition of formamides. **J. Sorrentino**, Z. Woydziak, J.I. Garcia

CHED **1129.** Study of the photodimerization of 4-vinylbenzylthymine and 4-vinylbenzyl trialkyl ammonium chloride using UV-Vis spectrophotometry and gel permeation chromatography. **N. Chen**, N.E. Lee

CHED **1130.** Polymer bound Wittig reaction under solvent free ball milling conditions. **K. Benson**, K. Leahy, J. Mack

CHED **1131.** Investigations of the conjugate hydrocyanation of α,β-unsaturated aldehydes in organic synthesis. **M.A. Hubbuck**, W.P. Serrano, T. Black, N.C. Kallan

CHED **1132.** Synthesis of nonsymmetric ferrocene derivatives from 1,1'-diacetylferrocene. **S. Ramos-de Dios**, I. Montes-Gonzalez, M.R. Otaño

CHED **1133.** Determining the benefits of alternative haircare conditioning practice. **D. Miller**, H. Sklenicka

CHED **1134.** Microwave-enhanced synthesis involving aliphatic alcohols & other compounds. L. Farber, **K. Hess**, **J.M. Wetherell**, **K. Konieczny**

CHED **1135.** Progress toward the synthesis of *N*-methyl improgan. **M.M. Siepsiak**, M.A. Vanalstine-Parris

CHED **1136.** Synthesis and investigation of sila-allyl anions. **C. Duke**, W.R. Winchester

CHED **1137.** Trends observed In solvent studies of 2-ethylhexyl chloroformate. **A. Wilson**, **K. Null**, M.J. D'Souza

CHED **1138.** Kinetics and mechanism of cyclohexyl chloroformate. **L.C. Malinowski**, **C.E. Gross**, M.J. D'Souza

CHED **1139.** Polyphenolic compounds from an acetone extract of *Hypericum pyramidatum*. **E. Fortier**, D.K. Ngo, J. Heneks, R. Force, S. Chen, G.E. Henry

CHED **1140.** Xanthones and a caffeic acid ester from an acetone extract of *Hypericum stragulum*. **S. Chen**, J. Heneks, R. Force, B. Rhodes, G.E. Henry

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CHED **1141.** Flavonoids and stilbenes from an acetone extract of *Hypericum stragulum*. **R. Force**, J. Heneks, S. Chen, B. Rhodes, G.E. Henry

CHED **1142.** Chemical constituents of *Scirpus atrovirens* leaves. **M. Bruer**, J. Kizina, S. Chen, G.E. Henry

CHED **1143.** Synthesis of indole derived fluorine-containing amino acids. **H. Cade**, M.A. Lnu, **M.H. Blocker**

CHED **1144.** Lewis acid-catalyzed decarboxylative addition of keto acid to trifluoromethyl imines. M.A. Lnu, **D. Van Leuven**

CHED **1145.** Use of Langlois' reagent in the synthesis of CF_3-containing bicyclic aromatic compounds. **L.R. Miner**, A.M. Wilson

CHED **1146.** Selective oxazole and thiazole formation from a common intermediate. **B. Sciarra**, A.M. Wilson

CHED **1147.** Methodology for trifluoromethylation. **T. Crandall**, A.M. Wilson

CHED **1148.** Ozonolysis of silyl enol ethers: Synthesis of 3-silyloxy-1,2- and 3-alkyl-3-silyloxy-1,2-dioxolanes. **K. Wilson**, D.P. Soulsby

CHED **1149.** Organic synthesis of novel SSRI analogs. **E.L. Kantor**, B. Jean, R. Lettan, J. Madura

CHED **1150.** Quorum sensing in *P. aeruginosa*: Synthesis of natural derivatives. **M.W. Coon**, E.G. Sega

CHED **1151.** Synthesis and evaluation of symmetrical biphenyltetrols as aggregation inhibitors for Alzheimer's amyloid-β peptide. **S.L. Wicks**, J.K. Logan, J.M. Hanna, R.K. Lammi

CHED **1152.** In search of objective measures of molecular structural similarity. **L. Smith**, **M.S. Erickson**

CHED **1153.** Survey of bracket and crust fungi for the presence of monacolin K and citrinin. **B.A. Clement**, **E. Jeong**, **A. Teh**, **T. Sitorus**, **K.A. Morris**

CHED **1154.** Survey of pesticide presence in local honey compared with migratory bee keepers. **W.L. Nason**, S.A. Waratuke

CHED **1155.** Evaluating the leaching of phthalates and bisphenol A from children's drinking cups. S.A. Waratuke, **N. Monteiro**

CHED **1156.** Comparison of BPA migration levels from polycarbonate food storage containers subjected to detergents, dishwasher, and microwave use. **E.D. Umali**, S.A. Waratuke

CHED **1157.** Antibiotic compounds isolated from fungal endophytes. **K.L. Bair**, S.J. Coval

CHED **1158.** Synthesis of flavanones from 2-hydroxychalcones using 1*H*-1-hydroxy-5-methyl-1,2,3-benziodoxathiole 3,3-dioxide. **J. Rhoads-Lorigan**, M.W. Justik

CHED **1159.** Derivatives of ferulic acid. **A. Feigley**, K.M. Halligan, J.J. Beck

CHED **1160.** Synthetic modifications of hypervalent iodine reagents. **A. Brkic**, M.W. Justik

CHED **1161.** Oxidative-substitution reactions of polyaromatic hydrocarbons with BF_3-activated iodonium ylides of 1*H*-1-hydroxy-5-methyl-1,2,3-benziodoxathiole 3,3-dioxide. **Z. Ekstrom**, M.W. Justik

CHED **1162.** Computational analysis of monomethylated and dimethylated Hückel and Möbius [12]-, [14]-, and [16]annulenes. **S. Luo**, G. Vinnacombe, C. Castro, W.L. Karney

CHED **1163.** Electronic characterization of organic materials. **R. Sechrist**, J.J. Reczek

CHED **1164.** Synthesis of small molecule inhibitors of LOX using BAPN and its derivatives. **N. Oragwam**, **H. Hashim**, D.M. Solano

CHED **1165.** Progress towards *N*-alkylbenzamides as potential antimalarials. **Z. Beggs**, M.J. Campbell

CHED **1166.** Preparation of trifluoromethylated vanillins for preparation of new curcumins. **J. Brown**, M.J. Campbell

CHED **1167.** Environmentally conscious one pot synthesis of isoxazolines in aqueous media. **S.E. Lewis**, **T.K. Carcamo**, **A. Avina**, D.M. Solano

CHED **1168.** Reduction of nitrobenzene derivatives using crystalline polymorphs of cobalt(II) sulfide and sodium borohydride. **L. Ramirez**, J. Gutierrez-Gonzales, J.G. Parsons, N. Izquierdo

CHED **1169.** Preparation and NMR studies of 2-benzoyl-1-naphthols. **M. Mifflin**, D.J. Crouse, T. Mathis

CHED **1170.** General route to *C*-nucleosides. **J. Sheena**, A. Washington, K.J. Friedrich

CHED **1171.** Synthesis and purification of cyclohexylphosphoserine for application as a potential phosphatidylserine analog. **T.A. Scott**, J.C. Amburgey-Peters

CHED **1172.** Formation of a protected carbobenzyloxy-L-serine-benzyl ester cyclohexyl H-phosphonate diester towards the synthesis of cyclohexylphosphoserine as a potential phosphatidylserine analog. **J.W. Polster**, J.C. Amburgey-Peters

CHED **1173.** Synthesis of a potential phosphatidylserine analog: Cyclohexyldiphosphoserine. **K.W. Murray**, J.C. Amburgey-Peters

CHED **1174.** Extraction of *N*-methylcytisine from *Caulophyllum thalictroides* (blue cohosh). **L. Sluis**, M.P. Maddox

CHED **1175.** Synthesis of homoleptic bismuth(III) sulfurylimide complexes. **D. Gingerich**, R. LaLonde

CHED **1176.** Rapid synthesis of *N*-(4-chlorobenzyl)-*N*-methylformamide. **K. O'Keefe**, M. Bobylev

CHED **1177.** TPEN and TPEN* ligands and ATRA in polar aprotic solvent system. **E. Gorse**, A. Kaur, G. Pros, T. Pintauer

CHED **1178.** Microwave promoted synthesis of diethyl phenylmalonate. **H. Meer**, **K.A. Moon**, C.C. Marvin

CHED **1179.** Synthesis of tetrabenazine via visible light photoredox catalysis. **L.R. Orgren**, E.E. Maverick, C.C. Marvin

CHED **1180.** Withdrawn.

CHED **1181.** Microwave promoted malonate arylation: Regioselectivity. **J.B. Pierce**, C.C. Marvin

CHED **1182.** "Click" synthesis of triazole-based cefotaxime derivatives. **N. Swope**, S.A. Brouet

CHED **1183.** Acetamide as a solvent in the rapid synthesis of *N*-(2,4-dichlorobenzyl) formamide. M.A. Falkenberg, **J.A. Collins**, L.I. Bobyleva, M.M. Bobylev

CHED **1184.** Rapid synthesis of *N*,*N*-dipiperonylformamide. **M.A. Bell**, N.L. Gillis, L.I. Bobyleva, M.M. Bobylev

CHED **1185.** Rapid synthesis of *N*,*N*,*N*-tri-(4-*t*-butylbenzyl)amine. **S. Park**, L.I. Bobyleva, M.M. Bobylev

CHED **1186.** Rapid synthesis of *N*,*N*,*N*-tri-(1-naphthylmethyl)amine. **H. Lee**, L.I. Bobyleva, M.M. Bobylev

CHED **1187.** Rapid synthesis of *N*,*N'*-(4-chlorobenzylidene)-bis-formamide. **S.W. Olson**, M.M. Bobylev

CHED **1188.** Synthesis of 1,1'-ferrocenyl chalcones derivatives as potential biological active compounds. **I. Lehman-Andino**, I. Montes Gonzalez

CHED **1189.** Synthetic approach toward attaching a pyridine based cation receptor to solid support. **M. Mills**, S.G. Tajc

CHED **1190.** Diastereoselective dipolar cycloadditions for the synthesis of pyrazoline and pyrazolidine pharmacophores. **E.F. Dohmeier**, A. Beebe, D.C. Seaman, C.A. Castro, G. Moura-Letts

CHED **1191.** Blue copper protein models: Characterization of copper (I/II) complexes of the N^2S_2 macrocycle 1,8-dithia-4,11-diazacyclotetradecane and derivatives. **J. Ziebiec**, I. Taschner, T.L. Walker

CHED **1192.** Mass scale-up of pyrazolidinones and *N*-alkylation tests. **K.M. Jensen**, C.P. Jasperse

CHED **1193.** Palladium cross-coupling reactions enhanced with aromatic co-catalysts. **A. Sterdjevich**, J.J. Reczek

CHED **1194.** Hydrodehalogenation of aryl halides using sodium borohydride. **A. Mayhugh**, D.B. Cordes

CHED **1195.** Preparation of a simple acetylenic poly(aryl ether). **B. Montz**, T.W. Nalli

CHED **1196.** Synthesis and characterization of novel boron cluster carboxylic acids. **G.E. Dwulet**, M.A. Juhasz

CHED **1197.** Liquid-liquid extraction and analysis of the antioxidant, resveratrol, from various red and white wines. F.C. Mayville, **N.E. Brandstetter**, **D.L. Mandracchia**

CHED **1198.** Soxhlet extraction and analysis of capsaicin from various pepper flesh. F.C. Mayville, **L.N. Amiano**, **C.P. Sulpizio**

CHED **1199.** Electrophilic aromatic substitution reactions with naphthalene and guaiazulene using ionic liquids. F.C. Mayville, **J. Park**, C.P. Saboe

CHED **1200.** Synthesis of four putrescine analogs using 95% and 100% ethanol. F.C. Mayville, **A.L. Cosentino**, R.J. Fischer, C.J. McCarthy, **H.C. Santos**

CHED **1201.** Synthesis of five spermidine analogs using 95% and 100% ethanol. F.C. Mayville, **N.S. Carvis**, **D.J. McGouldrick**

CHED **1202.** 4,4'- Bis(bromomethyl) diphenyl ether as a monomer for a new poly(arylene) ether. **J. Schultz**, T.W. Nalli

CHED **1203.** Hydrogenation using palladium nanoparticle catalysts: Functional group survey. **P.L. Ankney**, **C.L. Hathaway**, C.E. Harris

CHED **1204.** Synthesis of symmetrical biphenyls using phenylboronic acids and manganese(III) acetylacetonate. **N.J. Webster**, **A.M. Lelle**, **C. Ybarra Garcia**, C.E. Harris

CHED **1205.** Drug delivery systems utilizing modified nucleobase hydrogelators and polyamines: Synthesis of polyamines. **D. Benson**, D. Johnson, C.M. Lawrence

CHED **1206.** Utilization of nucleobase interactions to develop supramolecular polymer hybrids. **M. Porter**, G. Gilyot, C.M. Lawrence

CHED **1207.** Drug delivery systems utilizing modified nucleobase hydrogelators and polyamines: Synthesis of modified nucleobases. **D. Johnson**, D. Benson, C.M. Lawrence

CHED **1208.** Multiple methods for analysis of organic materials using the GC/MS. **T.L. Beck**, B.J. Karels, T.M. Pappenfus

CHED **1209.** Diastereoselective dipolar cycloaddtions for the synthesis of imidazoline and imidazolidine pharmacophores. **A. Beebe**, E.F. Dohmeier, D.C. Seaman, C.A. Castro, G. Moura-Letts

CHED **1210.** Synthesis of hydrazide heterocycle for development as an organocatalyst. **S.A. Brouet**, A. Warhausen, T.F. McMillan

CHED **1211.** Investigating the stereoselectivity of magnesium Oppenauer oxidations. **C.M. Webb**, K.J. Brown

CHED **1212.** Natural fiber welded chitin composites. **E. Brown**, M. Brusoski, E. Fox, C. Sweet, H.C. De Long, P.C. Trulove

CHED **1213.** Production of methyl-ester (biodiesel) using oleic acid and methanol and lipase B *Candida antarctica*. **J. Sekhon**, R.W. Hartmann

CHED **1214.** Stereoselective synthesis of fluorinated β-lactams. **A. Knulty**, J.C. Easdon

CHED **1215.** Synthesis, characterization, and phototoxicity studies of paraben derivatives. **K. Becker**, S. Merrill, C. Janson, A. Schaeffer, I. Hildebrandt, K. Pate, K.S. George Parsons

CHED **1216.** Progress toward the synthesis of fluorinated antimalarial analogs. **J. Roos**, H.E. Vaghoo

CHED **1217.** Synthesis of the benztropine derivative as a precursor of fluorescence labeled analogs to be used in dopamine transporter binding affinity assays. **W. Liang**, S. Xie

CHED **1218.** Synthesis of molecular electronic components for self-assembly onto metal electrodes. **K.S. Williams**, J.E. Meany, S. Woski

CHED **1219.** Thiosemicarbazone-derivatives from ferrocenyl chalcones as potential antibacterial and antimalarial agents. **A. Molina-Villarino**, I. Montes

CHED **1220.** Synthesis of (2-fluorophenyl) methanol followed by an investigation of hydrogen bonding via ^{1}H-NMR. **Y.V. Tsai**, .L. Johnson, R.N. Ferrill, R.E. Rosenberg

CHED **1221.** Synthesis of novel GLP-1 stimulants. **O. Zamulko**, **A.M. Heuer**, **D. Hinckley**, J.D. Goodwin, J.T. Ippoliti

CHED **1222.** Synthetic investigation of Diels Alder reactions with α-β unsaturated ketones. **L. Soong**, K. Cetto Bales

CHED **1223.** Synthesis and characterization of new oxadiazole-containing compounds. **M. Packard**, J.L. Crane

CHED **1224.** Synthesis of a novel blue light-emitter for use in organic light emitting diodes (OLED's). **M. Benda**, C. Pharr

CHED **1225.** Synthesis of fluorescent bisimidazole sensors for heavy metals. **S. Ansteatt**, B.N. Norris

CHED **1226.** Synthesis of an alkyne-containing isoprenoid mimic for the investigation of the role of substrate length on prenyl transferase activity. **K. Caron**, J. Wollack

CHED **1227.** Formylation of substituted phenols using mlcrowave irradiation. **E. Young**, V.P. McCaffrey

CHED **1228.** Progress towards the synthesis of a norbornene containing substrate for the enzyme protein farnesyltransferase. **L. Crepeau**, K. Caron, J. Wollack

CHED **1229.** DNA binding affinity and cleavage of aryl sulfoxides. **H. Rensch**, **A. Hurley Predecki**

CHED **1230.** Transesterification of hypophosphorous esters: The tales of secondary alcohols. **A.V. Carmona**, A.C. De La Cruz, S. Deprele

CHED **1231.** Polymeric melamine-metal catalysts in Suzuki-Miyaura couplings and azide-alkyne cycloadditions. **M.A. Trafford**, G.A. Edwards, J.M. Chalker

CHED **1232.** 1H NMR analysis of the methylation of acetic acid catalyzed by tin (II) bromide: A kinetic study. **N.L. Bayona**, R.W. Hartmann

CHED **1233.** Synthesis of biphenyl urea derivatives related to 3-iodothyronamine. **A.S. Niyibizi**, A. Snyder, M.E. Hart

CHED **1234.** Asymmetric design and synthetic studies of monoterpene indole alkaloid analogs. **S.L. Pilicer**, E.K. Leggans

CHED **1235.** Reaction of *O*-silylated cyanohydrins with epoxides as an alternative for the enantio- and diastereoselective preparation of aldols. **D.R. Melendez**, A.M. Hartel

CHED **1236.** Synthesis of enaminones using copper as a catalyst. **E. Lopez Quiroz**, S.R. Hussaini

CHED **1237.** Diversity oriented synthesis of an alkaloid-like library via cyclotrimerization of easily accessible aminonitriles. N.M. Chang, **A. Bates**, J.A. Santos, C.W. Livesey, G.J. Haun, C.B. Stein, N.A. Lopez, G. Moura-Letts

CHED **1238.** Cross-coupling reactions of fluorinated aryl chlorides and aryl chloride acetals with 1-hexylmagnesium bromide. **G. Carmassi**, K.J. Brown

CHED **1239.** Synthesis of highly substituted anthraquinone derivatives via microwave assisted self-condensation of benzoic acids. **L. Holokai**, J.J. Reczek

CHED **1240.** GC-MS analysis of phytosterol content of dried mushrooms. **A.M. Overgard**, T.W. Nalli

CHED **1241.** Preparation of functionalized dendrimers and their effectiveness in organocatalytic reactions. **A.R. Flynn**, **A. Kopp**, N. Brown, T.N. Jones, M. Cloninger

CHED **1242.** Direct esterification of H_3PO_2: A Dean Stark methodology. **J.N. Sanchez**, **A.M. Castillo**, S. Deprele

CHED **1243.** Synthesis of α -chalcones and derivatives via a microwave Knoevenagel condensation. **A.A. Bayly**, M.J. Pesch, A. Gogos, B.C. Weideman, S.R. Sieck

CHED **1244.** Diversification of thiol phosphonamidates. **J.L. Fulton**, K.R. Sittig, M.A. Hardy, S.R. Sieck

CHED **1245.** Characterization of α-substituted chalcones. **B.C. Weideman**, P. Leger, S.R. Sieck

CHED **1246.** Purposeful biofilm disassembly with unnatural alkyl and aromatic D-amino acids. **K. March**, M.A. Bertucci

CHED **1247.** Manipulation of n to π* orbital interactions in the hydrolysis of *para*-substituted *N*-acyl homoserine lactones. **S.R. Dunbar**, M.A. Bertucci

CHED **1248.** Intramolecular oxazolium salt/azomethine ylide cycloaddition reactions with varying dipolarophile tether position. **S.L. Wolfe**, D.L. Warner

CHED **1249.** Microwave accelerated deprotections of aryl silyl ethers. **A. Boyington**, R.D. Crouch

CHED **1250.** Look at biodiesel produced using *Chlorella vulgaris* microalgae. **M. Centore**, D. Fish

CHED **1251.** Structural elucidation of pyrrolizidine alkaloids from *Arnoglossum plantagineum*. **E.L. Feldkamp**, **K. Chattin**, **R.R. Christensen**, R.B. Kelley

CHED **1252.** Studies on "under air" direct arylation. **L. Armstrong**, J. Fritz, T. Murray

CHED **1254.** Reactions of the highly pyramidalized alkene pentacyclo[4.3.0.0^{2,4}.0^{3,8}.0^{5,7}]non-4-ene. M.A. Forman, **C. Adams**, **A. Savarese**

CHED **1255.** Studies toward the synthesis of altersolanol P. M. Hensinger, A. Smaligo, **S.M. Kennedy**

CHED **1256.** Studies toward the synthesis of Hunanamycin A and its derivatives. **S.M. Kennedy**, J. Dreer

CHED **1257.** Microwave synthesis and cytotoxicity studies of novel amino-substituted chalcones. **J.C. Bradshaw**, R.E. Tucker, J.E. Bradshaw

CHED **1258.** Synthesis and characterization of a reversible carceplex. **K. Nogales**, D. Nogales

CHED **1259.** Construction of the Choi framework. **S. Wytovich**, J. Tropp, M.S. Leonard

CHED **1260.** Progress towards the synthesis of 2-amino-1,3-dihydroxyphosphonates via oxazolidinone phosphonates. **B.A. Gibson**, **S.M. Hurrle**, K.J. Graham, T.N. Jones

CHED **1261.** Progress on the synthesis of a fluorescent lead(II)–trapping coumarocryptand. **J. Wilson**, M.R. Baar

CHED **1262.** Antiaromatic dications containing sulfur: Dications of sulfur analogues of tetrabenzo[5.5]fulvalene. **W. Mobley**, N.S. Mills, V. Romano

CHED **1263.** Relationship between delocalization and antiaromaticity in 5,5'-bisindenylidene dications. **P. Poliak**, C. McKay, N.S. Mills

CHED **1264.** Exploring and optimizing new palladium-catalyzed reactions. **R.T. Dove**, W.E. Brenzovich

CHED **1265.** Optimizing the purification of diarylacetic acid derivatives. **A. Denton**, W.E. Brenzovich

CHED **1266.** Synthesis and characterization of curcumin ferrocenyl analogs. **J. Rivera Hernandez**, M.R. Otaño, I. Montes, R. Gutiérrez, Y. Rivera-Tores, D.J. Sanabria Rios, E.E. Colón Lorenzo, A.E. Serrano Brizuela, M.D. García Maldonado, A.R. Guadalupe Quiñones

CHED **1267.** Factors affecting aggregation of beta-sheets. **B.R. Linton**, E.R. Kuhn

CHED **1268.** Hydrogen bonding principles and synthetic beta-sheet mimics. **E.J. Schneider**, B. Linton

CHED **1269.** Benzylideneanilines and benzonitrile oxides: Solid-state structure and reactivity studies. **K. Kassekert**, W.H. Ojala

Technical program information known at press time. The official technical program for the 249th ACS National Meeting is available at: www.acs.org/denver2015

CHED **1270.** Effects of molecular structure on crystal structure and solid-state reactivity of some nitrogenous organic compounds. **K. Van Auken**, W.H. Ojala

CHED **1271.** Solid-state structures and reactivity of some nitrogen-containing organic compounds. **B. Vickerman**, W.H. Ojala

CHED **1272.** Structures and reactivity of some nitrogenous organic solids. **J. Dhami**, W.H. Ojala

CHED **1273.** Synthesis of aziridinomitosene anticancer analogs that vary at the C6/C7 positions. **S. Irving**, R. Olsen, R. Reeves, D.L. Warner

CHED **1274.** Developing a synthesis of α-diazoamides. **L. Terrab**, S. Moss, J. Unger

CHED **1275.** Transition metal-catalyzed coupling of organic sulfonates and metal azides. **F. Xu**, R. Rowlands, J. Unger

CHED **1276.** Studies toward total synthesis of axinelloside A and its analogs. Z.**A. Rumlow**, L. Wiles, M. Walczak

CHED **1277.** Synthesis of core-substituted naphthalene diimide derivatives. **L. Abocado**, J.J. Reczek

CHED **1278.** Surface orientation analysis of naphthalene diimides using infrared spectroscopy. **R. Antonio**, J. Reczeck

CHED **1279.** Investigations of green and microscale methods in the synthesis of several flavones. **P. Martinez**, M. Davis, N. Gammons, P. Powers

CHED **1280.** Computational study on the high temperature isomerization of phenanthrene. B. Fregoso, C. Castro, W.L. Karney

CHED **1281.** Antibacterial activity of cefotaxime and terpenes. **E. Haiderer**, E. Campau

CHED **1282.** Analysis of porphyrin doped thiophene nanoparticles as potential water oxidizing catalysts. **R. Bogdan**, W.M. Ames

CHED **1283.** Stabilized copper(I) N,S containing cryptands. **V. Keehn**, I. Taschner, T.L. Walker

CHED **1284.** Adapting a conventional synthesis of dihydrotetrazines to microwave conditions. **C. Bethea**, M. Druelinger, D.L. Dillon

CHED **1285.** Energy decomposition analysis to predict the explicit solvent shell in the keto-enol tautomerism of acetylacetone in water, acetone, and chloroform. V. Deturi, **C.C. Jenkins**, **T. Reeves**

CHED **1286.** Synthesis, characterization, and analysis of diarylidenylpiperidone analogs of curcumin. **Z. Ligus**, D. Fish

CHED **1287.** Effect of aromaticity on the stability of isonitriles prepared from the deprotonation/metalation of oxazolic species. **W. Howitz**, R.S. Majerle

CHED **1288.** Synthesis of β-fluoroamines from alkenes. **J.M. Mutz**, M.L. Druelinger

CHED **1289.** Synthesis and characterization of potential polyol antifreeze coatings on glass substrates. **D. Vandemark**, E. McGurk, J. Hall, P.W. Baures

CHED **1290.** Analogs for blue copper protein: Thio-pendant arm derivative of 9[ane]S_2N. **K. Tomczak**, I. Taschner, T.L. Walker

CHED **1291.** Role of acetic acid in kinetic isotope effects observed in Pd(I/Pr)$(OAc)_2(H_2O)$ catalyzed oxidation of alcohols. **B. Lampkin**, J.A. Mueller

CHED **1292.** Investigation of the role of Hagemann's ester as a catalyst for natural product synthesis. M. Samoriski, **D. Fish**

CHED **1293.** Synthesis of symmetric and asymmetric porphyrins. **C.L. Carter**, E.M. Mitchell

CHED **1294.** Synthesis and properties of donor-pi-acceptor polyene dyes with azacycloalkane donors. **G.R. Ashley**, D.J. Keith, C.O. Adereti, H.O. Bradley, A.C. Friedli

CHED **1295.** Synthesis of secondary amines. **A. Westlie**, J.T. Ippoliti

CHED **1296.** Template-catalyzed polymerization of modified DNA nucleosides. **A. Cragoe**, M.P. Maddox

CHED **1297.** Synthesis and experimental and computational analysis of curcumin derivatives and their difluoroboron complexes. **K. Paavola**, R. Ciochina, K.E. Johnson

CHED **1298.** Concerted nature of isocyanate reactions with alkenes. **K. Alexander**, C.J. Licata, R.D. Robinson, D.F. Shellhamer

CHED **1299.** Cu(I)-complexes as photoredox catalysts: An alternative to $Ru(bpy)_3^{2+}$. **M.S. Maple**, D. Hockersmith, T. Peelen

CHED **1300.** Synthesis and analysis of a series of *N*-acetyl D-glucosamine derivatives as organogelators. **K. Mays**, A. Chen, G. Wang

CHED **1301.** Synthesis and characterization of glucose triazole derivatives as organogelators. **H. Mangunuru**, D. Liu, A. Espiritu, G. Wang

CHED **1302.** Self-healing polymers: Studies of the Diels-Alder reaction between furan and *N*-4-fluorophenylmaleimide. **T.A. Wells**, W.G. Hollis, P.A. Deck, J.B. Stegall

CHED **1303.** Self-healing polymers: Synthesis of highly-fluorinated dienes and their model Diels-Alder reactions. **D.E. Layo**, W.G. Hollis, P.A. Deck, J.B. Stegall

CHED **1304.** Synthesis of resveratrol. **B.L. Bradley**, G.L. Milligan

CHED **1305.** Synthesis of 5- and 6-(4-fluorophenyl)-*N*-acetylglyoxylamides. **N. Ngo**, A. Umhire-Juru, S. Hernandez, L. Desrochers, N. Kumar, D. Black, T.E. Goodwin

CHED **1306.** Synthesis of 5- and 6-(4-methoxyphenyl)-*N*-acetylglyoxylamides. **A. Umuhire-Juru**, S. Hernandez, L. Desrochers, N. Kumar, D. Black, T.E. Goodwin

CHED **1307.** Synthesis of aspartame *N*-acetylglyoxylamides: A sweet reaction. **S. Hernandez**, A. Umhire-Juru, L. Desrochers, N. Kumar, D. Black, T.E. Goodwin

CHED **1308.** Green synthesis of spiropyrrolizidines from isatin, proline, and *E*-4-phenylbut-3-en-2-ones. **J. Murdock**, L. Desrochers, T.E. Goodwin

CHED **1309.** Enantioselective synthesis and characterization of phase 1 warfarin metabolites. **R. Nshimiyimana**, L. Desrochers, G.P. Miller, T.E. Goodwin

CHED **1310.** Synthesis of 5- and 6-(4-trifluoromethylphenyl)-*N*-acetylglyoxylamides. **F. Musariri**, A. Umhire-Juru, S. Hernandez, L. Desrochers, N. Kumar, D. Black, T.E. Goodwin

CHED **1311.** Salt formation of potential acetylcholine esterase inhibitors. **S. Hickmann**, L.P. Dennis, T.L. Greiman, T.K. Nguyen, D.M. Sikazwe, B.F. Wood, **J.M. Davis**

CHED **1312.** Design and synthesis of potential acetylcholine esterase inhibitors. **L.P. Dennis**, K.N. Gorena, S. Hickmann, T.K. Nguyen, G.L. Tristyn, D. Hernandez, D.M. Sikazwe, B.F. Wood, **J.M. Davis**

CHED **1313.** Preliminary testing of *N*-benzyl isonipecotate derivatives as a potential acetylcholine esterase inhibitors. **T.K. Nguyen**, L.P. Dennis, T.L. Greiman, S. Hickmann, V.G. Martinez-Acosta, D.M. Sikazwe, B.F. Wood, **J.M. Davis**

CHED **1314.** Molecular docking of isoform-selective histone deacetylase 2 (HDAC2) inhibitors. **N. Brusman**, **E.M. Hogle**, R. Kline, E.J. Merino, S.F. Paula, L. Ma

CHED **1315.** Kinetic control mechanism: 1,2 vs. 1,4 addition in conjugated dienes. **J. Painter**, D.J. Oostendorp

CHED **1316.** Use of dimethoxymethane in place of chloromethyl methyl ether to prepare methoxymethyl (MOM) esters. **N. Meckes**, G.L. Milligan

CHED **1317.** Isonitrile ligands in iron-catalyzed Kumada couplings of N-aryl chloride. **K.C. Dornhofer**, M.C. Perry

CHED **1318.** Role of dialkylmagnesium species in the cobalt-catalyzed Kumada coupling of aryl bromides. **J.M. Myles**, M.C. Perry

CHED **1319.** Synthsis of NHC ligands for use in iron- and cobalt-catalyzed cross-coupling reactions. **J.A. Montemurro**, M.C. Perry

CHED **1320.** Synthesis of (-)-duryne and homologues. M. Keener, D.B. Ball

CHED **1321.** Microwave synthesis of *N*-phenyl succinimides and malenamides in undergruate organic chemistry laboratory. T.F. Guetzloff, B. Dudding, **M. Guetzloff**, M.W. Fultz

CHED **1322.** Synthesis and characterization of furan-based ligands for use in lactide polymerization. **B. Kasting**, A. Anderson-Wile

CHED **1323.** Withdrawn.

CHED **1324.** Caged phosphates in organic molecules. **A. Dame**, B.R. Sculimbrene

CHED **1325.** Catalytic asymmetric monophosphorylation of diols. **M. Lougee**, B.R. Sculimbrene

CHED **1326.** Synthesis of an amine-containing cyclooctyne via an intramolecular Nicholas reaction and subsequent dipolar cycloaddition with benzyl azide. **S. Huang**, G. Ortiz, K.M. Shea

CHED **1327.** Evaluation of copper photocatalysts in the enantioselective α-alkylation of aldehydes. **M.R. Hurst**, C.L. Kotelman, K.H. Jensen

CHED **1328.** γ-Cyclodextrin mediated photoheterodimerization between cinnamic acids and coumarins. **A. Clements**, M. Pattabiraman

CHED **1329.** Probing the effects of conformation on concerted proton-electron transfer. **M. Vettleson**, I. Rhile

CHED **1330.** Characterizing the excited states of multiple carbene and nitrene reactive intermediate precursors: A computational study. **V.E. Pane**, S. Vyas

CHED **1331.** Complex decalin formation through the use of an asymmetric Rauhut-Currier reaction. **A. Friant**, W.P. Malachowski

CHED **1332.** Development of π-stacking compounds for stationary phase modification. **T.G. Trimble**, G. Lohani, B.A. Logue, K.H. Jensen

CHED **1333.** Synthesis of polymers for organic light emitting diodes. **A. Place-Burtner**, **A. Ephron**, **A. Schroeder**, **D. Speed**, **J. Mimms**, **N. Jackson**, A.K. Schrock, M.T. Huggins

CHED **1334.** Synthesis and recrystallization of diapocynin and its derivatives. **C.R. DeClerck**, **B.L. Coffaro**, **D.K. Johnson**

CHED **1335.** Gold catalyzed cross-coupling using arenediazonium salt as the oxidant. **E.Y. Aguilera**, X. Shi

CHED **1336.** Exploration of long chain dialdehydes for use as linkers in catalytic metallodiporphyrins. **C.E. Gehman**, W.M. Ames

CHED **1337.** Structural changes induced by 8-Oxo-7,8-dihydroadenosine in RNA oligonucleotides may result in loss of function of RNA aptamers. **A. Chauca-Diaz**, Y.J. Choi, M. Resendiz

CHED **1338.** Biological degradation of acetaldehyde in marine waters. **M.K. Senstad**, W.J. De Bruyn, C.D. Clark, S. Hok, O. Barashy

CHED **1339.** Reverse anomeric effect-mediated synthesis of carbohydrate 1,2-orthoesters. **M.J. Obrinske**, W. Du

CHED **1340.** Solvent-free synthesis of biologically active stilbene derivatives. **J.L. Dickson**, S.A. Angel

CHED **1341.** Synthesis of 2,5-disubstituted 3-fluorothiophenes from 2-thienyl carbamates via a directed fluorination/cross-coupling approach. **N. Onuska**, J. Zhang, A.J. Seed, P. Sampson

CHED **1342.** Au(I) catalyzed imine formation from α-diazoesters and azide. **E.J. McClain**, X. Shi

CHED **1343.** Expansion of electrophile scope in the transition metal-catalyzed coupling of Corey-Seebach *umpolung* reagents. **E. McKinstry**, J.R. Schmink

CHED **1344.** Intramolecular halogen bonding of fluorinated haloarenes in solution. **R.A. Thorson**, G.R. Woller, Z.L. Driscoll, B.E. Geiger, C.A. Moss, A.L. Schlapper, E.D. Speetzen, E. Bosch, M. Erdelyi, N.P. Bowling

CHED **1345.** Manipulating the electronic properties of aryleneethynylenes with halogen bonding. **G.R. Woller**, N.P. Bowling

‡ *Cooperative Cosponsorship*

CHED **1346.** Intramolecular halogen bonding of non-activated aryl halides in solution. **E.R. Robinson**, D.L. Widner, N.P. Bowling

CHED **1347.** Metal binding and electronic properties of aryleneethynylene trapezoids. **Z. Driscoll**, E. Bosch, N.P. Bowling

CHED **1348.** Novel method of stereochemical management of Morita-Baylis-Hillman chemistry: Controlled acrylate ester synthesis. **R. Vaclav**, J.A. Struss

CHED **1349.** Total synthesis of the cyclic depsipeptide natural product Aspergillicin A, and investigation of its cell permeability, pharmacokinetic property, and bioactivity. **C.L. Etienne**

CHED **1350.** Multicomponent reaction to produce diversely substituted 2-imidazolines. **A. Ellsworth**, R.A. Mosey

CHED **1351.** Click, click, xyclize: Amino wster-serived β-ketosultams via Dieckmann cyclization of the corresponding methylsulfonamides. **T.R. Atkinson**, M.Y. Hur, J.H. Jun, P.R. Hanson

CHED **1352.** Synthesis of functionalized biscavitands. **M. Escamilla**, J. Buenaflor, L.M. Tunstad

CHED **1353.** Structural studies of oligonucleotides of RNA containing 7,8-dihydro-8-hydroxyadenosine. **Y. Choi**, A. Chauca-Diaz, M. Resendiz

CHED **1354.** Investigating the use of copper photoredox catalysts in an enantioselective reaction. **S.A. Souder**, K.H. Jensen

CHED **1355.** Synthesis of conformationally constrained diarylether cyclophanes. **H.I. Caldera**

CHED **1356.** Anion-responsive liquid crystals. **K. Grabias**, **L. Lam**, P. Cohn, H. Martinez

CHED **1357.** Synthesis and characterization of novel polyester polyols. **B. Thompson**, **K.D. Ulrich**, W.D. Coggio

Section A

Colorado Convention Center
Halls C/D

Undergraduate Research Posters

Physical Chemistry

Cosponsored by SOCED

N. Di Fabio, *Organizer*

12:00 - 2:00

CHED **1358.** Asymptotic behavior of travelling wave solutions to reaction-diffusion equations. **M.M. Nason**, S. Bricher

CHED **1359.** Interfacial interactions and adhesion properties of selected monomer and polymers probed by SFG spectroscopy and atomic force microscopy. K.A. Cimatu, **K. Hafer**, S. Chan, C.A. Ng

CHED **1360.** Why is there order in the purple membrane? A biological application of ultrafast Raman imaging. **K. Wilhelm**, W.R. Silva, R.R. Frontiera

CHED **1361.** Structures and CH...O interactions of fluorinated ethylene…carbon dioxide complexes as determined by microwave spectroscopy. **R.E. Dorris**, C.L. Christenholz, A.M. Anderton, R.A. Peebles, S.A. Peebles

CHED **1362.** Electronic spectroscopy of gold sulfide (AuS). **B. Pearlman**, **I. Wyse**, T.D. Varberg, D. Kokkin, T. Steimle

CHED **1363.** Investigation of the spectroscopic properties of newly synthesized pyrimidines. **L. Streacker**, N.M. Karn

CHED **1364.** Gas-phase reactions of Cu+ (^{1}S, ^{3}D) with CF_3CH_2Cl, $CF_3CH_2CH_2Cl$, and $CF_3CH_2CH_2Br$: Proximity effects in substrates with competitive reactive sites. **B.A. Scheuter**, X.S. Redmon, W.S. Taylor

CHED **1365.** Photodecomposition of phenylalanine on the surface of titanium dioxide. **C. Arp**, **B. Molnar**, H.M. Bevsek

CHED **1366.** State-specific reactions of Cu^+(^{1}S,^{3}D) with SF_6 and SF_5Cl: Thermochemical control over product formation. **X.S. Redmon**, B.A. Scheuter, W.S. Taylor

CHED **1367.** Thiol based adsorbate detection using Surface Enhanced Raman Spectroscopy. **M. Gray**, E. Bean, A. Deckert

CHED **1368.** Electron stimulated desorption and post-Irradiation analysis in a single ultrahigh vacuum chamber. **C. Belvin**, J. Zhu, C. Arumainayagam

CHED **1369.** Metastable fragmentation and photofragmentation of photoionized thiophene clusters. **M.W. Krone**, D.A. Hales

CHED **1370.** Computational study of nitrogen oxide decomposition by copper exchange ZSM-5 zeolites. **J. Rumley**, H.K. Hernandez

CHED **1371.** Determination and prediction of infinite dilution equivalent conductivities for ions in water at high temperatures and pressures. **S.J. Davis**, G.H. Zimmerman

CHED **1372.** Characterization of novel cyano-based room temperature ionic liquid electrolyte for lithium-ion batteries. **A. deKeratry**, T. Bergholz, C. Korte

CHED **1373.** Revisiting water radiolysis. **J. Lukens**, **M. Marković**, **S. Abdullahi**, C. Arumainayagam

CHED **1374.** Silica sol-gels containing calcein blue as surface-enhanced Raman spectroscopy (SERS) sensors for metal ions. **E.R. Carlson**, E.J. Atkinson, B.D. Gilbert

CHED **1375.** Xenon-129 NMR and surface tension of aqueous micelle solutions. **J. Wetmore**, T. Endreo, S. Grant, A. Calhoun

CHED **1376.** Ammonia radiolysis of astrochemical interest. **H. Cumberbatch**, **Z. Peeler**, **K. Tran**, C. Arumainayagam

CHED **1377.** Kinetic modeling of catalytically active aerogels. **Y. Cao**, M.K. Carroll, A.M. Anderson

CHED **1378.** Kinetics of aminopropyl-triethoxy silane on porous silicon and subsequent reaction with 4-(methylthio) benzoyl chloride studied using FTIR. **S. Kennemuth**, B. McCauley, A. Deckert

CHED **1379.** Colloid particle motion and aggregation in silica aerogels: Experiment and simulation. **K.A. Mengle**, J.N. Richardson, J. Kegerreis

CHED **1380.** Determination of the hydrogen bond effect on nitrile vibrational frequency through solvatochromic models. **H. Sun**, R.S. Moog

CHED **1381.** Computational analysis of conformational tunneling of glyoxylic acid. **V.T. Lim**, K. He, W.D. Allen

CHED **1382.** Surface IR spectroscopy and computational study of MHDA on GaAs(100) surface. **H.M. Barroso**, H.K. Hernandez

CHED **1383.** Diffusion of alkylbenzenes in *n*-alkanes. **P.M. Register**, B.A. Kowert

CHED **1384.** Characterization of an ethanol-benzene complex using matrix isolation infrared spectroscopy. **M. Silbaugh**, J.C. Amicangelo

CHED **1385.** Conformational elucidation of diphenylureas in varying solvent environments. **D.L. Ali**, J.F. Galan, M.I. Galinato

CHED **1386.** Synthesis and extraction of metallocarbohydrynes. **C. Shelmire**, B. May

CHED **1387.** Reaction mechanism for the conversion of creatine to N-formyl-N-methylglycine by hypochlorous acid in aqueous solution. **M.C. Williamson**, C.A. Lareau, L.A. Clough, A.J. Becker, G.H. Purser

CHED **1388.** Energetic, structural, and spectral data for noble gas hydride cations in the interstellar medium. **R.A. Theis**, W. Morgan, R.C. Fortenberry

CHED **1389.** Spectroscopic and microscopic analysis of aggregation effects in N-alkylated perylene diimides. **A. Austin**, **J.M. Szarko**

CHED **1390.** Role of low-energy (< 20 eV) electrons in astrochemistry. **K.D. Tran**, S.M. Abdullahi, C. Arumainayagam

CHED **1391.** Calculating the J=0 vibrational states of noble gas trimers using an energy selected basis. **J. Yudichak**, J. Montgomery

CHED **1392.** Analysis of the metal sulfate-sodium silicate "reverse chemical garden" reaction. **S. Partovi**, H. Basinger, C. Jensen, G. Miter, S. Ogden, M.A. Horn

CHED **1393.** Matrix isolation studies of tetrakis(dimethylamino)titanium IV & ozone. **H. Mosley**, B.S. Ault

CHED **1394.** Investigating the influence of lithium intercalation on dispersive electron mobility kinetics in dye-sensitized solar cells. **M.A. McFarland**, I.J. McNeil

CHED **1395.** Thermodynamics contribution to the stability of PrP^c in model plasma membranes. P. Soto, **R. Gonzales**

CHED **1396.** Computational and crossed molecular beam study in the synthesis of boronylallene. **B. Ganoe**, S. Maity, R. Kaiser, R.J. Bartlett

CHED **1397.** Characterization and the effect of pH and temperature on the degradation of creatine ascorbate, di-creatine ascorbate and creatine di-ascorbate. **M.A. Henneberry**, A.S. Wallner

CHED **1398.** Investigating the neutron inelastic scattering crossSections for ^{54}Fe through γ-ray spectroscopy. **A.J. French**, S.F. Hicks, B.P. Crider, T.J. Howard, S.H. Liu, M.T. McEllistrem, R.L. Pecha, E.E. Peters, F.M. Prados-Estévez, T.J. Ross, Z.C. Santonil, J.R. Vanhoy, S.W. Yates

CHED **1399.** Compositional characterization of cobalt lithium phosphate thin films using atomic absorption spectroscopy. **A.M. Bluhm**, **J.M. Clements**, C. Heideman

CHED **1400.** Driving forces of the stability of Alzheimer's Aβ aggregates in model membranes. **C.R. Bertsch**, B. Aoki, P. Soto

CHED **1401.** Vacuum ultraviolet photolysis matrix isolation infrared spectroscopy of GeH_4 in argon and nitrogen atrices. **P. Mott**, J.C. Amicangelo

CHED **1402.** Sum frequency generation at the DMSO/air interface: Theory meets experiment. **T. Ueltschi**, A.L. Mifflin, P.Z. El-Khoury, H. Wang

CHED **1403.** Determination of the limiting equivalent conductivity and thermodynamic equilibrium constant for the formation of $LaCl^{2+}$ Ion-pairs in water. E. Thompson, G.H. Zimmerman

CHED **1404.** Accurate quantum models of methylphosphonate adsorption onto a stable rutile surface. **S.W. Clifford**, M.N. Srnec, E.S. Gawalt, J.D. Evanseck

CHED **1405.** Synthesis and characterization of indium phosphide quantum dots for use In laser diodes. **J. Charlonis**

CHED **1406.** Rovibrational analysis of $SiOH^+$, $HSiO^+$, and other third row atom hydroxides. **M. Kitchens**, R.C. Fortenberry

CHED **1407.** Impact of tetrazine location in benzobisaxozole possessing cruciforms. **J. Ellett**, A.L. Tomlinson

CHED **1408.** Proposal for a more efficient acoustic array design to determine flow through a cylindrical conduit. **K.J. Ham**, **A. Shue**, K. McGill

CHED **1409.** Kinetics and dynamics of the photorearrangement reactions of aryl-substituted thiophenes. **D.J. Morrow**, J.M. Wasylenko, C.G. Elles

CHED **1410.** Characterization of a methanol-hexafluorobenzene complex using matrix isolation infrared spectroscopy. **C.M. Kindle**, J.C. Amicangelo

CHED **1411.** Microparticle transport across ionic liquid based interfaces. **M. Ngan**, D. Frost, L. Dai

CHED **1412.** Location of deuterated ammonia in Sagittarius B2. **A. Clements**, E. Mills

CHED **1413.** Synthesis of chloromethylsilyl isocynate. **S. Askarian**, G. Guirgis, T. Barker

CHED **1414.** Sustained photocurrent in CdS/α-Fe_2O_3 stacked thin films on titania-coated transparent conductive substrates. **T.C. Douglas**, C. Harris

Section A

Colorado Convention Center
Halls C/D

Undergraduate Research Posters

Polymer Chemistry

Cosponsored by PMSE, POLY and SOCED

N. Di Fabio, *Organizer*

12:00 - 2:00

CHED **1415.** Gel properties of polyisoprene and stearic acid shape memory composite. **B.J. Hukill**, N. Brostowitz, K.A. Cavicchi, R.A. Weiss

CHED **1416.** Smart hydrogel thin films for organophosphorus nerve agent detection. **C. Whitaker**, **N.R. Kaufmann**, **J.J. Snyder**

CHED **1417.** Synthesis and characterization of polyaniline-TiO_2 nanocomposites. **J. Dickens**, A. Stimmell, A.O. Sezer

CHED **1418.** Ring-opening metathesis polymers (ROMP) with organic radical groups for treatment of traumatic brain injuries (TBI). **K.A. Orr**, H.J. Schanz

CHED **1419.** Synthesis and characterization of 3-trifluoromethylstyrene copolymers. **K.M. Dubiak**, R.W. Kopitzke

CHED **1420.** Novel polymeric redox mediator for use in biofuel cells. **A.J. Halmes**, M. Retherford, D.T. Glatzhofer

CHED **1421.** Phase-selective studies of polyisobutylene-bound dyes using antileaching agents. **C. Torres-Lopez**, M.L. Harrell, D.E. Bergbreiter

CHED **1422.** Synthesis of hierarchically porous polymer network for carbon dioxide capture. **A. Sliwinski**, H. Gao, D. Lee

CHED **1423.** Synthesis of four-armed calixarene-core polylactide/polyethylene glycol star block copolymers using click chemistry. **K.A. Bogner**, A.C. Falls, P.S. Corbin

CHED **1424.** Investigating the polymerization mechanism of cyanoacrylate with fingerprint constituents. **K. McCarthy**, E.M. Persson, A.S. Dutton

CHED **1425.** Synthesis of a macroinitiator and its use in the preparation of poly(styrene-b-methacrylonitrile): An advanced undergraduate laboratory project in polymer chemistry. **B.A. Arce**, L. Calvo, H.N. Gray, S.C. Butler

CHED **1426.** Synthesis of asolectin-containing latexes by emulsion polymerization. **A. Johns**, M. Channell, M. Ming, R. Quirino

CHED **1427.** Synthesis and applications of ionic liquid monomers in free radical polymerizations. **M. Sea**, B. McFarland

CHED **1428.** Synthesis of high molecular weight poly(ε-caprolactone) star polymers and their degradation properties. **R.L. Collette**, K.A. Boduch-Lee

CHED **1429.** Synthesis and polymerization of *(E,E)*- [6.2]-(2,5)furanophane-1,5-diene. **N. Doppler**, J. Glans

CHED **1430.** Biocompatible material used for drug delivery. **A. Gomez**, G. Craft, J. Harmon

CHED **1431.** Poly(ionic) liquids: Imidazoles with ester linkages. **M.A. Andrews**, M.J. Campbell

CHED **1432.** Synthesis of metal-organic frameworks for adsorption of disease-relevant peptides. **B.J. Karels**, Z. Mensinger, **M.W. Smith**

CHED **1433.** CdSe quantum dot band edge tuning through photooxidation on nanopatterned polymers for applications in hybrid cell photovoltaics. **J. Custer**, J.D. Batteas, N. Stingelin

CHED **1434.** Synthesis of sustainable monomers for a polyurethane. **C. Johnston**, E. Black, L. Salzl, C.P. Schaller

CHED **1435.** NMR study of the active form of the polymerization catalyst formed between Tp*Rh(cod) and 4-ethynyltoluene. **H.K. Blakely**, R.M. Tarkka

CHED **1436.** Titanium and tantalum complexes bearing optically active tartrates as catalysts for the polymerization of D,L-lactide. **T. Bumpus**, M. Holcomb, B.M. Chamberlain

CHED **1437.** Lactones derived from fatty acids: New monomers for the production of bioplastics. **C. Seitzinger**, A. Linderman, R. Johnson, T. Bumpus, M. Holcomb, K. Walker, L. Boran, J. Johnson, B.M. Chamberlain

CHED **1438.** Ion conducting polymer electrolytes as electroactive polymers. **T. Makkapati**, D.C. Teeters

CHED **1439.** Synthesis and characterization of sol-gel based $AlFPO_4$ glasses. **G.B. Adkins**, C.B. Brennan

CHED **1440.** Polycation-DNA interaction thermodynamics: tailoring gene delivery systems. **K. Mueller**, L. Prevette

CHED **1441.** Study in the polymer crystallization kinetics and the birefringence of polyethylene glycol. **R.E. Kisling**, R. Wismer

CHED **1442.** Diarylethene containing π-conjugated polymers: The effects of binding site on photochromic and electrochemical behavior. **S.D. Myers**, K.G. Ohashi, S.M. Baksa, I.M. Walton, J.B. Benedict, D.G. Patel

CHED **1443.** Synthesis of 7-{bicyclo[2.2.1]hept-5-en-2-yl}-7-oxoheptanoic acid ligand monomer and attachment to lead sulfide nanoparticles. **G. Borkowski**, R.W. Kopitzke

CHED **1444.** Temperature effects on the impact properties of polymer coatings used in armor protection. **J.F. Chamberlain**, M.J. Schroeder

CHED **1445.** Synthesis of polymer capable of underwater adhesion. **C. Burns**, D. Fish

CHED **1446.** Spatially specified natural fiber welding via inkjet printing. **T. Price**, E. Fox, E. Brown, K. Sweely, P.C. Trulove, H.C. De Long

CHED **1447.** Synthesis and utilization of ionic microgel dispersions for uptake and release of active species. H. Chen, **M. Kelley**, L. Dai

CHED **1448.** Radiopaque shape memory polymers. **L. Allison**, K.R. Houston, V.S. Ashby

CHED **1449.** Carbon fiber precursors derived from lignin and acrylonitrile vinylimidazole blends. **M. Garcia Casas**, B. Batchelor, S. Mahmood, D. Yang

Section B

Sheraton Denver Downtown Hotel

Century

Experiments for Physical Chemistry Laboratory

Assessment, Computational Chemistry, & Kinetics

S. S. Hunnicutt, R. M. Whitnell, *Organizers*

A. Grushow, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CHED **1457.** Using three types of instructional videos to assist students' laboratory preparedness in a physical chemistry lab. R.S. Cole, **M.N. Muniz**, J.A. Schmidt, E. Keuter

1:55 CHED **1458.** Assessing a problem-based learning NMR & MRI laboratory experiment. **S.E. Erhart**, G.A. Lorigan, E.J. Yezierski

2:15 CHED **1459.** What factors affect the escapability of a molecule from a liquid? A molecular dynamics experiment for the physical chemistry laboratory. **R.M. Whitnell**, M.S. Reeves

2:35 Intermission.

2:45 CHED **1460.** 3D printing to create computationally derived models in the physical chemistry laboratory. **W.T. Grubbs**, S.M. Ryan

3:05 CHED **1461.** Computational exercise to explore the nature of hydrogen bonding. **M. Ayoub**

3:25 CHED **1462.** Can we make stew with these beans? An introduction to experimental inquiry for the physical chemistry laboratory. **M. Pacheco**, S.S. Hunnicutt, R.M. Whitnell

3:45 CHED **1463.** Kinetics of the carbon dioxide hydration reaction: Quantitative experiment for the undergraduate physical chemistry laboratory. **D. Bopegedera**, F.D. Tabbutt

4:05 CHED **1464.** How to make the most appealing fruit salad: An inquiry-based enzyme kinetics physical chemistry laboratory. **R.S. Cole**, S.S. Hunnicutt

4:25 Concluding Remarks.

Section A

Sheraton Denver Downtown Hotel

Gold

ACS Award for Achievement in Research for the Teaching and Learning of Chemistry: Symposium in Honor of Vickie M. Williamson

Cosponsored by WCC

Financially supported by Pearson Publishing

M. R. Abraham, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CHED **1450.** Visualizing chemistry: From idea to research to practice. **D.M. Bunce**

1:55 CHED **1451.** Limitations of engagement as a goal for design: Visualizations and beyond. **S. Hinze**

2:15 CHED **1452.** Providing opportunities for students to increase their understanding of chemistry: Guided inquiry, computer simulations and animations, and active learning. **T.J. Greenbowe**, J.I. Gelder, M.R. Abraham, D.H. Exton, B. Baldock

2:35 CHED **1453.** Lines, labels, and arrows: The role of graphical devices in visualizations. **L.L. Jones**, S. Akaygun, V. Fishback, D. Falvo, J.P. Suits

2:55 Intermission.

2:55 CHED **1454.** Research into practice: Visualization of the molecular world using animations and simulations. **R. Tasker**

3:15 CHED **1455.** Effects of e-homework systems on male and female students' understanding of the particulate nature of matter. **D.S. Mason**

3:35 CHED **1456. Award Address** (ACS Award for Achievement in Research for the Teaching and Learning of Chemistry sponsored by Pearson Education). Quest for student understanding of the particulate nature of matter. **V.M. Williamson**

Section C

Sheraton Denver Downtown Hotel

Spruce

Online Course Development and the Effects on the On-Campus Classroom

P. Sorensen, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CHED **1465.** Scholarship of teaching: Online courses as means of publishing innovations. **J.S. Hutchinson**

2:00 CHED **1466.** Analysis of peer-to-peer interactions in introductory online courses. **D.A. Canelas**

2:25 CHED **1467.** Toward the development of academic social networks: A new paradigm for online STEM eLearning. **D.M. York**

2:50 CHED **1468.** Generalized organic chemistry for a global student population: Organic chemistry on Coursera. **M. Evans**

3:15 CHED **1469.** Withdrawn.

3:40 Intermission.

3:50 CHED **1470.** Intro to solid state chemistry: A mastery-based learning and assessment model. **M.J. Cima**

4:15 CHED **1471.** Development of an online hypermedia environment as a complement to the traditional textbook and its impact on the on-campus classroom. **J.A. Suchocki**

4:40 CHED **1472.** Online-on campus dialogue: Lessons from Harvard's Science and Cooking course. **P. Sorensen**

Section D

Sheraton Denver Downtown Hotel

Denver

Undergraduate Research Papers

Biochemistry and Chemical Education

Cosponsored by SOCED

C. V. Gauthier, J. V. Ruppel, *Organizers*

N. L. Snyder, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CHED **1473.** Potential use of phenazine derivatives in the inhibition of the La Crosse virus. **N. Hami**

1:45 CHED **1474.** Posttranslational modification of nitrogenase in Rhodobacter sphaeroides. **T.C. Godfrey**, S. Ensign

1:55 CHED **1475.** Assignment of the HN-HSQC NMR spectrum of heat stable protein kinase inhibitor (PKI). **B. Stultz**, **J. Kim**, G. Veglia, M.B. Neibergall

2:05 Intermission.

2:15 CHED **1476.** Chalcones and analogs of caffeic acid phenethyl ester with xanthine oxidase inhibiting and radical scavenging properties: Tools capable of suppressing oxidative stress in cells. **J.E. Webster**, **L. Snider**, E. Hofmann, T.D. Do, S. Linn, S.F. Paula

2:25 CHED **1477.** Bioconjugating biotinylated gold nanoparticles (Au-NPs) to fluorescent streptavidin: Study of Au-NPs interaction with and photothermal effects on cells. **E.J. Vences**, B. Mellis, M. Steiger

2:35 CHED **1478.** Determining junctional tension in skin cells using Ecad-TSMod. **D.E. Morales-Mantilla**, B.W. Heck, W. Aw, D. Devenport

2:45 Intermission.

2:55 CHED **1479.** Direct amidation of carboxylic acids via microwave-assisted synthesis: Greener organic laboratory options. **S.M. Strobel**, **D. Parr**, I.J. Levy

3:05 CHED **1480.** Undergraduate laboratory experience on kinetics: Using the FeIII-TAML system with common food dyes. **H. Chang**, D. Tshudy, T.J. Collins

3:15 CHED **1481.** Preventing general chemistry students from sinking into the chemical ocean. **C. Gabel**, **L. Roon**, **M. Flores**, **J. Daniel**, **J. Richards**, D. Hyde, V. Wolf

3:25 Concluding Remarks.

Section E

Sheraton Denver Downtown Hotel

Columbine

ACS Award for Encouraging Disadvantaged Students in Chemistry: Symposium in Honor of Catherine H. Middlecamp

Four-Part Harmony (or Disharmony)

Cosponsored by CMA and WCC

Z. M. Lerman, C. H. Middlecamp, *Organizers, Presiding*

1:30 CHED **1482.** Harmonious world of chemistry with Cathy Middlecamp. **Z.M. Lerman**

1:50 CHED **1483. Award Address** (ACS Award for Encouraging Disadvantaged Students into Careers in the Chemical Sciences sponsored by the Camille and Henry Dreyfus Foundation). Four-part harmony (or disharmony). **C.H. Middlecamp**

2:10 Intermission.

2:20 CHED **1484.** Disadvantaged students: A faculty perspective. **M.H. O'Leary**

2:30 CHED **1485.** Disadvantaged students: Who are they and what prevents their learning and achievement. **B. Kean**, M.H. O'Leary

2:40 CHED **1486.** Disadvantaged students: The whole is more than the sum of the parts. **A. Jacob**

2:50 Panel Discussion.

3:05 Intermission.

3:15 CHED **1487.** Disadvantaged students: Undergrad to grad — a personal view. **D.R. Arnelle**

3:25 CHED **1488.** Disadvantaged students: Mentors come in many shapes and notes. **R. Hernandez**

3:35 CHED **1489.** Disadvantaged students: Diversity in many shapes and forms. **T.P. Yoon**

3:45 Panel Discussion.

4:00 Intermission.

4:10 CHED **1490.** Disadvantaged students: Mentoring and place-based engagement in Alaska. **L.K. Duffy**

4:20 CHED **1491.** Disadvantaged students: Jumping into the deep end. **L. Nicholas-Figueroa**

4:30 CHED **1492.** Disadvantaged students: The view moving forward. **M.A. Fisher**

4:40 Panel Discussion.

Section F

Sheraton Denver Downtown Hotel

Gold

Chemistry Education: International and Multi-cultural Perspectives

S. Raje, *Organizer*

S. Sandi-Urena, *Organizer, Presiding*

S. Hansen, *Presiding*

1:30 CHED **1493.** Implementing ASCIv2 to measure students' attitudes towards chemistry in large enrolment chemistry subjects at an Australian university. S. Chadwick, **A. Baker**, **J. Alexander**

1:50 CHED **1494.** Developing a curriculum for an international service learning (ISL) program in artisanal and small-scale gold mining (ASGM) communities. **A.M. Kiefer**

2:10 CHED **1495.** Good CoP: A successful community of practice in a faculty of science. **A.T. Baker**

2:30 CHED **1496.** Role of internationalization in the development of pedagogical content knowledge of pre-service chemistry teachers. **S. Akaygun**, M. Gootzen

MONDAY EVENING

Section A

Sheraton Denver Downtown Hotel

Gold

STRETCH Your Students' Polymer Knowledge by Putting Some BOUNCE into Your Curriculum

Polymer Science Education and the NGSS

Cosponsored by PMSE, POLY‡, RUBB and SCC‡

Financially supported by Intersociety Polymer Education Council

S. C. Rukes, *Organizer, Presiding*

4:30 Introductory Remarks.

4:35 CHED **1497.** PolyWhat? What in the world is a polymer. **S.C. Rukes**

5:25 CHED **1498.** Polymers: New twists on old favorites. D. Goodwin, **S.C. Rukes**

6:15 Intermission.

6:25 CHED **1499.** How are plastic toys made? The manufacturing of plastics. A. Nydam, **S.C. Rukes**

7:10 CHED **1500.** Bioplastics: From the farm to the store shelf. E.J. Escudero, **S.C. Rukes**

7:45 Panel Discussion.

7:55 Concluding Remarks.

Section A

Colorado Convention Center

Halls C/D

Sci-Mix

W. E. Jones, I. J. Levy, A. L. Marsh, *Organizers*

8:00 - 10:00

92-93, 95- 97, 100, 104, 107-108, 111-112, 115-116, 118, 121, 124, 127-128, 133-134, 136, 140, 142-143, 148, 152-154, 156, 158-160, 163-164, 169-170, 173-174, 178, 182. See previous listings.

1704, 1706, 1810, 1814, 1816- 1818, 1824, 1827-1828. See subsequent listings.

Section A

Colorado Convention Center

Halls C/D

Successful Student Chapters

N. Di Fabio, *Organizer*

8:00 - 10:00

CHED **1501.** Reaching out through outreach to the DFW community. **C. Ashbrook**, S. Mathis, S. DeSpain, A.L. Green, E. Fung, P. Patel, M. Chandra, S. Price, T. Le, R. Itoh, K. Vu, K. Upton, C. Simmons, T.A. Schneider, T. Gurney, J. Fry, K.N. Green, B. Janesko

CHED **1502.** Pasadena City College Student Chapter: Successful activities on campus and in the community. **K. Tsang**, **P. Donabedian**, **J. Portillo**, M. Anderson, D. Lyfeldt, P. Castro, **V.I. Jaramillo**

‡ *Cooperative Cosponsorship*

CHED **1503.** Expanding our community involvement. **T. Ebener**, M.E. Johll, P.K. Yong, T.L. Thacker, J. Damron, M. Allen, R. Marlett, L. Tomaszewski, A. Schalk, A. Molln

CHED **1504.** Student chapter events and activities done at Tennessee Tech University. **K. Richards**, **M.P. Butner**, **S.B. Reynolds**, **S.M. Amin**, **B.C. McGill**, **V. Sublett**, **A. Reno-Demick**, **A.J. Ferry**, **A.J. Crook**, **D.J. Swartling**

CHED **1505.** Non-Newtonian fluids as a student affiliates chapter event: Chemistry, logistics, and outreach. **A.M. McCollum**, **A.M. Longo**, **K.J. Goosherst**, **L.M. Jablonski**, **M.L. Kaak**, **A. Li**, **D.G. Sacenti**, **D.B. Green**, **J.M. Fritsch**

CHED **1506.** ACS student affiliates chapter of Seattle Pacific University. **S. Eng**, R. Hawkins, R. Kenyon, **K.M. Pierce**

CHED **1507.** American Chemical Society Student Chapter at The University of Texas at Tyler. **P. Martin**, B. Western, J.J. Smee, L.E. Boyd

CHED **1508.** Activites of Ferris State University student affiliate chapter. **E.K. Utke**, L. Bass, **K.J. Robb**

CHED **1509.** Discover gold with the Alchemist Club at Missouri Western State University. **A.J. Luke**, **S. Warren**, S.P. Lorimor

CHED **1510.** NSF Community College Innovation challenge: A proposal. A.J. Sanders, **J. Weber**, **S. Comshaw-Arnold**

CHED **1511.** Saint Francis University Chemistry Club: Safe but fun. **S. Ciraula**, **C. Fry**, **D. Mosier**, E.P. Zovinka

CHED **1512.** Discerning student interest in science activities. **M. Love**, **A. Bilbrough**, **A. Wilson**, M.J. D'Souza

CHED **1513.** Wayne State University ACS Student Affiliates. **K. Mullan**, **S.A. White**, **R. Dixon**, **Y.K. Elghoul**, **A.R. Breckenridge**, M. Farhat, **R. Donovan**, **H. Ahmed**, **J.A. Degg**, **J.L. Fischer**

CHED **1514.** Belmont SMACS: Engaging in awesome science. A.B. Moore, **V.T. Lim**, L. Patel

CHED **1515.** Molloy Chemical Society. **A. Stockhausen**, M. Pogash

CHED **1516.** SIUE Chemistry Club: Promoting science education on campus and beyond. **A. Fox**, D. Wright, M. Ontl, A. Cox, S.B. Luesse

CHED **1517.** American Chemical Society Student Chapter at Peninsula College. **B. Weintraub**

CHED **1518.** Gruen Chemistry Society: Student affiliate activities at Olivet College. **M. Piper**, A. George, Z. Kitzmiller, T. Thorn, S.M. Lewis

CHED **1519.** Millersville University ACS Student Chapter 2014-2015. **D. Hofmann**, **J. Charlonis**, **J. Dreer**, H. Ashberry

CHED **1520.** Improving leadership and programming: Finding the balance between quality and ability. K.B. Bramble, L. Saint-Fort, K.A. Leets, **G.D. Gibbs**

CHED **1521.** Online fundraising activities to support student travel and research at Illinois State University. **E. Jugovic**, L.M. Stateman, E.C. Sullivan, J. Kim

CHED **1522.** Student Affiliates of the American Chemical Society San José State University Chapter. **A. Hui**, N. Nguyen, M. Lim, Q. Lam, D. Lee, C. Lionel, G. Muller

CHED **1523.** Aquinas Chemistry Society: 2015 successful chapter poster. **N. Pierce**

CHED **1524.** ACS Student Chapter of the University of St. Thomas: At the center of the energy and medical capital of the world. **A. Rivera**, K. Foss, C. Chidi, P. Zaibaq, J. Hoang, C. Anderson, B. Mellis, E. Ledesma

CHED **1525.** Florida Southern College student chapter growth 2014-2015. **S. Wilson**, **K. Fussell**, **J.C. Sessums**, W. Teh, J. Yudichak, G. Beggs, B. Crosby, J.M. Montgomery

CHED **1526.** Small but mighty Centenary College Chemistry Club. **B.M. Bourgoyne**, P.R. Pritchett, R.S. Thompson, T.R. Johnson, T.M. Ticich

CHED **1527.** NCW 2013 at UPR Humacao: A sweet celebration. **C. Algarín**, S. Luquis, J. Suarez

CHED **1528.** Speaker series at Northeastern: Inspiring the next generation of chemists. **M. Naniong**, **W. Timson**, R. Timson, J. Conway, J. Conway

CHED **1529.** American Chemical Society University of New Mexico Chapter. **D. Martin**, A.C. Segura, E. Milarch, A. Fernandez, D.A. Garcia

CHED **1530.** ACS Wilkes Student Chapter applying green chemistry principles. **B.S. Clem**, **A. Fadel**, T. Weaver, K.M. Rehrig, A. Dinescu, C. Henkels

CHED **1531.** SMACS attacks chemistry. **T.A. Knippenberg**, **S. Ansteatt**, B.N. Norris

CHED **1532.** Events and outreach of the University of Colorado Denver SAACS Chemistry Club. J. Henderson, M.K. Maron, **R. Rodriguez**

CHED **1533.** Restarting the student affiliate in the oldest town in Texas. **D.A. Fry**, C. Huckaby, J. Moreland

CHED **1534.** University of Central Arkansas ACS chemistry chapter: Using an inter-chapter relations grant to increase chemical outreach. **A.D. Rolland**, J. Castillo, H.H. Agrama, J.D. Henderson, J.G. Schmidt, K.S. Dooley, K.L. Steelman, F.M. Yarberry

CHED **1535.** Leading a successful ACS Student Chapter. **J. Ewing**, A.J. Garrett, **J.R. Ligas**, **M.P. Snyder**, A.J. Sanders

CHED **1536.** Cultivating and communicating chemistry on campus and in the community. **D. Walter**, T. Meece, M.D. Perry, S.E. Hubbard

CHED **1537.** New Mexico Highlands University Chemistry Club: Starting a student chapter. B. Maki, **P. Dimas**

CHED **1538.** Successful student chapter, Suffolk University 2014. **S. Shrestha**, J. Bautista, E.M. Persson, T.E. West, K. McCarthy, T. Nguyen, A.S. Dutton

CHED **1539.** Eastern Oregon University ACS Student Member Chapter: Promoting community outreach and professional networking. **T. Winegar**, M.L. Gathright, D.A. Ladendorff, S.A. Sorensen, A.G. Cavinato

CHED **1540.** Saint Louis University brings the wonder of chemistry to local Saint Louis students. **N. Schlarman**, L. Green, B. Znosko

CHED **1541.** Surface modification to impact our community. **A.G. Colon**, P.N. Gonzalez Colon, M.A. Miranda Belandria, C. Pellicier Rodriguez, J.I. Ramirez Domenech, E.J. Ferrer Torres

CHED **1542.** Ecofriendly chapter: Education and implementation for a sustainable world. **L. Ramirez Santiago**, A.D. Almodovar Ortiz, P.N. Gonzalez Colon, J.I. Ramirez Domenech, E.J. Ferrer Torres

CHED **1543.** PCUPR student affiliate chapter celebrates a summer festival. **N. Rivera**, **J.K. Vale**, N.I. Negrón, L. Santos

CHED **1544.** Metamorphosis: Our chapter evolution. **A. Zapata Feliciano**, J. Vélez, G. Lopez-Perez, E. Francheschini, S. Ramírez de Arellano, S. Vargas-Padilla, N. Caraballo, A.M. Gonzalez

CHED **1545.** ChEmory: Emory University's undergradute chapter of the American Chemical Society. **K.E. Leon**, J. Elinburg, Y. Lin, K. Woolard

CHED **1546.** Exploring chemistry through candy at Carroll University. **A. Ott**, **K. Rude**, J. Rountree, S. Marton, G.T. Marks

CHED **1547.** Successful student chapters abstract: Hofstra University student members of the American Chemical Society. E. Zhou, **B. Biju**, L.E. Carlucci, E.K. Reagan, P. Fernandes, D. Prado, B. Xuan, S.T. Lefurgy, E.C. Mundorff

CHED **1548.** Student Affiliate Chapter of the American Chemical Society: Minot State University. **K.T. O'Keefe**, S.W. Olson, K.A. Dockter, M.A. Bell, J.M. Miller, S. Park, H. Lee, J.A. Collins, M.M. Bobylev

CHED **1549.** Georgia College's outstanding student chapter: "Sweeter" than Georgia peaches. **J.L. Minnick**, K. Taylor, H.E. Pekarek, J. Minnick, P. Skersick, K. Ehret, C.H. Lisse

CHED **1550.** Miami Chemical Society from Miami University (Ohio). **M.M. Shroder**, B.D. Center, R. Comer, A.A. Simoni

CHED **1551.** SMSU Chemistry Club: Activities of an outstanding student chapter of the ACS. **S.C. Kenea**, M.M. Bruns, N.J. Beyer

CHED **1552.** First Loras College chemistry carnival: The chemistry of candy. **M. Rea**, D.J. Oostendorp

CHED **1553.** Stimulating interest and enthusiasm for chemistry. **R.J. Wood**, **T. Glasgow**, **V. Linero**, **J. Castro**, **J. Allen**, U. Swamy

CHED **1554.** Successful chapter activities of the Monmouth University Chemistry Club. S.J. Ebner, **K. Flynn**, N. Famularo, K. Muratore, D. Szwajkajzer, G.A. Moehring

CHED **1555.** University of Puerto Rico- Río Piedras ACS Student Chapter: A role model to our society. **R.E. Martinez-Quinones**, **W.M. Pedreira-Garcia**, **E. Santiago-Aponte**, **I. Lehman-Andino**, I. Montes

CHED **1556.** Reactions to increase the yield of involvement. **Z. Hicks**, **B.H. Cameron**, M. Simmons, U. Phan

CHED **1557.** Tethering community and academic pursuit: A story of success. **D. Fager**, **R. Morrison**, **A. MacInnis**, **K. McAndrews**, C. Schnitzer

CHED **1558.** Arkansas Tech University Chemistry Club: Encouraging and broadening participation through outreach and on campus activities. S. Zulfer, T. Schultz, E.W. Turner, B.D. Curry, S.L. Moran, M. Fuller, **C.A. Mebi**

CHED **1559.** Promoting science with the "Chemistry CirCus". **C. Garcia**, **J.D. Guerra**, **V.M. Gonzalez Vazquez**, L. Griego, J.S. Enriquez, J.E. Becvar

CHED **1560.** Outreach, teaching, and university connection programs for two-year college students. **T. Bledsoe**, **J.S. Bloodsworth**, **C.M. Marshall**, P.E. Flores Gallardo, L.D. Burke

CHED **1561.** Traditions and innovations guiding the way to success for Nittany Chemical Society at Penn State. **T. Breidenbaugh**, C.S. Mallis, K. Lan

CHED **1562.** Onward and upward: Revitalizing a small student chapter. **J. Wells**, **C.J. Forsythe**

CHED **1563.** Western Washington University Student Chapter of the American Chemical Society. T. Clinkingbeard, C. Grote, N.P. Bradshaw, N. Schorr, **S.R. Emory**, E. Raymond

CHED **1564.** Priory of Biology & Chemistry at East LA College: Organically fun. **H. Castellanos**, **M. Lopez**, **I. Gonzalez**, K.N. Olsen, **A.M. Rivera Figueroa**

CHED **1565.** Getting your chapter involved the community: Examples of community involvement by the Elmira College ACS student affiliate chapter. **A. Davenport**, C. Zorn, C.E. Stilts

CHED **1566.** Instilling chemistry into our biggest natural resource. **A.R. Chappell**, **K.N. Weeber**

CHED **1567.** Central Washington University SA-ACS 2014-2015: Developement of standard operating procedures (SOPs) for the safe, educational and fun performance of chemistry demonstrations. C. Verwey, **C.D. Carman**, A. Wilson, C.E. Malmberg, N. Beebe, S. Bouchey, D. Chavez, J. Siegenthaler, P.W. Swain, T.L. Sorey

CHED **1568.** Importance of community outreach and encouragement of the sciences. **J. Kao**, **K. Gensemer**, **B. DeMauro**, S.A. Fleming

CHED **1569.** Barry University Chemistry Club: Celebrating twenty years of excellence. P. Nwokoye, H. Dao, V. Hoelscher, Q. Su, J. Sanchez, **G. Fisher**, T. Hamilton

CHED **1570.** How to retain members and make them feel included. **J.L. Farley**, A. Shepard, A.T. McDonald, J. Callus, M. Smoker

CHED **1571.** Chemical demonstration program for continuing education. **C. Cookenmaster**, M. Pendleton, M. Bache, E. Milligan, D.M. Bartley

CHED **1572.** SAACS Is $Au_{@}$ at SHU. L. Farber, **K. Konieczny**, A. Buonaccorsi, **J. Fierro**, **N. Doppler**, **J.M. Wetherell**, **K. Scinto**, **K. Hess**, D.N. Beier, M. Stewart, S. Bergman, C. Ruvolo, K. Campos

CHED **1573.** Forensic chemistry division; A new outreach in our campus. **J. Chabrier Rodriguez**, E. Medina, C. Osorio Cantillo, J.I. Ramirez Domenech, E.J. Ferrer Torres

CHED **1574.** Xavier University of Louisiana's student chapter: Enriching the legacy. **L.M. Mensah**, C. Pace, K. Lam, T.J. Harris, K. Crosby, E. Murphy, D. Johnson, M.R. Adams, J.A. Privett, C.M. Lawrence

CHED **1575.** UTPB Chemistry Club: Promoting chemistry in west Texas. K.A. Beran, **S. Moreno**, B.J. Garcia, M. Hagle, S. Siegler

CHED **1576.** Successful activities of the Waynesburg University ACS Chapter. **G. Strouse**, C. Petrone, K. Wilson, T. Bromenschenkel, **N. Frazee**, E.A. Baldauff

CHED **1577.** Lock Haven University Chemistry Club. **J. Seidel**, J. Caffyn, K. Range

CHED **1578.** Student Chemists Association at The College of New Jersey. **T. Maney**, **H. Sajjad**, **C. Kirby**, A.R. O'Connor, B.C. Chan

CHED **1579.** Erskine College ACS Chapter: Not just winging it anymore. **D.A. Roe**, D.K. Gentry, A.D. Houston, T.R. Hayden, J.E. Boyd

CHED **1580.** PLU Chemistry Club: Redistributing knowledge according to Le Châtelier's Principle. **S.D. Murphy**, **S. Huang**, N.A. Yakelis, A.M. Munro

CHED **1581.** Collegiate Chemistry Bowl, Demomania, Chemagic show, eminent speaker and networking luncheon part of UT-Martin hosting the undergraduate program at SERMACS. S.K. Airee, **K.A. Harris**, K.H. MccCrillis, L. Gargus

CHED **1582.** Career development and networking for chemistry, biochemistry, engineering, and pharmacy majors: KU Chem Club. **M. Holtz**, V. Tallavajhala, A. Petrulis, C. Barrett, P.R. Hanson, R.S. Black

CHED **1583.** Saint Vincent College Chemistry Club. **A.J. Rupprecht**, A.N. Dobracki, M. Brady, S.J. Gravelle

CHED **1584.** Green chemistry: Prevention for a cleaner future. **R. Jimenez-Hernandez**, **M. Torres-Caban**, B.J. Ramos-Santana

CHED **1585.** Forging leaders: Diamonds for society. **D.E. Morales-Mantilla**, **D. Morales-Rosa**, B.J. Ramos-Santana

CHED **1586.** Stay calm and get your grizzly growl on: Georgia Gwinnett College chemistry outreach. **G.E. Rudd**, **C. Fussell**, **S. Jiva**

CHED **1587.** Catawba College Chemistry: The fuel that will stand the test of time. **A.L. Williamson**, B. Baumgarten

CHED **1588.** Chemistry outreach efforts at North Dakota State University. S. Walker, R. Hessman, M. Mann, **M.J. Kleinsasser**

CHED **1589.** Fundraising methods at North Dakota State University. J. Wrage, T. Kim, S. Walker, **M.J. Kleinsasser**

CHED **1590.** Modeling a successful student chapter. M. Vang, **A. Lolinco**, B.J. Cole, P. Ounkham, R. Espinoza, K.M. Kazaryan, I. Kuchkovskaya, N. Chhay, M.L. Golden, D. Golden

CHED **1591.** University of Utah American Chemical Society Student Chapter: Successful student chapter poster. **C.J. White**, **F. Fernandez**, B. Ronna, B.L. Richeson, Z. Headman, C. Jennings, A. Jo, H. Hansen, R.Y. Chung, G. Clement, M.R. Kiley, H.L. Sebahar, J.D. Rainier, T.G. Richmond

CHED **1592.** Truman State University Student Chapter. **J.M. McGowan**, C. Witt, E.P. Riekeberg

CHED **1593.** Successful student chapter of the American Chemical Society, South Dakota School of Mines and Technology: Promoting chemistry and reading. **M. Braasch-Turi**, J. Meyer, **M.A. Huber**, **P.R. Holland**

CHED **1594.** Science of service: Gordon College's student chapter of the American Chemical Society. **D. Gray**, B.J. Marshall, L.T. Walsh, E. Fjellstad, D. Andujar, M.C. Enright

CHED **1595.** Chemistry: the final frontier: These are the chronicles of the Chemistry Club at South Texas College, its enduring mission – to spread knowledge, educate the unknowing, serve its community, and go where no chemistry club has gone before. **L. Avila**, R. Gonzalez, A.Y. Navarro, N. Salazar, A. Gonzalez

CHED **1596.** MTSU SMACS activities 2014-2015: Turning 40 isn't so bad. **H.O. Bradley**, D. Wilson, T. Chitpanya, G. Goodin, H.N. West, X. Aguilar, G. White, K. Ding

CHED **1597.** Exploits of the UM-Flint Demo Squad: Dragons, duties, and dewars. **A.N. Rizo**, J.L. Tischler, M.R. Wilhelm, C. Wilhelm, B. Shiflett, A. Shah, A. Hernandez, D. Duzdar, A. Burch, A. Singh, S.S. Grathoff, G. Martin

CHED **1598.** Park University C.H.E.M. Club: Using sweets to promote chemistry and conservation in the community. **S.M. Hansen**, J. Bautista, A. Davis, W. Washington, G.D. Claycomb, D.K. Howell

CHED **1599.** Journey of ACS student members at Duquesne University. **S.E. Kochanek**, B.R. Jagger, K.P. Devlin, A.B. Jansto, S.A. Richards, A.A. Dalal, C.M. Gaetano, M. Hockman, E.E. Gorse, A. Williams, J. Nielsen, S.C. Ratvasky, M.N. Srnec, P.G. Johnson, E.S. Gawalt, J.D. Evanseck

CHED **1600.** Increasing participation in the Chemistry and Biochemistry Club at Minnesota State University Moorhead. **A.N. Anderson**, **D.M. Anderson**, J. Bodwin

CHED **1601.** University of Central Florida's student chapter of the American Chemical Society. **K.J. LaBelle**, S.M. Kuebler

CHED **1602.** Community outreach projects of the ACS: RUM Chapter. **H.M. Quinones Rosaly**, D.C. Vazquez Gonzalez, T. Vélez, A.L. Garcia Duprey, H.A. Ocasio Rodriguez, M. Rodríguez, M. Lu, T. Massas, J.D. Núñez Cruz, J.A. Morales Vicens, J. Torres Candelaria

CHED **1603.** Successful activities of SAACS at the University of Central Oklahoma. **K.M. Magiera**, T. Murray, D.G. New, J.M. Ferguson, E.M. McIntyre, R. Evans, K. Jackson, C. Jones, J.M. Laverty

CHED **1604.** University of Kentucky Students of the American Chemical Society: Expanding undergraduate chemistry linvolvement at UK. **D. Wallace**, B.S. Guiton

CHED **1605.** Angelo State University ACS Student Chapter. B.R. Holle, **E. Osborne**, K.A. Boudreaux

CHED **1606.** Angelo State University Green Chemistry Student Chapter. S.I. Pena, **E. Osborne**, K.A. Boudreaux

CHED **1607.** Sweet success: NCW 2014 at Tarleton State University. **T.B. Roberson**, C.E. Earp, R.N. Goodrich

CHED **1608.** Student members of the American Chemical Society: University of Arizona chapter. **T.N. Szyszka**, R. Gonzalez, S. Herman, N. Tyler, D. Timonina, I. Garcia

CHED **1609.** Confectionary chemistry: Spreading the sweet joys of chemistry to Bristol, RI. **M. Levano**, T. Malewschik, I. Kieffer, C. Murphy, S.K. O'Shea

CHED **1610.** Newberry College Chapter of the American Chemical Society. **B.E. Lacy**, A. Privette, O. Valentin, D. Terrell, C.P. McCartha, Z.S. Davis

CHED **1611.** Texarkana College Chemistry Club, 2013-4 Activites Poster. **K. Parker**, J. Ordonez, M. Buttram

CHED **1612.** Chemistry and community outreach. **P.M. Doherty**, R. Byrnes, D. Szlosek, J. Howland, G. Smith, A. Makaretz

CHED **1613.** Making a better student chapter. **H. Mitchell**

CHED **1614.** PLNU chemistry club is involved in San Diego. M.J. Rouffet, **C. Kay**, **K. Alexander**, **B. Chicoine**, **K.C. Dornhofer**, **R.D. Robinson**

CHED **1615.** Honoring our professors and faculty: 75 years as a student chapter and 40 years of service from Jane Schley. **D. Alton**, **T.M. Dierker**, **A.M. Katsimpalis**, **S. Maurice**, **J. Samona**, **K.R. Evans**, **M.J. Mio**

CHED **1616.** Cleaning up Belle Isle: A UDM chemistry club project. **D. Alton**, **T.M. Dierker**, **J.M. Henning**, **A.M. Katsimpalis**, **S. Maurice**, **J. Samona**, **K.R. Evans**, **M.J. Mio**

CHED **1617.** St. Edward's University American Chemical Society Student Chapter. **K.L. Weber**

CHED **1618.** Propagating education in chemistry. **O.M. Price**, L.M. Berreau

CHED **1619.** Starting a Successful Student Chapter 101. **M. Lulsdorf**, **T. Harrison**

TUESDAY MORNING

Section A

Sheraton Denver Downtown Hotel

Silver

GSSPC: Designed by Nature, Developed by Science: Interdisciplinary Perspectives on Biocatalysis

Cosponsored by ANYL, BIOL, CATL, ENVR, I&EC, MEDI, ORGN and PRES

K. J. Clear, *Organizer*

K. Antonio, C. Ayres, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 CHED **1620.** Organelle bioelectrocatalysis. **S.D. Minteer**

9:15 Discussion.

9:25 CHED **1621.** Designing artificial metalloenzymes and their applications in biocatalysis for alternative energies. **Y. Lu**, A. Bhagi-Damodaran, S. Chakraborty, Y. Yu, I.D. Petrik, P. Hosseinzadeh, J. Reed, C. Cui, N.M. Marshall

10:05 Discussion.

10:15 CHED **1622.** Design and development of metal-metal bonded catalysts for transforming small molecule. **C. Lu**, R. Siedschlag, R. Cammarota, L.J. Clouston

10:55 Discussion.

Section B

Sheraton Denver Downtown Hotel

Century

Chemistry Education Research: Graduate Student Research Forum

E. Humphreys, S. E. Nielsen, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 CHED **1623.** Assessing the effectiveness of POGIL-PCL workshops. S.S. Hunnicutt, **S. Stegall**

8:55 CHED **1624.** How instructors and materials influence the development of scientific arguments and conceptual understanding of thermodynamics in POGIL classrooms. **C.L. Stanford**, N.M. Becker, J. Byers, A.C. Moon, M.H. Towns, R.S. Cole

9:15 Intermission.

9:35 CHED **1625.** Development and implementation of the enzyme-substrate interactions inquiry activity for a biochemistry survey course. **E. Humphreys**, K.J. Linenberger

9:55 CHED **1626.** Topic-specific pedagogical content knowledge (PCK) in chemistry: A characterization of chemical bonding PCK in high school teachers. **R.T. Smith**, E.J. Yezierski

10:15 CHED **1627.** Investigating the tutor-learning effect: Identification of predictors of tutors' productive behaviors. **J. Velasco**, M.N. Stains

10:35 CHED **1628.** Investigating student perceptions and opinions regarding recitation techniques in general chemistry. **J.M. Blechle**, N.E. Levinger, E.R. Fisher

10:55 CHED **1629.** Metamorphosis: Transforming a general chemistry lab to a blended course. **S. Burchett**, J.L. Hayes, K.H. Woelk

11:15 Concluding Remarks.

Section C

Sheraton Denver Downtown Hotel

spruce

ACS-CEI Award for Incorporating Sustainability into Chemistry Education

Cosponsored by CEI

K. E. Peterman, *Organizer, Presiding*

8:30 CHED **1630.** Sustainability and undergraduate chemistry education: How far we have come, and what work remains. **M.A. Fisher**

9:00 CHED **1631.** It's about *connections*: Sustainability in a liberal arts curriculum. **K. Anderson**

9:30 CHED **1632.** Empowering undergraduates for sustainability research and education. **D.A. Vosburg**

10:00 CHED **1633.** Incorporating Green chemistry and sustainability into the undergraduate curriculum at UC Berkeley. **J. Arnold**, A. Stacy, A.M. Baranger, M.C. Douskey, M. Robak

10:30 CHED **1634.** Using the chemistry curriculum as the starting point for engaging students and their families in pro-environmental behaviors. **P.L. Daubenmire**

Section D

Sheraton Denver Downtown Hotel

Denver

NSF Programs That Support Undergraduate Education

R. K. Boggess, *Organizer*

C. A. Burkhardt, *Organizer, Presiding*

8:30 Introductory Remarks.

8:40 CHED **1635.** Using TUES funds to create undergraduate scholarship. **S.M. Schelble**, K. Elkins, R.D. Walker, M. Wieder, E. Tsai

9:10 CHED **1636.** Implementing Raman spectroscopy into the chemistry curriculum. **E.M. Rezler**, A.C. Terentis, S. Hyvarinen, J.E. Haky

9:40 Intermission.

9:50 CHED **1637.** PhET interactive simulations: Using research-based simulations to transform undergraduate chemistry education. **Y. Carpenter**, E.B. Moore, R. Parson, K.K. Perkins

10:20 CHED **1638.** Active learning project of the Analytical Sciences Digital Library. **T.J. Wenzel**

10:50 CHED **1639.** Student learning and attitudes in real world vs. virtual laboratories. **K.J. Winkelmann**, W. Keeney-Kennicutt, C. Ahlborn, D. Fowler

11:20 Concluding Remarks.

Section E

Sheraton Denver Downtown Hotel

Columbine

George C. Pimentel Award in Chemical Education: Symposium in Honor of I. Dwaine Eubanks

Sputnik to Smartphones: A Half-Century of Chemistry Education

Cosponsored by HIST‡

Financially supported by ChemSource, Inc.

M. Orna, *Organizer, Presiding*

8:30 CHED **1640.** How things were then, and why history matters. **M. Orna**

8:55 CHED **1641.** Getting it right: A paradigm for the education of chemists. **J.A. Bell**

9:20 CHED **1642.** Chapter 6: New models for teacher preparation and enhancement. **B.P. Sitzman**

9:45 CHED **1643.** Access and diversity: Role of the two-year college. **A.K. El-Ashmawy**

10:10 CHED **1644.** College chemistry for non-scientists. **A.T. Schwartz**

10:35 Intermission.

10:50 CHED **1645.** What can the learning sciences tell us about teaching chemistry? **M. Cooper**

11:15 CHED **1646.** Enhancing and assessing conceptual understanding. **D.M. Bunce**

11:40 CHED **1647.** Visualization: The key to understanding chemistry concepts. **L.L. Jones**, R.M. Kelly

12:05 CHED **1648.** ACS's role in improving chemistry education — synergism between governance and staff. R.D. Archer, **M.K. Lester**

Section F

Sheraton Denver Downtown Hotel

Gold

Citizens First: Communicating Climate Science to the Public

Cosponsored by CEI‡

A. Hoffman, T. Scherban, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 CHED **1649.** Climate change: Opportunities and challenges for ACS and its members. **B.Z. Shakhashiri**

8:55 CHED **1650.** Communicating science in the public sphere: An elective course for science and engineering majors. **R.S. Black**, C.J. Bode, V.H. Smith

9:15 CHED **1651.** Facilitating chemistry club climate change outreach. **B. Chandler**

9:35 CHED **1652.** Infrared radiation and greenhouse gases: An introductory chemistry laboratory experiment. **M.R. Bruce**, T. Wilson, A.E. Bruce, S. Bessey

9:55 CHED **1653.** Communicating climate science by educating chemists in the Puget Sound. **C.E. Flener-Lovitt**, N. Milanovich

10:15 Intermission.

10:25 CHED **1654.** Communicating climate science to non-science groups. **J.B. Miller**

10:45 CHED **1655.** Challenges and success factors of student run climate change demonstrations and exhibits. **K.L. Klingenberg**, S.J. Underwood, R. Reddick, T. Greenwood, E. Dannen, A. Hoffman, T. Scherban

11:05 CHED **1656.** Cli-Sci Teacher Workshops: Outreach activities and demonstrations in the Illinois heartland. **C. Shaw**, B. Chandler, B. Gottemoller

11:25 CHED **1657.** Climate Science Toolkit: A sucessful project in Puerto Rico. **S.M. Delgado-Rivera**, **M.D. Rodriguez Guzman**, **I.D. Montes-González**, A.J. Gonzalez Nieves, J.G. Perez Colon, O.J. Morales Martinez, J.C. Aponte-Santini

11:45 CHED **1658.** Energy and the environment: Exploring climate change. **A. Kahl**

12:05 CHED **1659.** Communicating climate change: More than a message in a bottle. **L.E. Pence**

12:25 Concluding Remarks.

12:30 Information Sharing.

TUESDAY AFTERNOON

Section A

Sheraton Denver Downtown Hotel

Silver

GSSPC: Designed by Nature, Developed by Science: Interdisciplinary Perspectives on Biocatalysis

Cosponsored by ANYL, BIOL, CATL, ENVR, I&EC, MEDI, ORGN and PRES

L. Woods, *Organizer*

A. Gans, M. Pillers, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 CHED **1660.** Enzyme mechanisms: From physical chemistry to evolution and new drug targets. **A. Kohen**

2:15 Discussion.

2:25 CHED **1661.** Harnessing polyketide thioesterases to produce complex molecules. **C.N. Boddy**, G. Heberlig, T.P. Hari, M. Horsman

3:05 Discussion.

3:15 CHED **1662.** Lov story in biocatalyis: Natural product biosynthesis and protein engineering coming together. **Y. Tang**

3:55 Discussion.

4:05 CHED **1663.** Innovations in biocatalysis for pharmaceutical applications. **G.W. Huisman**

4:45 Discussion.

4:55 Concluding Remarks.

Section B

Sheraton Denver Downtown Hotel

Century

Chemistry Education Research

General Chemistry

J. Barbera, N. P. Grove, *Organizers*

J. P. Suits, *Presiding*

1:30 Introductory Remarks.

1:35 CHED **1664.** Case studies of problem solving strategies used by college professors, graduate, and undergraduate students in chemistry. **T. Gupta**

‡ *Cooperative Cosponsorship*

1:55 CHED **1665.** Gaining insight into visual problem solving by combining eye-tracking with multimodal data analysis. **S.J. Hansen**, F. Moore, P. Gordon, O. Anderson

2:15 CHED **1666.** Numerical comparisons of eye fixation sequences from chemistry problem solving. **J. Baluyut**

2:35 CHED **1667.** Study of self-explaining skill development in college level introductory chemistry courses via latent transition analysis. **A. Villalta-Cerdas**

2:55 CHED **1668.** Using an interactive simulation to support student development of expert practices for balancing chemical equations. **Y. Carpenter**, E.B. Moore, K.K. Perkins

3:15 Intermission.

3:30 CHED **1669.** Students' growth in scientific reasoning and the implications for chemistry instruction. **J.H. Carmel**, E.J. Yezierski

3:50 CHED **1670.** Characterizing students' explanations of energy change at the atomic-molecular level. **N.M. Becker**, K. Noyes, M. Cooper

4:10 CHED **1671.** Integrating scale-themed instruction into the undergraduate general chemistry curriculum using active learning methodologies. **J.M. Trate**, P. Geissinger, A. Blecking, K.L. Murphy

4:30 CHED **1672.** Exploring an inverted classroom model in General Chemistry II using POGIL style activities and undergraduate Learning Assistants. **U. Swamy**

4:50 CHED **1673.** Stop cheating! An evaluation of a scientific integrity writing strategy in General Chemistry I. **M.L. Edwards**

5:10 Concluding Remarks.

Section C

Sheraton Denver Downtown Hotel
Spruce

Perspectives on Climate Change Literacy and Education: Local to International

G. P. Foy, *Organizer*
K. E. Peterman, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CHED **1674.** Fracking and carbon sequestration, oh my: Connecting general chemistry students to climate change topics. **K. Anderson**, D.B. King, J.E. Lewis, G.H. Webster, S. Sutheimer, D.E. Latch, C.H. Middlecamp, R.S. Moog

1:55 CHED **1675.** Climate change and public health: The importance of literacy domestically and globally. **N. Diklich**, K.E. Peterman, G.P. Foy

2:15 CHED **1676.** Climate change impacts on biodiversity and mitigation efforts. **C. King**, K.E. Peterman, G.P. Foy

2:35 CHED **1677.** Energy discussions at the 20th Conference of Parties. **B. Hartweg**

2:55 CHED **1678.** Effects on agriculture from climate change. **S. Bariana**, G.P. Foy, K.E. Peterman

3:15 Intermission.

3:25 CHED **1679.** Campaign strategy, outreach, and advocacy efforts at the UN Climate Conference. **R.B. Sobel**

3:45 CHED **1680.** Geopolitical effects of climate change in the Arctic. **K.T. O'Keefe**, G.P. Foy, K.E. Peterman

4:05 CHED **1681.** How climate change will exacerbate the food, energy, and water nexus. **J. Mcdonald**

4:25 CHED **1682.** Future stance on climate change. **K. Teppert**, G.P. Foy, K.E. Peterman, D. Husic

4:45 Panel Discussion.

5:05 Concluding Remarks.

Section D

Sheraton Denver Downtown Hotel
Denver

NSF Programs That Support Undergraduate Education

C. A. Burkhardt, *Organizer*
R. K. Boggess, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 Description of NSF Programs.

1:55 Question/Answer Session.

2:15 CHED **1683.** Framing the chemistry curriculum: Year 1. **M.A. Griep**

2:45 CHED **1684.** 49erTeach: Building capacity for teachers of chemistry and physics through NSF's Noyce teacher scholarship program. **K. Asala**

3:15 Intermission.

3:25 CHED **1685.** Denver Metro Chem Scholars, an NSF S-STEM program at a large urban PUI. **R.D. Walker**, A.J. Bonham

3:55 CHED **1686.** NSF programs that support undergraduate education. **M. Cullin**

4:25 CHED **1687.** Implementing and assessing the efficacy of open access ChemWiki textbook resource. G. Allen, A. Guzman, M. Molinaro, **D.S. Larsen**

4:55 Concluding Remarks.

Section E

Sheraton Denver Downtown Hotel
Columbine

George C. Pimentel Award in Chemical Education: Symposium in Honor of I. Dwaine Eubanks

Sputnik to Smartphones: A Half-Century of Chemistry Education

Cosponsored by HIST‡

Financially supported by ChemSource, Inc.

M. Orna, *Organizer, Presiding*

1:30 CHED **1688.** Impact of technology on chemistry instruction. **R.A. Pribush**

1:55 CHED **1689.** Laboratory instruction: Less verification, more discovery. **L.P. Eubanks**

2:20 CHED **1690.** Evolution of undergraduate research as a critical component in the education of chemistry students. **B.E. Holmes**

2:45 CHED **1691.** Standards and expectations. **P. Smith**

3:10 Intermission.

3:25 CHED **1692.** Trajectory of testing in chemistry education. **T. Holme**

3:50 CHED **1693.** Inquiry activities based on Simulations and Animations. **J.I. Gelder,** M.R. Abraham, T.J. Greenbowe

4:15 CHED **1694.** Developments in chemical education: Influences, successes, and failures in adaptations in other countries. **D. Waddington**, H.W. Heikkinen

4:40 CHED **1695. Award Address** (George C. Pimentel Award in Chemical Education sponsored by Cengage Learning and the ACS Division of Chemical Education). Challenges for the next generation. **D. Eubanks**

Section F

Sheraton Denver Downtown Hotel
Gold

Overcoming Obstacles in Student Learning in Physical Chemistry

A. L. Marsh, A. Noble, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 CHED **1696.** Rethinking homework: The impact of content, format, and process on physical chemistry learning outcomes. **T.D. Shepherd**

1:55 CHED **1697.** Preparing students for effective engagement in group problem solving. **A.R. Noble**

2:15 CHED **1698.** Influences of student discourse in overcoming barriers in physical chemistry. **C.L. Stanford**, N.M. Becker, J.D. Byers, A.C. Moon, M.H. Towns, R.S. Cole

2:35 Intermission.

2:45 CHED **1699.** POGIL in the physical chemistry laboratory. **A. Grushow**, S.S. Hunnicutt, R.M. Whitnell

3:05 CHED **1700.** Quantum first physical chemistry at a regional liberal arts college. **A.L. Marsh**

3:25 CHED **1701.** Learning by doing: Teaching physical chemistry using guided inquiry with frequent feedback. **S.S. Hunnicutt**

3:45 Intermission.

3:55 Panel Discussion.

4:15 Concluding Remarks.

TUESDAY EVENING

Section A

Sheraton Denver Downtown Hotel
Gold

General Papers

S. A. Fleming, *Organizer*
C. Hamann, *Presiding*

6:00 Introductory Remarks.

6:05 CHED **1702.** Multistep synthesis of benzoyl peroxide for the second semester organic laboratory. **J. Wollack**

6:25 CHED **1703.** Where's the ketone: A laboratory showing the control of reaction intermediates in Grignard reactions with esters. **R.D. Barrows**, L. Giacomine, D. Hanson, A. Sylvester

6:45 CHED **1704.** Carbocation rearrangements in the undergraduate laboratory: GC/MS and NMR deduction of products from electrophilic aromatic substitution in a discovery laboratory experiment. M.V. Maskornick, V. Polito, I.J. Rhile, **C.S. Hamann**

7:05 Intermission.

7:15 CHED **1705.** Importance of sampling: The first lab in the analytical chemistry class. **R. Indralingam**

7:35 CHED **1706.** Organic chemistry and the native plants of the Sonoran Desert: A new model for the undergraduate laboratory. **T.L. Minger**, V. Nedelkova, J. Zikopoulos

7:55 CHED **1707.** Safety for chemical demonstrations. **D.A. Katz**

8:15 Intermission.

8:25 CHED **1708.** Synthesis and the three-separate independent purification of 3-nitrooacetanilide: An exercise in recrystallization, extraction and radial chromatography in the undergraduate organic chemistry labs. **R.B. Miller**

8:45 CHED **1709.** Teaching research in organic chemistry with a "guided-research" laboratory experience. **R. LaLonde**

9:05 CHED **1710.** Investigating enzyme assays. **W.A. Patton**

9:25 CHED **1711.** Introduction of the professional quote format and compound screening to project-based experiments in the biochemistry laboratory. **K.R. Gallagher**

9:45 CHED **1712.** Design and implementation of a multi-method enzyme kinetics project for a junior-level studio laboratory. **D.R. Goode**, R.L. Hutcheson, C.V. Crisan, J.D. Mimbs

WEDNESDAY MORNING

Section A

Sheraton Denver Downtown Hotel
Silver

Green Chemistry: Theory and Practice

Cosponsored by CEI‡

Financially supported by NSF-CCI Center for Sustainable Polymers at the University of Minnesota; ACS Green Chemistry Institute; I&EC Green Chemistry Subdivision

J. E. Wissinger, *Organizer*
E. J. Brush, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 CHED **1713.** Green chemistry of biodiesel production. **V. Gude**, E. Martinez-Guerra

8:55 CHED **1714.** Biorefinery: A molecular design platform for green surfactants and soft materials. **G. John**

9:15 CHED **1715.** Greener synthesis of photochromic, fluorescent, and industrially important organic compounds for one- and two-semester organic chemistry laboratories. **J. Bennett**, D. Dragotta, E. Stopler

9:35 CHED **1716.** Nickel-catalyzed Suzuki–Miyaura cross-coupling in a green alcohol solvent for an undergraduate organic chemistry laboratory. **N.K. Garg**

9:55 Intermission.

10:05 CHED **1717.** Paper to plastics: An interdisciplinary outreach program in sustainable research. **J. Byers**, E. Weerapana, F.B. Tamburini, T.B. Kelly, N. Chinnaswamy, T. Fazekas

10:25 CHED **1718.** Hands-on, inquiry-based laboratory experiment for chemistry and engineering students comparing "green" and "nongreen" Noble metal nanoparticle synthesis methods. **M.L. Edwards**, **S.A. Paluri**

10:45 CHED **1719.** Green chemistry principles illustrated through the synthesis of renewable triblock copolymers: an inquiry-based experiment. **J.E. Wissinger**, D.K. Schneiderman, M.T. Wentzel

11:05 CHED **1720.** Decision-making based on evaluation of the benefits, costs, and risks associated with the use and production of chemicals. **H. Sevian**, S. Cullipher, V. Talanquer

11:25 Panel Discussion.

11:45 Concluding Remarks.

Section B

Sheraton Denver Downtown Hotel
Century

Chemistry Education Research

Concept Inventories

J. Barbera, N. P. Grove, *Organizers*
J. R. Raker, *Presiding*

8:30 Introductory Remarks.

8:35 CHED **1721.** Development of a chemistry concept inventory online database. **K.J. Linenberger**

8:55 CHED **1722.** Student alternative conceptions of theory application during first year General Chemistry: Does anything really change? **W.E. Schatzberg**

9:15 CHED **1723.** Development of stereochemistry concept inventory using principles of effective test construction and results from national surveys. **A. Leontyev**, R.M. Hyslop

9:35 CHED **1724.** Detecting incorrect ideas in stereochemistry. **A. Leontyev**, R.M. Hyslop

Section B

Sheraton Denver Downtown Hotel
Century

Chemistry Education Research

Online Homework

J. Barbera, N. P. Grove, *Organizers*
J. R. Raker, *Presiding*

10:10 CHED **1725.** Students' short and long term impressions, attitudes, percieved learning, and actual performance using two online homework systems: Embedded text vs. linked text. **C. Zumalt**, V.M. Williamson

10:30 CHED **1726.** Developing student-generated content in sapling learning. **D.M. Zurcher**, B.P. Coppola, A.J. McNeil

10:50 CHED **1727.** Form vs. function: A comparison of Lewis structure drawing tools and the cognitive loads they induce. **P. Duffy**, A. Coleman, T. Gampp, J.M. Tiettmeyer, N.P. Grove

11:10 CHED **1728.** How many tries are optimal for on-line homework? **C.H. Atwood**, J. Moody

11:30 Concluding Remarks.

Section C

Sheraton Denver Downtown Hotel

Spruce

Process-Oriented Guided Inquiry Learning (POGIL)

R. S. Moog, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 CHED **1729.** Introduction to POGIL and The POGIL Project. **R.S. Moog**

8:55 CHED **1730.** High school chemistry POGIL activites on a dollar store budget. **A.S. Schwab**

9:15 CHED **1731.** Using knowledge surveys to assess student knowledge gains from POGIL activities. **B.D. Gilbert**

9:35 CHED **1732.** Quantum, spectroscopy, bonding with POGIL in first semester physical chemistry. **N.E. Levinger**

9:55 Intermission.

10:05 CHED **1733.** POGIL on a large scale. **S.M. Taylor**, C.A. LaBrake, D. Vanden Bout

10:25 CHED **1734.** Using POGIL in a large lecture setting: The benefits and the challenges. **T.A. Madison**

10:45 CHED **1735.** Guided inquiry in chemistry: Teaching assistant training courses for undergraduates. **S.S. Hunnicutt**

11:05 Panel Discussion.

Section D

Sheraton Denver Downtown Hotel

Denver

Instructors and Researchers: Advancing Graduate Education in Chemistry

S. Hansen, S. Sandi-Urena, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 CHED **1736.** ETTA: Educational Training for Teaching Associates. P. Varma-Nelson, **L. Easterling**, J.R. Gregory

8:55 CHED **1737.** Orientation and teacher training programs for graduate students. **M.L. Miller**, R. Hirko

9:15 CHED **1738.** Evaluation methods and findings for interdisciplinary graduate training programs at UBC. **J.J. Stewart**, A.K. Bertram, L. Schafer, K.J. Knox, G. Birol, S. Burke, C. Underhill

9:35 CHED **1739.** Graduate teaching assistants' potential benefits and professional development associated with teaching general chemistry laboratories. **S. Sandi-Urena**, T. Gatlin

9:55 Intermission.

10:05 CHED **1740.** It takes a village: Transition from graduate student to practitioner. **G. Bhattacharyya**, G.M. Bodner, A. Verdan

10:25 CHED **1741.** Bringing chemical research into the undergraduate teaching lab: A graduate student perspective. **J. Zhu**, S. Hansen, L. Kaufman, J. Ulichny

10:45 CHED **1742.** How my teaching role has impacted my graduate student experience. **M.L. Miller**, D.P. Cartrette, O. Odeleye, T. Cox, M. Stutelberg

11:05 Concluding Remarks.

Section E

Sheraton Denver Downtown Hotel

Columbine

Using Technology in the Undergraduate Laboratory

A. Oxley, C. E. Stilts, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 CHED **1743.** Agent-based modeling as a tool for a discovery-based TLC experiment. **D. Brownholland**, M. Goadrich

8:55 CHED **1744.** Home-built instruments as group projects in instrumental analysis courses. **M. Chia**, A. Blank, A. Sabelhaus, B. Wiefering, C.A. Morris

9:15 CHED **1745.** Implementation of cost-effective tablet technology for the development of electronic laboratory notebook skills and to promote active learning at the undergraduate level. **R.N. Dansby-Sparks**, R.M. Meier

9:35 CHED **1746.** Flipping the General Chemistry laboratory. **A. Oxley**

9:55 Intermission.

10:05 CHED **1747.** 3D printed colorimeters for use in the freshman chemistry lab. **J.D. Mendez**

10:25 CHED **1748.** Designing and implementing effective virtual laboratory experiments in general chemistry. **K.J. Winkelmann**, W. Keeney-Kennicutt

10:45 CHED **1749.** Organic lab transformation. **J. Potratz**

11:05 CHED **1750.** Electronic grading of laboratory reports to account for variation in student data. **E.M. Epp**, K. Nippert

11:25 CHED **1751.** Using QR codes and online videos in the undergraduate organic chemistry lab. **C.E. Stilts**

11:45 Concluding Remarks.

Section F

Sheraton Denver Downtown Hotel

Gold

Computational Chemistry in the Undergraduate Curriculum: What is Working and How Do We Assess It?

Cosponsored by PHYS

J. L. Sonnenberg, *Organizer*

J. B. Foresman, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 CHED **1752.** What makes an electron a valence electron? Introducing students to computational chemistry in the POGIL-PCL framework. **M.S. Reeves**

8:55 CHED **1753.** Withdrawn.

9:15 CHED **1754.** Utilizing electronic structure calculations in undergraduate inorganic chemistry. **J.T. York**

9:35 Intermission.

9:50 CHED **1755.** Web based computational job submission for the undergraduate laboratory. **M.J. Perri**, S.H. Weber

10:10 CHED **1756.** Quantum and computational chemistry: A difficult and necessary classroom union. **M.F. Tuchler**

10:30 CHED **1757.** Gaussian-based laboratory exercises in physical chemistry. **S.M. Basu**

10:50 Intermission.

11:05 CHED **1758.** Computational chemistry in the physical chemistry course. **T. Engel**, L. Johnson

11:25 CHED **1759.** 15-year retrospective of computational chemistry in the undergraduate curriculum at The University of Tulsa. **G.H. Purser**, G.R. Medders

11:45 CHED **1760.** Assessment of student knowledge and opinions of computational chemistry in a physical chemistry for engineer's course. **E.P. Wagner**

12:05 CHED **1761.** Atomistic level computational chemistry for visualization and calculation in the undergraduate chemistry laboratory. **L. Tribe**

WEDNESDAY AFTERNOON

Section A

Sheraton Denver Downtown Hotel

Silver

Green Chemistry: Theory and Practice

Cosponsored by CEI‡

Financially supported by NSF-CCI Center for Sustainable Polymers at the University of Minnesota; ACS Green Chemistry Institute; I&EC Green Chemistry Subdivision

E. J. Brush, *Organizer*

J. E. Wissinger, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CHED **1762.** Adapting green chemistry metrics for nanoparticle synthesis. B. Reid, **S.M. Reed**

1:55 CHED **1763.** New shoots from old vines: Greening reactions in the organic chemistry laboratory. **T.N. Jones**, K.J. Graham, C.P. Schaller, E.J. McIntee

2:15 CHED **1764.** Case study: Green chemistry — theory and practice in an undergraduate laboratory. **O. Oluwaniyi**, S.O. Famuyiwa

2:35 CHED **1765.** Educating general chemistry students about green chemistry through their laboratory experience. **S.A. Henrie**

2:55 Intermission.

3:05 CHED **1766.** Need for green chemistry at the undergraduate level. **I.T. Sidhwani**, R. Sharma

3:25 CHED **1767.** Incorporation of green principals across a chemistry curriculum at a small liberal arts college. **J. Wollack**

3:45 CHED **1768.** Project GreenLab: A regional student-faculty collaboration in green chemistry curriculum development, research, and outreach education. **E.J. Brush**

4:05 CHED **1769.** Green chemical education in curriculum: Cracking siloed education. **C.D. Jensen**

4:25 Panel Discussion.

4:45 Concluding Remarks.

Section B

Sheraton Denver Downtown Hotel

Century

Chemistry Education Research

Organic and Biochemistry

J. Barbera, N. P. Grove, *Organizers*

T. Bussey, *Presiding*

1:30 Introductory Remarks.

1:35 CHED **1770.** Acid-base topic in the context of a nursing chemistry course. **C.E. Brown**, M.L. Henry, R.M. Hyslop

1:55 CHED **1771.** Comparative study of organic chemistry representations and students' cognitive load. **P. Duffy**, N.P. Grove

2:15 CHED **1772.** Student understanding of glycolysis: Organic chemistry tasks in a biochemistry context. **J.R. Raker**, B.R. Van Norman

2:35 CHED **1773.** Biochemistry instructors' perceptions of their classroom use of analogies. **T.J. Bussey**, M. Orgill

Section B

Sheraton Denver Downtown Hotel

Century

Chemistry Education Research

Chemistry Majors

J. Barbera, N. P. Grove, *Organizers*

T. Bussey, *Presiding*

3:10 CHED **1774.** Concept mapping: A learning strategy for teaching Instrumental Chemical Analysis course. **T. Saleh**

3:30 CHED **1775.** Student grade perceptions throughout a chemistry program (Freshman-Master's). **J.A. Webb**, A.G. Karatjas

3:50 CHED **1776.** Investigating the enacted and stated curriculum in physical chemistry. **S.E. Erhart**, E.J. Yezierski

4:10 Concluding Remarks.

Section C

Sheraton Denver Downtown Hotel

Spruce

Research on Learning in the Laboratory

M. J. Chrzanowski, S. Sandi-Urena, A. Villalta-Cerdas, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 CHED **1777.** Improving general chemistry students' inquiry skills and confidence with research-inspired experiments. **K.J. Winkelmann**, M.H. Baloga, C. Giannoulis, T. Marcinkowski, P. Cohen, G. Anquandah

1:55 CHED **1778.** Current research on learning in the chemistry college laboratory. **S. Sandi-Urena**

2:15 CHED **1779.** Incorporation of instructional videos to encourage students' coordination of theory and evidence in the physical chemistry laboratory. R.S. Cole, **M.N. Muniz**, J.A. Schmidt, E. Keuter

2:35 Intermission.

2:45 CHED **1780.** Examining student analogical reasoning in introductory chemistry laboratory. **M.R. Bruce**, S. Avargil, A.E. Bruce, F.G. Amar

3:05 CHED **1781.** Perceptions of students and teaching assistants regarding a project-based undergraduate laboratory. **S.R. Mooring**, N.L. Burrows

3:25 CHED **1782.** Reform in general chemistry laboratory instruction: How do students experience change between an expository laboratory and a cooperative project-based laboratory? **M.J. Chrzanowski**, S. Sandi-Urena

3:45 Discussion.

Section D

Sheraton Denver Downtown Hotel

Denver

Undergraduate Research in Chemistry: Expanding Opportunities and Broadening Participation

Models Supporting and Expanding Undergraduate Research

B. L. Gourley, R. M. Jones, *Organizers, Presiding*

1:30 Introductory Remarks.

1:40 CHED **1783.** First-Year Research Experience (FYRE) program: A gateway to undergraduate research and enhanced STEM development at the University of Oklahoma. **N. Kothapalli**, **A. Burgett**, **R. Halterman**

2:00 CHED **1784.** Guiding a senior undergraduate in chemical education and computational chemistry research. J.P. Beck

2:20 CHED **1785.** PRISM: CSUSB strengthening the scientific workforce. **K.R. Cousins**, Y. Kim

2:40 CHED **1786.** Integrating undergraduate research with teaching and learning: Unanticipated opportunities to broaden participation. **L.E. Echegoyen**, S.B. Aley, C.E. Botez, G. Corral, H.H. Meeuwsen, D. Villagran

Section D

Sheraton Denver Downtown Hotel

Denver

Undergraduate Research in Chemistry: Expanding Opportunities and Broadening Participation

Undergraduate Research in the Curriculum

B. L. Gourley, R. M. Jones, *Organizers, Presiding*

3:00 CHED **1787.** Freshman research immersion: Transforming freshman into researchers. **M.E. Fegley**, **J.R. Amey**, W.E. Jones, N.E. Stamp

3:20 CHED **1788.** Research-based analytical chemistry laboratory: Incorporation of students' self-designed projects into curriculum. **R. Gao**

3:40 CHED **1789.** Increasing reach: Dealing with resource limitations and scalabilty issues by bringing collaborative research into the teaching laboratory. **R.E. Bachman**

4:00 CHED **1790.** Components of a research-rich undergraduate chemistry curriculum. **T.J. Wenzel**

4:20 Concluding Remarks.

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‡ *Cooperative Cosponsorship*

Section E

Sheraton Denver Downtown Hotel

Columbine

Nanotechnology in Undergraduate Education and Research

D. S. Heroux, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CHED **1791.** Nanotechnology experiments for inorganic chemistry laboratory. **D.S. Heroux**

1:55 CHED **1792.** Synthesis and exploration of Au nanoparticles in an open-ended junior-level capstone lab. **C.S. Seney**, J.D. Mimbs

2:15 CHED **1793.** Harnessing the power of partnerships and technology in nanoscience education. **K.A. Pacheco**, **J. Ristvey**

2:35 Intermission.

2:45 CHED **1794.** Debating societal impacts of nanotechnology through role playing. **K.J. Winkelmann**

3:05 CHED **1795.** Synthesis and comparative study of ZnO/Au, ZnO/Ag, MgO/Au, and MgO/Ag core-shell nanoparticles with their functionalization with antibiotics. **C. Pellicier Rodriguez**, M. Feliciano Sanchez, E. Medina, J.I. Ramirez Domenech, C. Osorio Cantillo, E.J. Ferrer Torres

3:25 CHED **1796.** Investigating the antimicrobial properties of silver nanoparticles with respect to *Desulfovibrio* genus bacteria. **J. Snitker**, M. Montes

3:45 Concluding Remarks.

Section F

Sheraton Denver Downtown Hotel

Gold

Computational Chemistry in the Undergraduate Curriculum: What is Working and How Do We Assess It?

Cosponsored by PHYS

J. B. Foresman, *Organizer*

J. L. Sonnenberg, *Organizer, Presiding*

1:30 CHED **1797.** Computational chemistry should start in high school. **R.R. Gotwals**

1:50 CHED **1798.** Computational chemistry throughout the curriculum. **K. Range**

2:10 CHED **1799.** Computational modelling across the curriculum: General, organic and physical chemistry. M.W. Ducey, D.R. Myers, **J.S. Rhoad**, **J.N. Woodford**

2:30 Intermission.

2:45 CHED **1800.** Computational chemistry in an undergraduate curriculum: Strategies for deliverable skills. **M.M. Ivey**, J.L. Sonnenberg

3:05 CHED **1801.** Examples of instructional units in computation and modeling for the undergraduate chemistry curriculum. **L.S. Pelter**, M.W. Pelter

3:25 CHED **1802.** 20 years of computational chemistry at a public regional university: Thoughts and experiences. **M. Pelter**, L. Pelter

3:45 Intermission.

4:00 CHED **1803.** Computational chemistry: Practical issues in leveraging the Cloud. **R. Thackston**, B. Kimmons, R.C. Fortenberry

4:20 CHED **1804.** PSI4Education: Computational chemistry labs using free software. **R.C. Fortenberry**, **T.D. Shepherd**, A. Ringer McDonald, M. Kennedy, D. Sherrill

4:40 CHED **1805.** Challenges and rewards of the computational chemistry undergraduate thesis project. **R.C. Brown**

5:00 CHED **1806.** NCSI workshops are ready to help train faculty to use computational chemistry in the classroom. **C. Metz**, S.C. Sendlinger, E.T. Bell-Loncella, R. Panoff

THURSDAY MORNING

Section A

Sheraton Denver Downtown Hotel

Gold

General Papers

S. A. Fleming, *Organizer*

C. R. Pharr, *Presiding*

8:00 Introductory Remarks.

8:05 CHED **1807.** Building connections in biology and chemistry courses in the second year curriculum. **S.R. Sieck**

8:25 CHED **1808.** Chemical analysis of paint: Development of multidisciplinary class sessions for chemistry and art students. **B. Sieve**, J. Hedges, **C.A. Morris**

8:45 CHED **1809.** Interdisciplinary experimental approach for undergraduate chemistry students. **C. Lobato**, N. Romero-Ceronio, A. Gomez-Rivera, L. Roa-De la Fuente

9:05 Intermission.

9:15 CHED **1810.** Flipped classroom for large organic chemistry class. **S. Xie**

9:35 CHED **1811.** Half flipped: Using videos and online quizzes to maximize in class problem solving time. **C.R. Pharr**

9:55 CHED **1812.** Flipping general chemistry to improve student success. **C.M. Zaleski**

10:15 Intermission.

10:25 CHED **1813.** Unit Conversion Literacy Project: A partnership model for driving curricular change. **G. Baker**

10:45 CHED **1814.** Engaging science students and the public through science-themed art. **D.B. Cordes**

11:05 CHED **1815.** Sophomore organic chemistry to synthesize that? **J.K. Murray**

11:25 CHED **1816.** Capstone experience for the sophomore organic chemistry sequence emphasizing written and oral expression. **L.R. Eller**

Section B

Sheraton Denver Downtown Hotel

Century

General Papers

S. A. Fleming, *Organizer*

M. T. Mongelli, H. Stokes-Huby, *Presiding*

8:00 Introductory Remarks.

8:05 CHED **1817.** Exploring DNA and protein structures with PyMOL. **J.A. Himmelberger**

8:25 CHED **1818.** Teaching general chemistry in context using the ChemConnections Activity Workbook. **K.L. Braun**, H. Mernitz, S. Anthony

8:45 CHED **1819.** Demonstrating the intelligence capabilities of the Q-electronic tutor. **T.R. Farhat**

9:05 Intermission.

9:15 CHED **1820.** Polycraft: Utilizing online gaming to enable next generation polymer chemistry education. **W. Voit**

9:35 CHED **1821.** Teaching and learning with a tablet. **H. Stokes-Huby**, **M.T. Mongelli**

9:55 CHED **1822.** Incorporating peer-review homework assignments into a large enrollment freshman chemistry course. **C.T. Cox**, R.N. Zare, K. Murphy

10:15 Intermission.

10:25 CHED **1823.** Student designed organic laboratories as an alternative research project. R.B. **Lettan II**, S. Sagcan, S. Candiello

10:45 CHED **1824.** Designing accessible linteractive chemistry simulations for all students – including students with disabilities. **E.B. Moore**, A. Paul, K. Perkins

11:05 CHED **1825.** Perceptions of competency for male and female chemistry majors: Does he receive more credit? **R.P. Beeton**, S. Hilwig, T. Martinez

Section C

Sheraton Denver Downtown Hotel

spruce

General Papers

S. A. Fleming, *Organizer*

J. D. Mendez, *Presiding*

8:00 Introductory Remarks.

8:05 CHED **1826.** Guided inquiry laboratory experiment water analysis and hands-on experience for K-12 students in the Advancing Mathematics and Science Skills Program. **S.O. Fakayode**, M. Kanipes-Spinks

8:25 CHED **1827.** Collaboration between historically black colleges and universities and local school districts to promote K–12 science education, North Carolina, USA. **S. Fakayode**, V. Snipes, M. Kanipes-Spinks

8:45 CHED **1828.** Quantitative approach to the study of the effectiveness of using the Dual Credit General Chemistry I Program at Missouri Western State University as a recruiting tool. **J.L. Torres y Torres**, M.W. Ducey

9:05 Intermission.

9:15 CHED **1829.** Electrolytic reactions of reagent precursors for preparation and standardization of commonly used reagents in an undergraduate laboratory. S. Melaku, **R. Dabke**

9:35 CHED **1830.** Towards increasing student engagement in the general chemistry laboratory with environmental research. **R. Driscoll**, J. Hall Tomasik, A. Miller, S.A. Majorski, D.J. Lecaptain

9:55 CHED **1831.** Utilizing 3D printing to create demonstrative models for freshman chemistry courses. **J.D. Mendez**

10:15 Intermission.

10:25 CHED **1832.** Integrative and exploratory junior-level studio laboratory for student-centered learning and scientific growth. **D.R. Goode**, D.E. Moore, C.S. Seney, A.M. Kiefer

10:45 CHED **1833.** Solution concentration uncertainty: An experiment to illustrate the concepts of precision and propagation of error through measurement of the molar extinction coefficient of $Cu(NH_3)_4Cl_2$. **J.J. Stankus**

11:05 CHED **1834.** Laboratory experiment: Carbonates and the ideal gas law. **T. Hodgkins**

11:25 CHED **1835.** Open source drug discovery with undergraduates and high school students. **A.E. Williamson**, M.H. Todd, P. Willis, O. Consortium

CHAS

Division of Chemical Health and Safety

D.M. Decker, F. K. Wood-Black and J. M. Pickel, *Program Chairs*

MONDAY AFTERNOON

Section A

Embassy Suites Denver–Downtown Convention Center

Silverton Ballroom 1

Legalized Marijuana & Health & Safety

Cosponsored by CCS

N. R. Langerman, R. W. Phifer, *Organizers, Presiding*

1:30 Introductory Remarks.

1:40 CHAS **1.** Taking care of Mary Jane's workers. **J. Lieberman**

2:10 CHAS **2.** Safety considerations in the development of sensible workplace drug testing policies for legalized marijuana. **R.W. Phifer**

2:40 CHAS **3.** Marijuana health and safety for licensed and regulated businesses. **C. Villano**

3:10 CHAS **4.** State mandated testing of retail marijuana in Colorado. **A. LaFrate**

3:40 Intermission.

3:55 CHAS **5.** Safety and health standard of cannabis extractions with an emphasis on CO_2. **A. Cahoj**

4:25 CHAS **6.** Recent improvements in chromatography: Advancing chromatographic data quality to make a safer Cannabis product. A. Rigdon, **R. Lake**, R. Freeman, F. Carroll, T. Kahler

4:55 CHAS **7.** GC methods for Cannabis safety and potency testing. **A. Rigdon**, J. Cochran, C. Hilliard, W. Schroeder, C. Schroeder, T. Flood

5:25 Concluding Remarks.

MONDAY EVENING

Section A

Colorado Convention Center

Halls C/D

Sci-Mix

J. M. Pickel, *Organizer*

8:00 - 10:00

CHAS **8.** Division of Chemical Health and Safety. **D.M. Decker**

CHAS **9.** Withdrawn.

CHAS **10.** Safety survey of chemistry teaching laboratories in Nepal. B. Giri, **K. Kandel**

CHAS **11.** Lessons learned from a hood fire and deflagration event. **J.M. Pickel**

CHAS **12.** Increasing sample throughput of Cannabis analyses on any LC system. **R. Lake**, A. Rigdon, R. Freeman, F. Carroll, T. Kahler

TUESDAY MORNING

Section A

Embassy Suites Denver–Downtown Convention Center

Silverton Ballroom 1

Ask Dr. Safety: EH&S Support of Nanotechnology R&D

Cosponsored by AGFD, CCS and PRES

H. J. Elston, N. R. Langerman, *Organizers, Presiding*

9:00 Introductory Remarks.

9:05 CHAS **13.** How hazardous can nanostructured titanium dioxide be to humans in a water purification application? **P. Zuniga**, J. Quesada-Kimzey

9:25 CHAS **14.** Ask Dr. Safety: EH&S support of nanotechnology R&D. **N.R. Langerman**, H.J. Elston

10:55 Concluding Remarks.

TUESDAY AFTERNOON

Section A

Embassy Suites Denver–Downtown Convention Center

Silverton Ballroom 1

Safety in Undergraduate Teaching

Cosponsored by CCS

F. K. Wood-Black, *Organizer, Presiding*

1:30 Introductory Remarks.

Technical program information known at press time. The official technical program for the 249th ACS National Meeting is available at: www.acs.org/denver2015

1:40 CHAS **15.** Moving from a danger culture to a safety culture. **R. Stuart**

2:00 CHAS **16.** Teaching basic technique: A view into preparing for a safer educational and work environment. **F.K. Wood-Black**, K. Black

2:20 CHAS **17.** Using traditional safety rules to teach more advanced concepts in chemical hygiene. **S.B. Sigmann**

2:40 CHAS **18.** Talk dirty to me: Teaching undergraduate students the importance of good hygiene in the teaching laboratory. **L. Gallion**, A.M. Wilson, M.J. Samide

3:00 CHAS **19.** Risk hazard assessment in the general chemistry laboratory. **S.D. Wiediger**, A. Hyett

3:20 Intermission.

3:35 CHAS **20.** Developing a safety synergy in the chemistry department at Stanford University. **C.T. Cox**, S. Chan

3:55 CHAS **21.** Safety Friday: Do in-class safety presentations impact student behavior and perceptions of laboratory safety? **A.M. Wilson**, P.M. Morgan

4:15 CHAS **22.** Student view of safety in the undergraduate laboratory. **T. Black**, F.K. Wood-Black

4:35 CHAS **23.** Case study: Impact of chemical safety training in undergraduate teaching. **O. Oluwaniyi**, O.O. Fadare

4:55 CHAS **24.** Nitric acid acts upon trousers: Learning about hazardous chemicals. **K.P. Fivizzani**

5:15 Concluding Remarks.

CINF

Division of Chemical Information

E. Davis, *Program Chair*

OTHER SYMPOSIA OF INTEREST:

Drug Discovery *(see COMP, Sun, Mon, Tue, Wed)*

Applications of Positron Emission Tomography in Drug Discovery (see MEDI, Sun)

New Models for Drug Discovery: Public, Private, and Non-Profit (see MEDI, Mon)

Putting Chemical Biology in Context *(see BIOL, Tue)*

Citizens First: Communicating Climate Science to the Public *(see CHED, Tue)*

ACS Award for Computers in Chemical & Pharmaceutical Research: Symposium in Honor of David A. Case *(see COMP, Mon, Tue)*

SOCIAL EVENTS:

Reception, 6:30 PM: Sun

Harry's Party, 5:30 PM: Mon

Luncheon, 12:00 PM: Tue

BUSINESS MEETINGS:

Business Meeting, 1:00 PM: Sat

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SUNDAY MORNING

Section A

Colorado Convention Center
Room 110

Getting to the Best Reaction: Tools for Finding a Needle in a Haystack

R. Schenck, *Organizer, Presiding*

10:00 Introductory Remarks.

10:05 CINF **1.** Automated design of realistic organometallic complexes and catalysts. M. Foscato, G. Occhipinti, V. Venkatraman, B.K. Alsberg, **V.R. Jensen**

10:30 CINF **2.** Different needles for different tailors: How specialized reaction search algorithms support scientists working in various research areas. **V. Eigner Pitto**, J. Eiblmaier, H. Kraut, H. Saller, P. Loew

10:55 CINF **3.** Classification of scientific journal articles for the NIST Thermodynamic Research Center. **A. Dima**, Y. Feng, S. Youssef, K. Kroenlein

11:20 CINF **4.** Mining electronic lab notebooks for synthetic needles (or gems). **P.J. McHale**

11:45 Concluding Remarks.

SUNDAY AFTERNOON

Section A

Colorado Convention Center
Room 110

Defining "Value" in Scholarly Communications: Evolving Ways of Evaluating Impact on Science

S. Rouhi, T. M. Vogel, *Organizers, Presiding*

1:00 CINF **5.** Withdrawn.

1:25 CINF **6.** Dynamic evaluation of impact for scholarly communications in the field of thermophysical properties. **R. Chirico**, V. Diky, J. Magee, A. Bazyleva, C. Muzny, K. Kroenlein

1:50 CINF **7.** Impact of crystal structures over the last, and next, 50 years. **S. Ward**, I. Bruno, C. Groom

2:15 CINF **8.** Give me kudos for taking responsibility for self-marketing my scientific publications and increase impact. **A.J. Williams**, W. Russell, M. Kenneway, L. Peck

2:40 Intermission.

2:55 CINF **9.** How do you define the value of something if it's free? Observations on Caltech's Institutional Repository. **D.T. Wrublewski**, G.S. Porter

3:20 CINF **10.** Redefining value: Alternative metrics and research outputs. K. Deards, R.M. Burks, S. Rouhi, W. Gunn

MONDAY MORNING

Section A

Colorado Convention Center
Room 110

Research Results: Reproducibility, Reporting, Sharing & Plagiarism

M. G. Hicks, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 CINF **11.** Addressing researcher Incentives for publishability over accuracy. **S. Davis** Bowman, B. Nosek

9:05 CINF **12.** Ethics in publishing: Editorial and related experiences. **P.S. Weiss**

9:35 CINF **13.** Data management and the research record in research misconduct investigations. **K. Busch**

10:05 Intermission.

10:20 CINF **14.** Irreproducibility in the scientific literature or: How often do scientists tell the truth, the whole truth and nothing but the truth? **R.G. Bergman**

10:50 CINF **15.** Interplay of prior information and new data in high-throughput small-molecule studies. P.A. **Clemons**

11:20 CINF **16.** STRENDA – proposing minimum information for reporting functional enzymology data. **C. Kettner**, M.G. Hicks

MONDAY AFTERNOON

Section A

Colorado Convention Center
Room 110

Research Results: Reproducibility, Reporting, Sharing & Plagiarism

M. G. Hicks, *Organizer*
C. Kettner, *Presiding*

1:30 CINF **17.** Reproducibility in organic synthesis. **R.L. Danheiser**

2:00 CINF **18.** Data and models, models and data. **T.R. Clark**, C. Kramer

2:30 CINF **19.** Reproducibility and the quality of chemical probes. **A. Edwards**

3:00 Intermission.

3:15 CINF **20.** MIRAGE – the minimum information required for a glycomics experiment: Rationale and progress. **W. York**, C. Kettner, R. Ranzinger

3:45 CINF **21.** Reporting and reuse of crystal structure data and knowledge. **I. Bruno**, S. Ward, C. Groom

4:15 CINF **22.** Reproducibility and variance of literature compound structure and bioassay data. **J.P. Overington**

MONDAY EVENING

Section A

Colorado Convention Center
Halls C/D

Sci-Mix

E. Davis, *Organizer*

8:00 - 10:00

1, 3-6, 11, 20. See previous listings.

CINF **23.** Chemical literature: A comparison of most important databases for searching the chemical literature from an undergraduate perspective. **N. Bharti**

CINF **24.** From lab to the libraries: A new route for chemistry librarianship. **N. Bharti**

CINF **25.** 3Dmol.js: Simple visualization and sharing of 3D molecular data. **D. Koes**, N. Rego

26, 34-37, 44. See subsequent listings.

TUESDAY MORNING

Section A

Colorado Convention Center
Room 110

Research Results: Reproducibility, Reporting, Sharing & Plagiarism

M. G. Hicks, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 CINF **26.** Sharing and reproducibility/replication: An NIH view. **P. Bourne**

9:05 CINF **27.** Globalization of Big Data: Access, integration, and quality control issues. **S. Boyer**, E. Bolton, R. Martin, E. Louie, T.D. Griffin, G. Fu, B. Yu

9:35 CINF **28.** Flagging and curating erroneous chemical and biological records using cheminformatics to ensure data reproducibility. **D. Fourches**

10:05 Intermission.

10:20 CINF **29.** Increasing open communication to facilitate reproducibility. **C. Soderberg**

TUESDAY AFTERNOON

Section A

Colorado Convention Center
Room 110

Molecular & Structural 2D & 3D Chemical Fingerprinting: Computational Storing, Searching, & Comparing Molecular & Chemical Structures

R. J. Bienstock, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CINF **30.** Insights into molecular similarity from crystal structures. **C. Groom**, S. Ward, I. Bruno, S. Vyas, N. Feeder

2:00 CINF **31.** Do chiral fingerprints and descriptors work? **S. Swamidass**, G.P. Miller, T. Hughes, J. Hartman, S. Cothren

2:25 Intermission.

2:40 CINF **32.** Similarity to SAR — interactive navigation of similarity relationships to guide optimization. **M.D. Segall**, E. Champness, J. Chisholm, C. Leeding, P. Hunt, A. Elliott, S. Dowling, H. Garcia

3:05 CINF **33.** Database fingerprint clustering methods using KNIME. **R.J. Bienstock**

3:30 CINF **34.** Highly visual representation methods for comparison of chemical structures and related properties. **J.W. Sager**, P. Mounteney, C.P. Snyder, T.E. Mansley

3:55 Concluding Remarks.

WEDNESDAY MORNING

Section A

Colorado Convention Center
Room 110

Development & Use of Data Format Standards for Cheminformatics

D. Martinsen, *Organizer, Presiding*

9:00 Introductory Remarks.

9:05 CINF **35.** Overview of the analytical Information markup language. **S.J. Chalk**

9:35 CINF **36.** Thermophysical property dissemination utilizing an XML-based standard. **K. Kroenlein**, R. Chirico, V. Diky, A. Bazyleva, J. Magee, C. Muzny

10:05 CINF **37.** Standard data format for computational chemistry: CSX. **S.J. Chalk**, N.S. Ostlund, M. Sopek, B. Wang

10:35 Intermission.

10:50 CINF **38.** Development of an ontology specific to computational chemistry. **M. Sopek**, S.J. Chalk, B. Wang, L. Nardozi, N.S. Ostlund

11:20 CINF **39.** Importance of data standards for large scale data integration in chemistry. **A.J. Williams**, V. Tkachenko, A. Pshenichnov, K. Karapetyan, C. Coba

11:50 Concluding Remarks.

WEDNESDAY AFTERNOON

Section A

Colorado Convention Center
Room 110

Development & Use of Data Format Standards for Cheminformatics

D. Martinsen, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CINF **40.** InChI as the chemical data format standard for cheminformatics. **S.R. Heller**

2:05 CINF **41.** Using HL7 SPL standard for modeling substance information. **Y. Borodina**, F.L. Switzer, G. Schadow

2:35 Intermission.

2:50 CINF **42.** JCAMP-MOL: A JCAMP-DX extension to allow integrated delivery of structural models and correlated spectral data. **R.M. Hanson**, R.J. Lancashire

3:20 CINF **43.** Communicating crystal structures: Successes, challenges, and opportunities. **I. Bruno**, C. Groom, S. Ward

3:50 CINF **44.** Building a standard for standards: The ChAMP project. **S.J. Chalk**, A. Williams

4:20 Concluding Remarks.

TOXI

Division of Chemical Toxicology

A. C. Bryant-Friedrich, *Program Chair*

MONDAY MORNING

Forensic Toxicology of Marijuana

Sponsored by SOCED, Cosponsored by BMGT and TOXI

CHAL

Division of Chemistry and the Law

K. E. Bianco and J. J. Hasford, *Program Chairs*

SOCIAL EVENTS:
Luncheon, 12:00 PM: Mon
Reception, 5:00 PM: Mon

BUSINESS MEETINGS:
Business Meeting, 5:00 PM: Sun

SUNDAY MORNING

Section A

Embassy Suites Denver–Downtown Convention Center

Cripple Creek Ballroom 1

Strengthening Your Patent Rights in Light of Recent Federal Circuit Court Decisions

A. Berks, X. Pillai, *Organizers, Presiding*

10:00 CHAL **1.** Review of recent Federal Circuit decisions relevant to what scientists need to know about patent filing and prosecution. **X. Pillai**, **A. Berks**

SUNDAY AFTERNOON

Section A

Embassy Suites Denver–Downtown Convention Center

Cripple Creek Ballroom 1

Hot Topics in Chemical and Pharmaceutical Patent Law

J. J. Hasford, *Organizer*

K. E. Bianco, *Organizer, Presiding*

1:00 CHAL **2.** Options for protecting your intellectual property. **K.E. Bianco**

1:30 CHAL **3.** Chemistry/pharma patents AND the "unpredictable arts"– increasing restrictions on patent protection for chemical compounds and compositions. **H. Tostmann**

2:00 CHAL **4.** Recent case law on non-obviousness of patented chemical and pharmaceutical formulations. **J.J. Hasford**

2:30 CHAL **5.** Recent Supreme Court cases in patent law. **S.P. Hasford**

MONDAY MORNING

Section A

Embassy Suites Denver–Downtown Convention Center

Cripple Creek Ballroom 1

A Patent Litigation Primer

K. E. Bianco, J. J. Hasford, *Organizers, Presiding*

9:30 CHAL **6.** Patent litigation primer: What every chemist needs to know. **K.E. Bianco**, **J.J. Hasford**

MONDAY AFTERNOON

Section A

Embassy Suites Denver–Downtown Convention Center

Cripple Creek Ballroom 1

Anti-Doping: A Unique Combination of Chemistry and the Law

J. D. Lee, J. J. McShane, *Organizers, Presiding*

1:00 Introductory Remarks.

1:15 CHAL **7.** Evolution of the world anti-doping code. **R. Young**

1:55 CHAL **8.** Deterring performance-enhancing drug use in sports: The role of science. **L. Bowers**

2:35 Intermission.

3:00 CHAL **9.** Deterring performance-enhancing drug use in sports: The role of investigations. **W. Bock**

3:40 CHAL **10.** Role of World Anti-Doping Agency accredited laboratories in the fight against doping. **D. Eichner**

4:20 Panel Discussion.

MONDAY EVENING

Section A

Colorado Convention Center

Halls C/D

Sci-Mix

K. E. Bianco, *Organizer*

8:00 - 10:00

CHAL **11.** Chocolate: Food of the gods. **H.M. Peters**, **S.B. Peters**

CHAL **12.** New changes in the "America Invents Act" for inventors. NewSection 102. **A. Berks**

CHAL **13.** Provisional patent applications for fun and profit! **A. Berks**

TUESDAY MORNING

Section A

Embassy Suites Denver–Downtown Convention Center

Cripple Creek Ballroom 1

Fundamental Concepts in Protecting Chemical Technologies

M. J. Incorvia, *Organizer, Presiding*

9:00 CHAL **14.** Patent vs. trade secret protection – the benefits and pitfalls. **B. Kugler**, **K. Pearson**

9:40 CHAL **15.** How to read a patent. **D. Swartz**, **M.J. Incorvia**

10:00 CHAL **16.** Maintaining intellectual property protection through confidentiality and non-use agreements. **D. Kellis**, **R. Brunelli**

10:30 CHAL **17.** Intellectual property ownership. **H. Covell**, **B. Lieb**, **R. Brunelli**

11:00 CHAL **18.** Rocky Mountain Regional Office of the US Patent and Trademark Office. **J. Posthumus**, **R. Slifer**

The Interface of Chemical and Biological Sciences International Disarmament Efforts

Sponsored by IAC, Cosponsored by ANYL, CHAL, CPRC and PRES

TUESDAY AFTERNOON

Section A

Embassy Suites Denver–Downtown Convention Center

Cripple Creek Ballroom 1

Legal and Business Considerations for Chemical Technologies

M. J. Incorvia, *Organizer, Presiding*

1:30 CHAL **19.** Supreme Court/Federal Circuit patent law update. **B. Lieb**, **R. Brunelli**

2:30 CHAL **20.** Global patenting strategy. **D. Swartz**

3:00 CHAL **21.** Intellectual property issues in acquisitions and financing. **J. Posthumus**, **R. Brunelli**, **D. Swartz**

3:30 CHAL **22.** Inventive step in the United States, Japan, and Europe. **Y. Shimizu**

The Interface of Chemical and Biological Sciences International Disarmament Efforts

Sponsored by IAC, Cosponsored by ANYL, CHAL, CPRC and PRES

WEDNESDAY MORNING

Section A

Embassy Suites Denver–Downtown Convention Center

Cripple Creek Ballroom 1

Patenting Chemical Inventions

K. L. Berkowski, S. Danek, *Organizers, Presiding*

9:00 CHAL **23.** You discovered something new in the lab… now what? **J.C. Hayes**

9:30 CHAL **24.** Patent eligible subject matter in the chemical arts. **S. Danek**

10:00 CHAL **25.** Examination of the obviousness requirement for patenting chemical compounds. **K.L. Berkowski**

10:30 CHAL **26.** Getting from bench-to-bedside. **V. Nielsen**

11:00 CHAL **27.** Technology transfer and industry collaborations: A new era in cooperative and sponsored research. **M. Carr**

WEDNESDAY AFTERNOON

Section A

Embassy Suites Denver–Downtown Convention Center

Cripple Creek Ballroom 1

Intellectual Property and Natural Resources: What Can I Protect and How?

J. L. Kennedy, D. Lorentzen, *Organizers, Presiding*

1:00 CHAL **28.** Protecting natural resources with patents. **J.L. Kennedy**, **D. Lorentzen**

2:00 CHAL **29.** Intellectual property strategy for technology employing natural resources. **J.L. Kennedy**, **D. Lorentzen**

THURSDAY MORNING

Section A

Embassy Suites Denver–Downtown Convention Center

Cripple Creek Ballroom 1

The Many Faces of CHAL: Where Chemistry Meets the Law

K. E. Bianco, *Organizer*

R. G. Bone, *Presiding*

9:00 CHAL **30.** First inventor to file: Two years on. **R.G. Bone**

9:30 CHAL **31.** Is your chemical process still patentable? **R.R. Charney**

10:00 CHAL **32.** *Inter partes* review: The story so far. **R.G. Bone**

10:30 CHAL **33.** Is your drug now indefinite? **R.R. Charney**

11:00 CHAL **34.** Double patenting trouble: Why terminal disclaimers matter more than ever. **R.G. Bone**

11:30 CHAL **35.** Separate powers, singular purpose: How Congress, the Executive, and the courts are revolutionizing pharmaceutical patent litigation. **C. Ray**

COLL

Division of Colloid and Surface Chemistry

R. Nagarajan, *Program Chair*

OTHER SYMPOSIA OF INTEREST:

Nanomaterials for Solar Energy Conversion and Storage *(see ENFL, Sun, Mon, Tue, Wed, Thu)*

Chemical Processes at Environmental Interfaces *(see ENVR, Sun, Mon)*

Probing Nano-Plasmonic Phenomena at the Single Molecule, Single Electron, and Single Photon Level *(see PHYS, Sun, Mon, Wed)*

Graphene and Carbon Nanotubes: Synthesis, Devices and Applications *(see PMSE, Sun, Mon, Thu)*

Stimulus-Responsive Assemblies and Materials *(see PMSE, Sun, Mon, Tue)*

WCC Rising Stars Awards Symposium *(see WCC, Mon)*

SOCIAL EVENTS:

Social Hour, 6:00 PM: Sun
Luncheon, 12:00 PM: Tue

BUSINESS MEETINGS:

Executive Committee Meeting, 5:00 PM: Sat
COLL Open Business Meeting, 5:30 PM: Sun

SUNDAY MORNING

Section A

Marriott City Center Denver

Colorado A/B

Molecular Engineering of Peptide Assembly

Financially supported by Institute for Molecular Engineering, University of Chicago

H. Cui, M. V. Tirrell, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 COLL **1.** Dendronized helix bundle assemblies designed de novo. **J.G. Rudick**

9:05 COLL **2.** Mimicry of biorecognition motifs with peptidic foldamers. **S.H. Gellman**

9:35 COLL **3.** Functional coiled-coil peptides controlled assemblies. **A. Kros**

10:05 Intermission.

10:20 COLL **4.** Thermodynamics of surface-tethered peptide-polymer conjugates. S.P. Carmichael, **M. Shell**

10:50 COLL **5.** Combating diseases with peptide– polymer conjugate. **H. Klok**

11:20 COLL **6.** Carving pi-ways into biomaterials: electronic delocalization via peptide self-assembly. **J.D. Tovar**

Section B

Marriott City Center Denver

Colorado I

Functionalization of Complex Nanosurfaces

Cosponsored by PRES

W. Parak, *Organizer*

L. Liz Marzan, *Organizer, Presiding*

8:30 COLL **7.** Colloidal effects in virus stability. **F. Stellacci**

9:00 COLL **8.** Self-assembly of nanoparticles in chiral and other superstructures. **N. Kotov**

9:30 COLL **9.** Ultraflexible reconfigurable magnetic nanoparticle filaments and networks by nanocapillary lipid bridging. **O.D. Velev**, B. Bharti, A. Fameau, M. Rubinstein

10:00 Intermission.

10:30 COLL **10.** Colloidal design and optimization for assembly of complex crystals. **S.C. Glotzer**

11:00 COLL **11.** Selective and differential functionalization of interior surface of hollow nanoparticles for nanoreactor applications. S. Kim, D. Lee, **I. Lee**

11:20 COLL **12.** Protein-based organic/inorganic hybrid nanocapsules for In vivo delivery applications. **Y. Nam**, J. Lee

11:40 COLL **13.** Interface engineering for nanocrystal stability in media spanning hexane to water. **L.M. Wheeler**, N.J. Kramer, U.R. Kortshagen

12:00 COLL **14.** Design of stimuli-responsive nanogels for bioapplications. J. Ramos, A. Pikabea, G. Aguirre, **J. Forcada**

Section C

Marriott City Center Denver
Colorado C/D

Metallic Nanostructures for Optical & Electrochemical Sensing & Alternative Energy Conversion

Cosponsored by PRES

Financially supported by Sigma-Aldrich

S. Pan, J. Zheng, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 COLL **15.** Shape engineering substrate-based plasmonic nanostructures. **K.D. Gilroy**, R.A. Hughes, D. Sil, E. Borguet, S. Neretina

8:55 COLL **16.** All-optical control of localized plasmonic resonance using photoalignment and liquid crystals. **T.J. Bunning**, L. De Sio, G. Klein, S. Serak, N. Tabirian, A. Cunningham, C. Tone, F. Ciuchi, T. Burgi, C. Umeton

9:15 COLL **17.** Unique temporal and spatial biomolecular emission profile on individual zinc oxide nanorods. M. Singh, **J. Hahm**

9:35 Intermission.

9:45 COLL **18.** Withdrawn.

10:05 COLL **19.** Unprecedented upconversion efficiency in lanthanide nanocrystals via uniform, optically inert shells. N. Johnson, S. He, **A. Almutairi**

10:25 COLL **20.** Creation of natural dye sensitized solar cell. **J. Uddin**

10:45 COLL **21.** Rapid and sensitive assessment of biological and environmental samples using microwave-accelerated bioassay technique. **M. Mohammed**, K. Aslan

Section D

Marriott City Center Denver
Denver III

Biomembrane Synthesis, Structure, Mechanics, & Dynamics

Interfacial Phenomena

S. Muralidharan, M. Nieh, A. N. Parikh, *Organizers*
N. Srividya, *Organizer, Presiding*

9:00 COLL **22.** Physical measurements of hydrophobin air-filled bubbles and oil-filled blobs. **X. Zhang**, S. Kirby, D. Gorman, Y. Chen, W. Huberty, F. Hung, S.L. Anna, L. Walker, P.S. Russo

9:30 COLL **23.** Interactions of aromatic compounds with water-air and water-phospholipid interfaces. **R.J. Perkins**, R. Rapf, S.S. Mansy, V. Vaida

10:00 Intermission.

10:10 COLL **24.** Cellular uptake mechanisms as controlled by nanostructures of a lipid mixture: Comparison between bicelles and vesicles. W. Aresh, Y. Liu, J. Sine, D. Thayer, A. Puri, Y. Huang, Y. Wang, **M. Nieh**

10:40 COLL **25.** Investigating effects of Al^{3+} on structure and fluidity of lipid membranes: FRAP and molecular dynamics. **H.K. Wayment-Steele**, Y. Jing, L.E. Johnson, S. Svedhem, M.S. Johal, M. Swann, B. Agnarsson, A. Kunze

11:10 COLL **26.** Characterization of solid-supported ultrathin films using MP-SPR. **N.M. Granqvist**, W.M. Albers, A. Jokinen, J.W. Sadowski

Section E

Marriott City Center Denver
Colorado G

Basic Research in Colloids, Surfactants & Nanomaterials

Metal Nanomaterials

Cosponsored by PRES

R. Nagarajan, *Organizer, Presiding*

9:00 COLL **27.** Production of highly dispersed silver nanoparticles recovered from photographic film wastes using a simple green method. **A.M. Atta**, **H.A. Al-Lohedan**, **A. Ezzat**

9:20 COLL **28.** AFM-based fabrication and probing of metallic nanostructures. **C.L. Berrie**, C.M. Edwards, S. Ulapane

9:40 COLL **29.** Controlling the electronic structure and chemical reactivity of small nanoparticles through atomic composition. **D. Kauffman**, D. Alfonso, C. Matranga, J. Trindell, R. Jin

10:00 COLL **30.** Withdrawn.

10:20 COLL **31.** Real time microfluidic investigation: The role of seed age on gold nanorod formation. **J. Watt**, R. Anderson, B. Hance, D. Huber

10:40 COLL **32.** Investigation of the surface effects of Ag nanoparticles in solution as a result of a NSF-TUES related funding opportunity. **C.S. Seney**

11:00 COLL **33.** Dissolution and antibacterial efficiency of silver nanoparticles: Influence of particle size, shape, and surface chemistry. **Q. Zhang**, W. Jang, V.L. Colvin

11:20 COLL **34.** Study of interparticle interactions between gold nanoparticles using liquid cell electron microscopy. Q. Chen, **H. Cho,** K. Manthiram, M. Yoshida, X. Ye, P. Alivisatos

11:40 COLL **35.** Size-focusing synthesis of gold nanoclusters with *para*-mercaptobenzoic acid. **L.M. Tvedte**, C.J. Ackerson

12:00 COLL **36.** Constructing 0, 1, and 2D silvers within interlayer dpaces of titania nanotubes. **S.A. Ferdousi**, K.L. Yeung

12:20 COLL **37.** Iridium-triggered facet transformation of Au nanocrystals via spontaneous oxidation-reduction process. **C. Yang**

Section F

Marriott City Center Denver
Colorado H

Particles at Fluid Interfaces

Cosponsored by PRES

M. A. Bevan, *Organizer*
J. Frechette, *Organizer, Presiding*

8:30 COLL **38.** Capillary migration of spheres on curved fluid interface. **K. Stebe**, N. Sharifi-Mood, I. Liu

8:55 COLL **39.** Interactions between soft microgel particles at fluid interfaces. O.S. Deshmukh, A. Maestro, D. van den Ende, M. Cohen Stuart, F. Mugele, **M.H. Duits**

9:20 COLL **40.** Molecular characterization of surfactant adsorption at the surface of emulsion particles. **G.L. Richmond**, J. Hensel, A. Carpenter

9:45 COLL **41.** Understanding Pickering emulsions using multiscale simulations. **A. Striolo**

10:10 COLL **42.** Tracking nanoparticles in 3D– techniques and applications. **J. Liddle**, S. Stavis, P. Mathai, A. Balk, L. Mair, C. Hangarter, J. Unguris

10:35 COLL **43.** Spontaneous emulsification and interface formation induced by colloids. **W. Kegel**

11:00 COLL **44.** DNA-functionalized nanoparticle assembly. **M. Olvera De La Cruz**

11:25 COLL **45.** Capillary foams: A new pathway toward functional porous materials. Y. Zhang, J.C. Meredith, **S.H. Behrens**

11:50 COLL **46.** Organized assemblies of colloids formed at the interfaces of micrometer-sized droplets of liquid crystal: Enabling the synthesis of patchy and nonspherical particles. **N.L. Abbott**

Chemical Processes at Environmental Interfaces

Chemistry and Imaging at Air/Liquid(Solid) Interfaces of Atmospheric Systems

Sponsored by ENVR, Cosponsored by COLL

SUNDAY AFTERNOON

Section A

Marriott City Center Denver
Colorado A/B

Molecular Engineering of Peptide Assembly

Financially supported by Institute for Molecular Engineering, University of Chicago

H. Cui, M. V. Tirrell, *Organizers, Presiding*

2:00 COLL **47.** Artificial organelles: Cellular expression and assembly of polypeptide microdomains. **J.A. MacKay**, Z. Li, A. Truong, J. Dhandhukia, M. Pastuszka, P. Shi, S. Hamm-Alvarez, C. Okamoto

2:30 COLL **48.** Self-assembling peptide materials for hydrogen sulfide delivery. **J.B. Matson**, J.M. Carter

2:50 COLL **49.** Photons, chemicals, and electric fields as functional stimuli in supramolecular materials. **S.I. Stupp**

3:20 Intermission.

3:35 COLL **50.** 3D cell entrapment as a function of the weight percent of peptide-amphiphile hydrogels. C.M. Scott, **E. Kokkoli**

4:05 COLL **51.** Targeting collagen strands by triple helix hybridization. **S. Yu**

4:35 COLL **52.** Design evolution of an antibacterial bioadhesive inspired by cationic peptide hydrogels. **J.P. Schneider**

5:05 COLL **53.** Self-assembling antimicrobial nanofibers based on supramolecular peptide assemblies. **H. Dong**

Section B

Marriott City Center Denver
Colorado I

Functionalization of Complex Nanosurfaces

Cosponsored by PRES

L. Liz Marzan, *Organizer*
W. Parak, *Organizer, Presiding*

2:00 COLL **54.** Ultrasonic modification and functionalization of surfaces and particle. **H. Moehwald**

2:30 COLL **55.** Functionalization of gold nanorods. **C.J. Murphy**

3:00 COLL **56.** Hybrid platforms based on metal nanoparticles-doped filter paper for sensing and catalysis. **I. Pastoriza Santos**

3:30 COLL **57.** Dynamically self-assembling nanoflasks. **R. Klajn**

4:00 COLL **58.** Compact coatings for quantum dots that resist nonspecific binding to proteins, cells, and tissues. **L. Ma**, A. Smith

4:20 Intermission.

4:50 COLL **59.** Functional nanoparticles: Synthesis and biomedical applications. **S. Sun**

5:20 COLL **60.** Multicoordinating amphiphilic polymers provide compact, highly stable, and reactive semiconductor and metal oxide nanocrystal-conjugates. W. Wang, A. Kapur, G. Palui, **H.M. Mattoussi**

5:50 COLL **61.** Intracellular sensing of ion concentration with nanoparticles. **W. Parak**

Section C

Marriott City Center Denver
Colorado C/D

Metallic Nanostructures for Optical & Electrochemical Sensing & Alternative Energy Conversion

Cosponsored by PRES

Financially supported by Sigma-Aldrich

S. Pan, J. Zheng, *Organizers, Presiding*

2:00 COLL **62.** Smart photon management for organic photovoltaic. **Y. Yang**, **Y. Yang**, J. You, Z. Hong

2:30 COLL **63.** Nanoscale oxynitrides with tunable composition and absorption spectra. **G. Dukovic**

3:00 COLL **64.** Light extraction from organic light-emitting diodes using plasmonic scattering layers. **L. Rothberg**, C. Favaro, C. Chang

3:30 Intermission.

3:40 COLL **65.** Nanostructured plasmonic antenna systems and catalytic electrode materials for enhancing solar water splitting. **S. Pan**

4:10 COLL **66.** Molecular imprinted polymers for plasmonic sensing. **A.J. Haes**

4:40 COLL **67.** On the possiblity of the para-aryl-dithiols cross-linking plasmonic nanoparticles as dithiolates. **D. Zhang**

Section D

Marriott City Center Denver
Denver III

Biomembrane Synthesis, Structure, Mechanics, & Dynamics

Model and Cellular Systems

S. Muralidharan, M. Nieh, A. N. Parikh, N. Srividya, *Organizers*
M. L. Longo, *Presiding*

2:00 COLL **68.** Air-stable droplet interface bilayers. **C.P. Collier**, C.I. Richards, S.A. Sarles, J. Boreyko

2:30 COLL **69.** From compartmentalized polymersomes to biomimetic artificial cell. M. Marguet, R. Peters, J. van Hest, **S. Lecommandoux**

3:00 Intermission.

3:10 COLL **70.** Probing interactions between nanoparticles and cellular membrane via single cell mechanics. **G. Liu**, Y. Liu, D. Anderson, A. Karsai, D. Uyeminami, L. Von Winkle, K. Pinkerton

3:40 COLL **71.** Rigidity signals drive differential ROCK signaling to regulate invadopodia activity. **A. Parekh**

4:10 COLL **72.** Phase separation in hybrid polymer/lipid vesicles: A rational to obtain lipid or polymer raft-like nanodomains. **J. Le Meins**, T. Dao, R. Salva, F. Fernandes, A. Brulet, M. Schmutz, M. Er-Rafik, M. Prieto, S. Lecommandoux, O. Sandre

Section E

Marriott City Center Denver
Colorado G

Basic Research in Colloids, Surfactants & Nanomaterials

Metal Oxide Nanomaterials

Cosponsored by PRES

R. Nagarajan, *Organizer, Presiding*

2:00 COLL **73.** Methods for rapid synthesis of nonaggregated nanozeolite Y. **B. Wang**, Y. Li, P.K. Dutta

2:20 COLL **74.** Design of suitable protocols to evaluate metal oxide nanoparticles in unmodified commercial sunscreens. **C. Sapcharoenkun**, P. Kasamechonchung, P. Kumnorkaew, P. Kopermsub

2:40 COLL **75.** Local and long range structure in metal oxide nanoparticles. **M.A. Langell**, M.A. Peck, M. Kumbier, D. Wilson

3:00 COLL **76.** Fabrication of abundant Zn vacancies in ZnO for p-type conductivity, room-temperature ferromagnetism and high photocatalytic activity. **L. Pan**, **J. Song**, **J. Zou**, S. Wang, Z. Huang, L. Wang, X. Zhang

3:20 COLL **77.** Application-scale size-selective fractionation of iron oxide nanoparticles using CO_2-expanded liquids. **P.S. Vengsarkar**, R. Xu, C.B. Roberts

3:40 COLL **78.** Improvements of TiO_2 nanoparticle dispersion stability in nonpolar solvents by long chain fatty acid functionalization. **N. Baek**, Y. Kim, S.F. Okeefe

4:00 COLL **79.** Mobility of antiscalant-modified $BaSO_4$ particles through saturated proppant pack. **C. He**, R.D. Vidic

‡ *Cooperative Cosponsorship*

4:20 COLL **80.** Enhanced photodecomposition activity induced by nanodimensional cerium oxide domains on titania surfaces. **C.A. Estes**, M.B. Mitchell

4:40 COLL **81.** Thiol adsorption on metal oxide nanoparticles and surfaces. **Y. Wang**, O. Grimm, J.E. Whitten

5:00 COLL **82.** Highly uniform gadolinium oxide nanoparticles as remarked remarkably enhanced MRI contrast agents for cellular MR imaging. **N. Taheri**, G. Stinnett, r. pautler, P. Decuzzi, V.L. Colvin

5:20 COLL **83.** Cr:$ZnGa_2O_4$ nanoparticles with controllable size and persistent luminescence. **Y. Mao**, B. Bahadur Srivastava

5:40 COLL **84.** Controlled synthesis of inorganic nanostructures using soft stretchable substrates. **S.A. Morin**, J.J. Bowen, J.M. Taylor

Section F

Marriott City Center Denver
Colorado H

Particles at Fluid Interfaces

Cosponsored by PRES

J. Frechette, *Organizer*
M. A. Bevan, *Organizer, Presiding*

2:00 COLL **85.** Electrostatic repulsion between colloids at the oil-water interface. **E.M. Furst**

2:25 COLL **86.** Janus particles as dynamically tunable solid surfactants. **D. Lee**

2:50 COLL **87.** Bicompartmental phase transfer vehicles based on colloidal dimers with anisotropic structural and interfacial properties. **N. Wu**

3:15 COLL **88.** Self-organisation of colloidal particles at liquid interfaces. **T.S. Horozov**

3:40 COLL **89.** Particle transport at oil/water interfaces driven by spatially varying surfactant adsorption or desorption kinetics. **R.D. Tilton**, S. Garoff, T.M. Przybycien, G. Duner

4:05 COLL **90.** Thermodynamics of Janus particles in 2D confinement. S. Razavi, R.S. Tu, **I. Kretzschmar**

4:30 COLL **91.** Remotely triggered colloidal disassembly from particle-laden microbubble. **V. Garbin**

4:55 COLL **92.** Measurements and models of reversible adsorption of nanoparticles at the oil-water interface. X. Hua, M. Bevan, **J. Frechette**

Section G

Marriott City Center Denver
Colorado F

ACS Award in Colloid and Surface Chemistry: Symposium in Honor of Paul S. Weiss

N. Kotov, *Organizer*
C. R. Kagan, *Presiding*

2:00 COLL **93.** Breaking Lord Rayleigh's Rule: Linked photochemical reactions that double the resolution of a lens. **C.G. Willson**, R.A. Mesch, X. Gu, W. Wang, T. Kawakami, Y. Hajiwara, M. Okazaki, H. Truong, Y. Li, S. Jockusch, **N. Turro**

2:40 COLL **94.** Designing precursors for the deposition of inorganic nanostructures by CVD, SPMCSD and EBID. **L. McElwee-White**

3:10 COLL **95.** Dynamic substrate control: Dual-tone hydrogel photoresists. C. Xue, D. Wong, S. Norris, **A.M. Kasko**

3:40 COLL **96.** Chemical lift-off lithography by collapsing soft-material molds. **W. Liao**, H. Jan

4:10 COLL **97.** Atomic picture of nuclear decay in stable 2D radioactive films. **E.H. Sykes**

Chemical Processes at Environmental Interfaces

Chemistry and Imaging at Air/Liquid(Solid) Interfaces of Atmospheric Systems

Sponsored by ENVR, Cosponsored by COLL

SUNDAY EVENING

Section A

Colorado Convention Center
Hall B2

Fundamental Research in Colloids, Surfaces & Nanomaterials

Cosponsored by PRES

R. Nagarajan, *Organizer*

6:00 - 8:00

COLL **98.** J-aggregate formation of cationic cyanine dyes on clay minerals. **N. Sato**, T. Fujimura, Y. Ohtani, T. Shimada, S. Takagi

COLL **99.** Dynamics of binary mixtures of cationic and anionic microgels at the air water interface. **K. Horigome**, D. Suzuki

COLL **100.** Solvent-free functionalization of multiwalled carbon nanotube buckypaper with amines. I.J. Ramírez-Calera, V. Meza-Laguna, E. Abarca-Morales, V.A. Basiuk, **E.V. Basiuk**

COLL **101.** Coordination functionalization of graphene oxide and nanodiamond with nickel(II) tetraazamacrocyclic complexes. N. Alzate-Carvajal, L.V. Henao-Holguín, V. Meza-Laguna, A. Moreno-Bárcenas, J.F. Pérez-Robles, E. Rybak-Akimova, **V.A. Basiuk**, E.V. Basiuk

COLL **102.** Characterization of covalently-functionalized mesoporous silica nanoparticles by solution-phase NMR methods. **S.E. Lehman**, Y. Tataurova, S.C. Larsen

COLL **103.** DFT study of noncovalent complexes of phthalocyanines with spherical fullerenes and short nanotube models. **V.A. Basiuk**

COLL **104.** Label-free detection of RNA by using liquid crystals. **Y. Liu**, **K. Yang**

COLL **105.** Interaction of a Ni(II) tetraazaannulene complex with spherical and elongated fullerenes: A DFT study. L.V. Henao-Holguín, **V.A. Basiuk**

COLL **106.** Imaging of liver cells using water soluble CdTe quantum dots. **A. Coover**, T.G. Lewis, T.J. Ripley, A.L. Asunskis, D.J. Asunskis

COLL **107.** Effects of composition on the gradient structure and surface properties of fluorinated polyacrylates latex blends film. **H. Yuanyuan**, Z. Chaocan, Y. Chen

COLL **108.** Effect of chain length, number of chains, and charge on the in vitro cytotoxicty of surface coating agents used for nanoparticles. **Y. Zhang**

COLL **109.** Fluorescent organic nanodots for sensing metals and a targeted immunofluorescence labeling. **H. Kim**

COLL **110.** Electrochemical and photocatalytic activity analysis of TiO_2-NiO/TiO_2. S. Buama, **P. Rangsunvigit**

COLL **111.** Studies on the mechanisms of forced transport of dye through solution modifications to a polymerized surface. **J. Siegenthaler**, D. Rivera

COLL **112.** Adsorption of poly(vinyl alcohol) onto polydimethylsiloxane substrates: Formation of continuous films, honeycomb structures, and fractal morphologies. **B. Sharma**, **A. Karki**, L. Nguyen, W. Chen

COLL **113.** Role of substrate receding contact angle in deposit patterns of sessile droplets containing stabilized gold nanoparticles. **E. Laudadio**, L. Zhang, W. Chen

COLL **114.** Smooth and uniform thiol-functionalized substrates for bioconjugations. **T. Tabassum**, **S. Xu**, W. Chen

COLL **115.** Probing the hydrodesulfurization properties of cobalt-nickel phosphides: Supported catalysts and encapsulated nanoparticles. **S. Danforth**, R. Liyanage, B. Ilic, P. Topalian, M.E. Bussell

COLL **116.** Capacitance and hydrogen evolution reaction characterization of electrodeposited nickel alloy thin films. **M. Gira**, J.R. Hampton

COLL **117.** Quantitative characterization of methanol oxidation catalysis on dealloyed NiCu films. **M. Milliken**, J.R. Hampton

COLL **118.** Nickel phosphide hydrotreating catalysts on phosphorus-modified oxide supports. **B.J. Morgan**, S. Danforth, B. Ilic, M.E. Bussell, P. Topalian

COLL **119.** Total holographic characterization of colloidal suspensions. **L.A. Philips**, F.C. Cheong, D.G. Grier

COLL **120.** Effects of shear and walls on the diffusion of colloids in microchannels. S. Ghosh, F. Mugele, **M.H. Duits**

COLL **121.** Glutathione-coated luminescent gold nanoparticles: A surface ligand for minimizing serum protein adsorption. **R. Vinluan**, J. Liu, C. Zhou, M. Yu, S. Yang, A. Kumar, S. Sun, A. Dean, X. Sun, J. Zheng

COLL **122.** Crystallization of proteins on iron nanocolumns using metal-assisted and microwave-accelerated evaporative crystallization for liproved size distribution. **K. Mauge-Lewis**, E. Toth, D. Seifu, **K. Aslan**

COLL **123.** Crystal engineering of L-alanine in the presence of multiple amino acid additives using metal-assisted and microwave-accelerated evaporative crystallization. A. Mojibola, E. Constance, T.E. Onuekwusi, I. Nicholson, M. Mohammed, **K. Aslan**

COLL **124.** De-crystallization of uric acid crystals in synovial fluid using gold colloids and low power microwave heating. B. Kioko, T. Ogundolie, M. Adebiyi, Y. Ettinoffe, C. Rhodes, B. Gordon, N. Thompson, M. Mohammed, **K. Aslan**

COLL **125.** Biodegradable polymer materials containing stabilized silver nanoparticles. A. Paul, **A. Vasiliev**

COLL **126.** Characterization and bioapplication of nanoscaled materials derived from green chemistry. **P. Hanumandla**, J. Dinn, **M. Ngassa**, D. Lopez, P. Nandakumar, J.L. Liu

COLL **127.** How small molecules self-assemble into nanofibers and form hydrogels. **Y. Gao**, B. Hammouda, J. Douglas, F. Horkay

COLL **128.** Computational study of hydroxyproline-pectin cross-linkage for drug delivery. **M.H. Andersen**, **L. Tribe**

COLL **129.** Tmpyp containing nanoparticles with enhanced photo –physical properties. M. Zhu, S. Shutthanandan, H. Zhang, G.H. Aryal, **J. Jayawickramarajah**

COLL **130.** Optical characterization of purified noble metal nanoparticles. **A. Thomas**

COLL **131.** Green synthesis of magnetic nanocomposites formulated with Indian medicine to perform cancer theranostic study. J.L. Liu, **K.Y. Amaravathi**, **H. Shravan**, S. Bashir, X. Du

COLL **132.** Plasmonic nanocrystal solar cells utilizing strongly confined radiation. **P. Moroz**, M. Zamkov, N.N. Kholmicheva, U. Rijal, A. Razgoniaev, A. Ostrowski

COLL **133.** Structure and behavior relationships among semifluorinated linear, dibranched and miktoarm amphiphiles. **W. Tucker**, A. McCoy, S. Fix, M. Stagg, M. Murphy, S. Mecozzi

COLL **134.** Effect of pH on the adsorption of cationic polyacrylamide to polyacrylic acid. **D. Seo**, H. Lee, H. Youn

COLL **135.** Role of alpha-hemolysin's phosphocholine binding pocket and cholesterol in lipid membrane adsorption and nanopore formation. **C. McCauley**, L. Keranen Burden, D. Burden

COLL **136.** Surface equilibrium and kinetic dynamics of alpha hemolysin on red blood cell membranes. **J. Ellingsen**, A.S. Freeman, L. Keranen Burden, D. Burden

COLL **137.** Morphological and electrochemical characterization of Laponite/polyaniline/graphene and graphene oxide nanocomposite materials. **I. Ramphal**, M.E. Hagerman

COLL **138.** Morphosynthetic studies of polyaniline/graphene oxide/Laponite nanoscaffolds. **Y. Hu**, **M.E. Hagerman**

COLL **139.** Study of selective heavy metal removal from seawater. X. Chen, **Y. Li**, W. Han, K.L. Yeung

COLL **140.** Interaction of ligand-capped metal nanoparticles with t2D atomic layered nanomaterials. **S.S. Low**, S. Gang, Y. Shon

COLL **141.** Gold nanoparticles size characterization using PCA and LDA techniques by UV-Vis spectroscopy. **H. Cavusoglu**, Y. Danisman, H. Sakalak, M. Yilmaz, M. Yavuz

COLL **142.** Dynamic observation of NIH3T3 cells adhesion behaviors on binary self-assembled monolayers modified gold surfaces. **W. Kao**, H. Chang, J. Shyue

COLL **143.** Ag nanoparticle nucleation vs. shell growth. **M. Shaughnessy**, D. Khon, N. Sharma, M. Zamkov

COLL **144.** Improving the catalytic activity of metal semiconductor nanocomposites. **J. Bocanegra**, D. Khon, E. Khon, M. Zamkov

COLL **145.** Preparation of highly efficient Winsor-IV type microemulsions for rapid wood penetration. **X. Du**, L.A. Lucia, R.A. Ghiladi, O.J. Rojas

COLL **146.** Variations in intermolecular interactions in the microtubule associated protein tau revealed by atomic force microscopy. **Z. Donhauser**

COLL **147.** First principles characterization of nontronite clay surfaces with varying Fe(II)/Fe(III) composition. **S. Ramadugu**, S.E. Mason

COLL **148.** Effect of solvent on the growth of isotropic/anisotropic core/shell nanoparticles via alternating layer techniques. **R. Tan**, S.K. Roberts, Y. Shen, M.Y. Gee, A.B. Greytak

COLL **149.** Nanoparticle mediated remote activation of thermophilic enzymes with alternating magnetic fields. **C. Collins**, C.J. Ackerson

COLL **150.** Template synthesis of gold nanoparticles using an organic molecular cage. **R. McCaffrey**, W. Zhang

COLL **151.** Progress toward clonable inorganic nanoparticles. **T. Ni**

COLL **152.** Role of surface groups in cycloaddition reactions over ZIF-8 films. **E.R. Webster**, F. Tian, L.B. Benz

COLL **153.** Adsorption and interaction of alcohols with ZIF-8 films and the role of surface groups. L.B. Benz, **H.L. Larson**, **A.M. Mosier**, F. Tian, E. Baxter, A. Cheetham

COLL **154.** Rational design and control of functional molecules on single metal nanoparticles. **Y. Zheng**

COLL **155.** Nanoporous hydrogen-reduced bismuth vanadate coupled with electrocatalysts as high-performance photoanodes for solar fuels. J. Gan, X. Lu, Y. Tong, **Y. Zheng**

COLL **156.** Ultrafast and temperature-dependent optical properties of Au_{67}, Au_{102} and Au_{144} clusters. **V.D. Thanthirige**, K. Kwak, D. Lee, E. Sinn, R. Guda

COLL **157.** Fabrication of inverse opal films with stop bands in the full spectral range of visible light using co-assembly technique. **U.S. Madduma-Bandarage**, Y. Vasquez

COLL **158.** Electric-field assembly and propulsion of chiral colloidal clusters. **F. Ma**, S. Wang, D. Wu, N. Wu

COLL **159.** Effect of surfactants on cyclopentane hydrates: Structure and properties. **E. Brown**, J. Wells, C.A. Koh

COLL **160.** Properties of Fe_3O_4@chitosan nanoparticles at oil/water interfaces. **A.R. Molina**

COLL **161.** Withdrawn.

COLL **162.** Elucidating reaction pathways for thermoelectric materials fabricated by bottom-up solution-phase solid-state synthesis. **C. Holder**, E. Rugen, D. Stevens, M.E. Anderson

COLL **163.** New approach for scientific research on RO membrane. **J. Okabe**, M. Nishida, T. Ogawa, T. Sasaki, M. Kimura

COLL **164.** Foundational layer formation of metal-organic coordinated thin films. **M.L. Ohnsorg**, **B. Bowser**, L. Gentry, M.E. Anderson

COLL **165.** Investigation of the stability of Ag nanoparticles in solution by isothermal titration calorimetry (ITC) and zeta-potential measurements. **J.D. Mimbs**, C.S. Seney, R. Vaithi, A. Weems, R.H. Goddard

COLL **166.** Study of fractal colloidal gels using DLS and SALS. **R. Ebini**

COLL **167.** Effects of H_2O and H_2 plasma surface modification of SnO_2 nanowires and spiked nanowires. **C.J. Miller**, E.P. Stuckert, E.R. Fisher

COLL **168.** Withdrawn.

COLL **169.** Analysis of polymeric phase separation within a thermoset polymer blend for applications in high performance low gloss coatings. **S.L. Giles**, J.H. Wynne, C.R. Clayton, N.W. Heller

COLL **170.** Controlling the unit cell lattice parameters in nanoscaled $Cu_xPd_{1-x}O$ by composition and crystallite size. **M. Kumbier**, G.L. Christensen, M.A. Langell

COLL **171.** Synthesis, characterization, and imaging applications of various silver nanoparticles morphologie. **D. Castillo**, L.M. Hernandez, M. Forero-Shelton, W.L. Vargas

COLL **172.** Chemical synthesis and High temperature structural stability of monodisperse ruthenium nanostructures. **N. Chou**, D. Zakharvoc, E. Stach, A. Harutyunyan

COLL **173.** Effect of doping density on current-voltage behavior and quantum yields of dye-sensitized single crystal TiO_2 electrodes. **K.J. Watkins**, B.A. Parkinson, M. Spitler

COLL **174.** Directed synthesis of bimetallic nanoparticles using poly(2-vinylpyridine) colloids. **A.K. Taylor**, D.A. Rider

COLL **175.** Modulating beta amyloid (Aβ) aggregation with metal ions and nanochelators. **M.R. Mackiewicz**, B.D. Jorgenson, E.A. Costa

COLL **176.** Surface-chemistry effect on cellular response of luminescent plasmonic silver nanoparticles. **S. Sun**

COLL **177.** Enhanced dispersion of cellulose nanocrystals for nanofibrilled cellulose nanocomposites. **W. Fang**, E. Kontturi, M. Linder, P. Laaksonen

COLL **178.** Microscopy study of poly(3-hexylthiophene) films processed from binary mixtures of organic solvents. **M.P. Gordon**, D.S. Boucher

COLL **179.** Distinct assembly and disassembly pathways of nanotube formed by drug amphiphile. **P. Zhang**, A. Cheetham, H. Cui

COLL **180.** Investigation of bone growth onto titanium rods investigated with model cell membranes. **M. Gulley**, A.G. Sostarecz

COLL **181.** Exploring the desolvation of BSA–ligand complexes using the quartz-crystal microbalance and dual polarization interferometer. **N. Stanton**, J. Kang, C.R. Selassie, M.S. Johal

COLL **182.** Withdrawn.

COLL **183.** Synthetic route for the growth of entirely I-III-VI semiconductor core/shell nanocrystals. **S.M. Hughes**, F. Rowe, S. Dvorak

COLL **184.** Synthesis of micrometer-sized CdSe nanosheet via cation exchange. **P. Tongying**, Y. Morozov, M. Zhukovskyi, M.K. Kuno

COLL **185.** Zein nanoparticles as superhydrophobic coating: a simple and ecofriendly way to antiwetting textiles surfaces. **G. Li**

COLL **186.** Laser-induced copper deposition from solution with the addition of non-ionic surfactants: Influence of hydrophilic properties. **S.V. Safonov**, S. Araslanova, F. Sergey

COLL **187.** DFT study of the dissociative adsorption of chlorobenzene and 1,2-dichlorobenzene on Si(100). **E. Butson**, N.F. Materer, Q. Zhu

COLL **188.** Ultrastrong epoxy nanocomposites containing self-assembled synthetic clay in smectic order. **P. Li**, K. White, C. Lin, D. Kim, R. Krishnamoorti, A. Muliana, R. Nishimura, H. Sue

COLL **189.** Withdrawn.

COLL **190.** Synthesis and characterization of homogeneous $Zn_xCu_{1-x}O$ solid-solutions. **D. Wilson**, M.A. Langell

COLL **191.** Size- and shape-controlled synthesis of Gold nanoparticles using chitosan as a stabilizer. **L. Liu**, J. Chaudhuri

COLL **192.** Influence of shelling temperature and time on the optical and structural properties of CuInS2/ZnS quantum dots. **C. Robinson**, C.D. Heyes

COLL **193.** Bright tunable photoluminescence in colloidal amorphous porous silicon nanostructures. **J. El Demellawi**, S. Chaieb

COLL **194.** Topical delivery of lipophilic carbonic anhydrase inhibitors with liposomal formulations. A. Shabana, S. Akocak, **M.A. Ilies**

COLL **195.** Model system development for urban films and environmental adsorption. J.S. Grant, **S.K. Shaw**

COLL **196.** Stretchable surface-chemical patterns. **J.J. Bowen**, J.M. Taylor, S.A. Morin

COLL **197.** Oxidative decomposition of $Au_{25}(SR)_{18}$ clusters in a catalytic context. **T. Dreier**, A. Wong, C.J. Ackerson

COLL **198.** Titania containing thin films for the detection of TATP and peroxide vapors. **N.F. Materer**, T.H. James, C. Cannon, D.W. Scott, Z. Alothman, A.W. Apblett

COLL **199.** Synthesis of large-pore SBA-15 silica at room temperature. **T. Man**, I. Stoyko, I. Nayshevsky, M. Kruk

COLL **200.** Surface reactions of gas-phase atomic radicals with alkanethiolate monolayers. **A. Gans**, S.A. Kandel

COLL **201.** Stability and transport properties of magnetic nanoparticles under high temperature, high salinity aqueous conditions for oil reservoir imaging. **Y. Fei**, S. Kong, E. Urena, E. Lin, V. Ngo, Y. Lu, C.J. Ellison, K.P. Johnston

COLL **202.** Layer-by-layer assembly of polyelectrolytes and different size and shape gold nanoparticles. **S.M. Budy**, D. Hamilton, Y. Cai, M.K. Knowles, S.M. Reed

COLL **203.** Multiwalled carbon nanotube incorporated "molecular fan" coatings for optimized thermal managment applications. **T. Eyassu**, T. Hsiao, K. Henderson, T. Kim, C. Lin

COLL **204.** Size dependence of gold nanoparticle interactions with a supported lipid bilayer: A QCM-D study. C.M. Bailey, E. Kamaloo, K. Waterman, K. Wang, **R. Nagarajan**, T.A. Camesano

COLL **205.** Extreme-wettable nanomolecular layer. H. Baik, **S. Chae**, Y. Kim

COLL **206.** Droplet size distributions of water-in-oil emulsions using low field NMR before and after gas hydrate formation. A. Abdul Majid, M. Saidian, C.A. Koh

COLL **207.** Methane activation on ceria surfaces modified with metal nanoparticles. **M. Nolan**, J. Carey, A. Van Veen

COLL **208.** Surface properties of hydrocolloid-stabilized magnetite Murrh capped nanoparticles. A.M. Atta, **H.A. Al-Lohedan**

COLL **209.** Epoxy/clay nanocomposites containing clay layers in smectic long-range order. M. Wong, **P. Li**, F. Lei, M. Miyamoto

Section B

Colorado Convention Center
Hall B2

Interfacial Biomolecular Recognition

Cosponsored by BIOL‡

Financially supported by Avanti Polar Lipids, Inc.

J. Ross, *Organizer*
B. E. Bowler, M. Kastantin, *Organizers*

6:00 - 8:00

COLL **210.** Isolation and investigation of distinct cytochrome *c*/cardiolipin interaction sites. **M. Elmer-Dixo**n, B.E. Bowler

COLL **211.** Role of lysine 72 in human cytochrome *c* alkaline conformational transition. **E.M. Nold**, B.E. Bowler

COLL **212.** ^{19}F Dendron probes for specific detection of enzyme activity. **H. Wang**, K.R. Raghupathi, J. Zhuang, S. Thayumanavan

COLL **213.** Biomolecular patterning via chemical lift-off lithography. **H.H. Cao**, W. Liao, N. Nakatsuka, S. Deshayes, A.M. Kasko, P.S. Weiss, A.M. Andrews

COLL **214.** Surface passivation and acidic conditions allow for the rapid synthesis of DNA-conjugated gold nanoparticles with high salt stability and DNA-binding specificity. **J. Deka**, R. Mech, L. Ianeselli, H. Amenitsch, F. Cacho-Nerin, P. Parisee, L. Casalis

COLL **215.** Sialic acid decorated polymer@goldNP as biofunctional hybrids: assembly, lectin and viral binding. **Z. Zhang**, B. De Geest

COLL **216.** Using fluorescent-labeled nanodiscs to study lipid interactions with yeast Cytochrome C. **H.B. Steele**, L. McClelland, K. Stipe, M.C. Terwilliger, B.E. Bowler, J. Ross

Section C

Colorado Convention Center
Hall B2

Metallic Nanostructures for Optical & Electrochemical Sensing & Alternative Energy Conversion

Cosponsored by PRES

Financially supported by Sigma-Aldrich

S. Pan, J. Zheng, *Organizers*

6:00 - 8:00

COLL **217.** Plasmonic enhancement of dye-sensitized solar cells using SiO_2@AuNP thin films. **B.D. Clark**, E.M. Spain

COLL **218.** Preparation of Fe(II)-impregnated granular activated carbon for arsenate removal from water. **H. Xu**

Section D

Colorado Convention Center
Hall B2

Plasmonic Catalysis and Sensing

C. Matranga, *Organizer*
E. Borguet, *Organizer*

6:00 - 8:00

COLL **219.** Enhanced photocurrent via plasmon excitation of ultrasmall PbS quantum dots on Au/TiO_2 electrode. **X. Li**, K. Suzuki, T. Toda, S. Yasuda, K. Murakoshi

COLL **220.** Nucleation and growth of silver nanoparticles by AB and ABC-type atomic layer deposition. **S. Masango**, R.P. Van Duyne, P.C. Stair

MONDAY MORNING

Section A

Marriott City Center Denver
Colorado A/B

Molecular Engineering of Peptide Assembly

Financially supported by Institute for Molecular Engineering, University of Chicago

H. Cui, M. V. Tirrell, *Organizers, Presiding*

8:30 COLL **221.** Supramolecular polypeptide structures assembled from folded, globular proteins. W. Park, **J. Champion**

9:00 COLL **222.** Elastin-based amphiphilic copolymers as precision building blocks for controlled self-assembly. E. Garanger, S. Mac Ewan, A. Chilkoti, **S. Lecommandoux**

9:30 COLL **223.** Growth factors engineered for super-affinity to the extracellular matrix enhance tissue healing. **P.S. Briquez**, M.M. Martino, J.A. Hubbell

10:00 Intermission.

10:15 COLL **224.** Effect of surfaces in modulating peptide assembly. **J.E. Shea**

10:45 COLL **225.** Materials with desired nanostructure through peptide design and solution assembly. D**.J. Pochan**

11:15 COLL **226.** Fibrillar protein and peptide co-assemblies: Design and applications in medicine. T. Sun, G. Hudalla, C. Mora Solano, **J. Collier**

Section B

Marriott City Center Denver
Colorado I

Functionalization of Complex Nanosurfaces

Cosponsored by PRES

W. Parak, *Organizer*
L. Liz Marzan, *Organizer, Presiding*

8:30 COLL **227.** Formation of protein coronas on gold nanorods stabilized by amphiphilic ligands. **K. Hamad-Schifferli**

9:00 COLL **228.** Direct delivery of proteins and nucleic acids to the cytosol using nanoparticle-stabilized capsules. **V.M. Rotello**

9:30 COLL **229.** In how far can we make nanoparticles mimic molecules? **Z. Nie**, C. Yi, Y. Liu, J. He

10:00 COLL **230.** Hierarchical architectures from ordered electroactive small molecules. **N. Martin**, C.M. Atienza, J. López, A. Insuasty, J. López-Andarias

10:30 Intermission.

11:00 COLL **231.** Modification of microgel surfaces with a self-assembling peptide. **K.C. Clarke**, L.A. Lyon

11:20 COLL **232.** Probing the dynamic and structure of nanoparticle protein corona by using single molecule spectroscopy. **A.D. Indrasekara**, S. Dominguez-Medina, L. Kisley, C.F. Landes, S. Link

11:40 COLL **233.** Lipid coated gold nanoparticles as models of faceted and highly curved membranes. **D. Hamilton**, S.M. Budy, S.M. Reed

12:00 COLL **234.** Role of ligands in the structure and properties of molecular silver nanoparticles and their assemblies. **T.P. Bigioni**

Section C

Marriott City Center Denver
Colorado C/D

Metallic Nanostructures for Optical & Electrochemical Sensing & Alternative Energy Conversion

Sensing, Electronics, & Photophysics

Cosponsored by PRES

Financially supported by Sigma-Aldrich

S. Pan, J. Zheng, *Organizers, Presiding*

8:30 COLL **235.** Theranostic gold nanorods for synergistic cancer treatment. **Z. Gu**

9:00 COLL **236.** Determining drug efficacy using plasmonically enhanced imaging of the morphological changes of cells upon death. **M. Aioub**, L. Austin, M.A. El-Sayed

9:30 COLL **237.** Functional DNA nanotechnology and its applications in environmental sensing and live cell imaging. **Y. Lu**, J. Zhang, L. Li, P. Wu, K. Hwang, H. Xing

10:00 Intermission.

10:10 COLL **238.** Role of the protein corona in mediating nanoparticle targeting. **W. Chan**

10:40 COLL **239.** Prolonged hot electron dynamics in plasmonic-metal/semiconductor heterostructures with implications for solar photocatalysis. **W. Wei**

11:10 COLL **240.** Enhanced light-matter interactions in nanoparticle arrays. **T.W. Odom**

11:40 COLL **241.** Renal clearable metal nanoparticles for cancer imaging. **J. Zheng**

Section D

Marriott City Center Denver
Denver III

Biomembrane Synthesis, Structure, Mechanics, & Dynamics

Vesicles and Related Systems

S. Muralidharan, M. Nieh, A. N. Parikh, N. Srividya, *Organizers*
D. L. Daleke, *Presiding*

9:00 COLL **242.** Functional reconstitution of integral membrane proteins in giant lipid vesicles by hydrogel swelling. **N. Malmstadt**

9:30 COLL **243.** Membrane shape instabilities induced by BAR domain proteins. **T. Baumgart**

10:00 COLL **244.** Nanoparticle-induced pore formation in lipid bilayers. **J. Schmidt**

10:30 Intermission.

10:40 COLL **245.** Nanolipoprotein particles entrapped within nanoporous silica gel. W. Zeno, S.H. Risbud, **M.L. Longo**

11:10 COLL **246.** Multiple faces of cholesterol in membrane fusion. **L.K. Tamm**

11:40 COLL **247.** Designing biotinylated lipids for selective partitioning to liquid ordered phase. **D.Y. Sasaki**, N. Momin, S. Lee, C. Hayden, J. Stachowiak, G.D. Bachand

‡ *Cooperative Cosponsorship*

Section E

Marriott City Center Denver
Colorado G

Plasmonic Catalysis and Sensing

Cosponsored by PRES

C. Matranga, *Organizer*
E. Borguet, *Organizer, Presiding*

8:30 COLL **248.** Photoinduced dynamics at metallic and semiconducting nanoparticles: time-domain ab initio studies. **O.V. Prezhdo**

9:05 COLL **249.** Plasmons, hot electrons, and artificial photosynthesis. **M. Moskovits**

9:40 COLL **250.** Ligand effects on the aqueous plasmonic catalysis by alloyed gold-copper nanorods. **S.V. Jenkins**, J. Chen

10:00 Intermission.

10:15 COLL **251.** Surprisingly efficient plasmon-induced hot electron transfer and photochemistry in semiconductor-Au nanoheterostructures. **T. Lian**

10:50 COLL **252.** Characteristics of reaction intermediates at plasmon-induced water oxidation processes. K. Suzuki, S. Yasuda, **K. Murakoshi**

11:25 COLL **253.** Surface-enhanced spectroscopies by rational nanoantenna design. **N.J. Halas**

Section F

Marriott City Center Denver
Colorado H

Particles at Fluid Interfaces

Cosponsored by PRES

M. A. Bevan, J. Frechette, *Organizers*
N. Wu, *Presiding*

8:30 COLL **254.** Synthesis of hybrid dumbbells with combined compositional and interfacial asymmetries. **S. Wang**, N. Wu

8:50 COLL **255.** Synthesis and characterization of chemically and physically bonded Janus particles. **L.M. Hernandez**, S. Razavi, I. Kretzschmar, W.L. Vargas

9:10 COLL **256.** Salt-induced detachment of non-touching colloidal particles from oil-water interfaces. **N. Elbers**, J. van der Hoeven, A. van Blaaderen

9:30 COLL **257.** Direct view of the nanobio interface. **F. Geiger**

9:50 COLL **258.** Carbon dioxide-in-water foams stabilized with interfacially active nanoparticles and surfactants. **A.J. Worthen**, P.S. Parikh, T.R. Dickey, D.A. DiCarlo, M. Prodanovic, S.L. Bryant, C. Huh, K.P. Johnston

10:10 COLL **259.** Studying the molecular orientation and behavior of ionic liquid films at solid- liquid interface. **R.S. Anaredy**, S.K. Shaw

10:30 COLL **260.** Interactions and ordering of soft microgels at oil-water interfaces. **W. Richtering**

10:50 COLL **261.** Synthesis of monodisperse, colloidal microcapsules, and their use in controlled encapsulation and release studies. **N. Elbers**, J. Jose, A. Imhof, A. van Blaaderen

11:10 COLL **262.** Nanoparticle induced charge redistribution of the air-water interface and its role in regulating nanoparticle spatial distributions. **M.A. Brown**

11:30 COLL **263.** Inverted pendant drop set-up for X-ray absorption spectroscopy of electrolyte solutions and their surfaces. **M.K. Bera**, M.R. Antonio

Section G

Marriott City Center Denver
Colorado F

ACS Award in Colloid and Surface Chemistry: Symposium in Honor of Paul S. Weiss

N. Kotov, *Organizer, Presiding*

9:00 COLL **264.** Plasmonic gold nanoparticles in the cancer cell: Following cell cycle, cell death, drug delivery dynamics and efficacy. **M.A. El-Sayed**

9:40 COLL **265.** Chemically modified 2D nanoelectronic heterostructures. **M. Hersam**

10:20 COLL **266.** Surface chemistry and interface engineering for high performance perovskite solar cells. **A.K. Jen**

11:00 COLL **267.** Adaptive wavelet approach for signal/image processing. **J. Gilles**

WCC Rising Stars Awards Symposium

Sponsored by WCC, Cosponsored by BIOT, COLL, GEOC, INOR, ORGN, PHYS, PMSE and PROF

Chemical Processes at Environmental Interfaces

Chemistry at Aqueous/Mineral(Solid) Interfaces

Sponsored by ENVR, Cosponsored by COLL

MONDAY AFTERNOON

Section A

Marriott City Center Denver
Colorado A/B

Molecular Engineering of Peptide Assembly

Financially supported by Institute for Molecular Engineering, University of Chicago

H. Cui, M. V. Tirrell, *Organizers, Presiding*

2:00 COLL **268.** Periodically sequenced peptides: A new tool for nanoscale materials synthesis. M. Kubilius, **R.S. Tu**

2:30 COLL **269.** Design of 3-helix micelles as viable nanocarriers. **T. Xu**

3:00 COLL **270.** Molecular design of peptide nucleic acid amphiphiles as self-assembled probes for electrophoretic miRNA detection. **J.W. Schneider**, B.A. Armitage, D.H. Ly, J.M. Goldman

3:30 Intermission.

3:45 COLL **271.** Multistimuli responsive polypeptides and stimuli responsive hydrogels. **T.J. Deming**

4:15 COLL **272.** Molecular engineering of peptide and protein therapeutics. **M.J. Webber**, D.G. Anderson, R. Langer, S.I. Stupp

4:35 COLL **273.** Biomimetic silica formation probed at the molecular level using SFG spectroscopy and MD simulation. H. Lutz, J. Baio, V. Jaeger, A. Roehrich, J. Pfaendtner, G. Drobny, **T. Weidner**

4:55 COLL **274.** Engineering mitochondria-penetrating peptides. **S.O. Kelley**

Section B

Marriott City Center Denver
Colorado I

Functionalization of Complex Nanosurfaces

Cosponsored by PRES

L. Liz Marzan, *Organizer*
W. Parak, *Organizer, Presiding*

2:00 COLL **275.** Charge shuttling across membranes by functionalized gold nanoparticles. **M. Brust**

2:30 COLL **276.** Hyaluronic acid-modified Fe_3O_4@Au core/shell nanostars for multimodal imaging and photothermal therapy of tumors. J. Li, Y. Hu, J. Yang, P. Wei, W. Sun, M. Shen, G. Zhang, **X. Shi**

2:50 COLL **277.** Nanostructured gold model catalysts on thin film substrates. **W.C. McKee**, M. Patterson, D. Huang, L. Liu, R. Kurtz, P. Sprunger, Y. Xu

3:10 COLL **278.** Nonwettable, oxidation stable, brightly-luminescent silicon nanocrystal film. **C. Qian**, W. Sun, G.A. Ozin

3:30 COLL **279.** Enzyme multilayer coatings prevent bacterial biofilm formation on urinary catheters. **K. Ivanova**, M. Fernandes, A. Francesko, T. Tzanov

3:50 Intermission.

4:20 COLL **280.** Chemical and structural transformations in colloidal inorganic nanocrystals. **L. Manna**

4:50 COLL **281.** Dithiocarbamate-anchored ligands on smooth and nanostructured gold surfaces. **A. Wei**

5:20 COLL **282.** Mesoporous membranes, zwitterionic monomers, and iniferter-initiated polymerization: Where does the polymerization proceed? **L. Silies**, H. Didzoleit, C. Hess, B. Stühn, A. Brunsen

Section C

Marriott City Center Denver
Colorado C/D

Metallic Nanostructures for Optical & Electrochemical Sensing & Alternative Energy Conversion

Spectroelectrochemistry, Imaging, & Surface

Cosponsored by PRES

Financially supported by Sigma-Aldrich

J. Zheng, *Organizer*
S. Pan, *Organizer, Presiding*
W. Wei, *Presiding*

2:00 COLL **283.** Spectroelectrochemistry and electrochemiluminescence of mixed-thiolate protected Au130 clusters. **G. Wang**, D. Wang, J. Padelford, T. Ahuja, T. Wang

2:30 COLL **284.** Imaging nanoscale energy transfer at the limits of temporal resolution and spatial accuracy. **K.L. Knappenberger**, J.W. Jarrett, S. Biswas, X. Lui, P.F. Nealey, R. Vaia

3:00 COLL **285.** Tailoring optical and plasmon resonances in core-shell and core-multishell nanowires for plasmonic light harvesting. **C. Yang**

3:30 Intermission.

3:40 COLL **286.** Single-particle photoelectrocatalysis. **P. Chen**

4:10 COLL **287.** Aqueous growth of fluorescence-tunable gold nanoclusters capped with lipoic acid-polyethylene glycol ligands. D. Mishra, F. Aldeek, G. Palui, **H.M. Mattoussi**

4:40 COLL **288.** Vivid, full-color plasmonic pixels. **S. Link**

Section D

Marriott City Center Denver
Denver III

Biomembrane Synthesis, Structure, Mechanics, & Dynamics

Dynamics

S. Muralidharan, M. Nieh, A. N. Parikh, N. Srividya, *Organizers*
D. Y. Sasaki, *Presiding*

2:00 COLL **289.** Substrate specificity of the plasma membrane phosphatidylserine flippase. **D.L. Daleke**

2:30 COLL **290.** Anionic phospholipid asymmetry and translocation in lipid membranes. **J.C. Conboy**

3:00 Intermission.

3:10 COLL **291.** Infrared study of membranes and membrane proteins. **F. Gai**

3:40 COLL **292.** Molecular transport through living cell membranes: Effects of molecular structure, membrane structure, and electrolyte composition. **H. Dai**

4:10 COLL **293.** Molecular interactions at model cell membranes. **Z. Chen**

Section E

Marriott City Center Denver
Colorado G

Plasmonic Catalysis and Sensing

Cosponsored by PRES

E. Borguet, *Organizer*
C. Matranga, *Organizer, Presiding*

2:00 COLL **294.** Plasmonic hetero-oligomer nanoparticle arrays for hydrogen sensing. **T.W. Odom**

2:35 COLL **295.** Optical gas sensors based on localized surface plasmon resonance. **A. Martucci**

3:10 COLL **296.** Localized surface plasmon resonance (LSPR) optical cetection of hydrogen. **D. Sil**, K.D. Gilroy, S. Sylla, S. Neretina, E. Borguet

3:30 Intermission.

3:45 COLL **297.** Thermal energy harvesting plasmonic based chemical sensors. M. Carpenter, **N. Karker**, G. Dharmalingam

4:20 COLL **298.** Plasmonic spectroscopy and photochemistry on highly damping platinum group metals. **K. Ikeda**

4:55 COLL **299.** Nanocomposite fiber optic pH sensor for high temperature applications. **C. Wang**, P. Ohodnicki, X. Su

Section F

Marriott City Center Denver
Colorado H

Advances in Formulations Science & Technology

Cosponsored by PRES

R. Y. Lochhead, *Organizer, Presiding*

2:00 COLL **300.** Advances in targeted multifunctional inhalation aerosols with nanotechnology and solid-state particle engineering design. **H.M. Mansour**

2:30 COLL **301.** Effects of formulation on the affinity of an SPD peptide fragment toward hair keratin: Experimental and molecular dynamics data. **A. Cavaco-Paulo**

3:00 COLL **302.** Design of thermal gelling polymer formulations for spray applications. **J.L. Curtis-Fisk**, M. Knarr, R. Adden, S.L. Jordan, T. Rogers

3:30 COLL **303.** Novel parameter to replace HLB. **K. Sakamoto**

4:00 COLL **304.** Watching paint age. **M.H. Keefe**, M. Linsen, M. Clark, J. Calderaio, J. Reffner

Section G

Marriott City Center Denver
Colorado F

ACS Award in Colloid and Surface Chemistry: Symposium in Honor of Paul S. Weiss

N. Kotov, *Organizer*
Y. Zheng, *Presiding*

2:00 COLL **305.** Development of multifunctional nano carrier platforms for cancer treatment. **A. Nel**

2:30 COLL **306.** Enabling biomolecule selection by small molecule-functionalized substrates: A decade of collaborative progress. **A.M. Andrews**, H. Cao, N. Nakatsuka, S. Deshayes, A. Vaish, M.J. Shuster, L.S. Slaughter, W. Liao, A.M. Kasko, P.S. Weiss

3:00 COLL **307.** Nanoparticle-mediated sorting of circulating tumor cell subpopulations. **S.O. Kelley**

3:30 COLL **308.** Graphene integration by molecular assembly. **P. Han**, K. Akagi, F. Federici Canova, H. Mutoh, S. Shiraki, K. Iwaya, P.S. Weiss, N. Asao, T. Hitosugi

4:00 COLL **309.** Reactions and functionalizations of graphene and surfaces. **K.N. Houk**

WCC Rising Stars Awards Symposium

Sponsored by WCC, Cosponsored by BIOT, COLL, GEOC, INOR, ORGN, PHYS, PMSE and PROF

MONDAY EVENING

Section A

Colorado Convention Center
Halls C/D

Sci-Mix

R. Nagarajan, *Organizer*

8:00 - 10:00
8, 26, 53, 64, 74-75, 78, 82, 106, 119, 164, 174-175, 191, 212, 220, 232-233, 243, 262, 269, 272-273, 302-303. See previous listings.
310- 311, 322, 341, 351, 365, 367, 378, 380-382, 390, 400, 411, 413, 419, 423, 430, 434, 437, 455, 458, 465, 468-469, 492, 502-503, 518, 521, 523-524, 535, 545-546, 549-550. See subsequent listings.

TECHNICAL PROGRAM

TUESDAY MORNING

Section A

Marriott City Center Denver
Colorado A/B

Molecular Engineering of Peptide Assembly

Financially supported by Institute for Molecular Engineering, University of Chicago

H. Cui, M. V. Tirrell, *Organizers, Presiding*

8:30 COLL **311.** Protein analogous micelles: Versatile, modular nanoparticles. **M.V. Tirrell**

9:00 COLL **312.** Enzymatic transformation and self-assembly of peptides for future cancer therapy. **B. Xu**, J. Zhou, X. Du, J. Shi, Y. Kuang

9:30 COLL **313.** Designability of peptide-based materials. **V.P. Conticello**

10:00 Intermission.

10:15 COLL **314.** Tumor-penetrating peptides in the targeting of drugs and theranostic nanoparticles. **E. Ruoslahti**

10:45 COLL **315.** Peptide-guided drug assembly. **H. Cui**

11:15 COLL **316.** Engineering underwater adhesives: Leveraging cation-π interactions to govern peptide cohesion. **M.A. Gebbie**, W. Wei, A.M. Schrader, T.R. Cristiani, J. Waite, J.N. Israelachvili

11:35 COLL **317.** Peptide-polymer amphiphiles as programmable synthons for biologically-responsive nanomaterials. **N.C. Gianneschi**

Section B

Marriott City Center Denver
Colorado I

Functionalization of Complex Nanosurfaces

Cosponsored by PRES

L. Liz Marzan, *Organizer*
W. Parak, *Organizer, Presiding*

8:30 COLL **318.** Interaction of colloidal nanoparticles with mammalian cells: Correlation of uptake and toxicity with physicochemical properties, such as surface coating. **N. Feliu**, S. Ashraf, C. Carrillo-Carrion, P. del Pino, B. Pelaz, W. Parak

8:50 COLL **319.** Impact of gold nanoparticles on cells: PEGylation's type matters. **P. del Pino**, W. Parak

9:20 COLL **320.** Silanization of layer-by-layer assemblies: Mechanisms and application for the fabrication of superhydrophobic surfaces. **A. Dirani**, A. Fernandes, P. Lipnik, C. Poleunis, B. Nysten, K. Glinel, A.M. Jonas

9:40 COLL **321.** Verification of anti-icing/icephobic properties of different chemical modified superhydrophobic surfaces. Y. Wang, Q. Wang, **Q. Chen**

10:00 Intermission.

10:30 COLL **322.** Super-high resolution of control assembled fluorescent-TMV using microlens. **R. Balaraman**, C. Zhou, P. Kohli

10:50 COLL **323.** Surface-enhanced Raman scattering nanoparticles as optical labels for imaging cell surface proteins. **G.C. Walker**, C. MacLaughlin

11:20 COLL **324.** Surface modification of inorganic nanoparticles for biomedical applications. **B. Pelaz**, M.G. Soliman, P. del Pino, W. Parak

11:40 COLL **325.** Engineering the optical properties of gold nanoparticles by assembling into highly packed 2D arrays of different structure. **M.A. Mahmoud**

12:00 COLL **326.** Protein resistant nanoparticle surfaces designed for the assembly of biodegradable plasmonic gold nanoclusters. **R. Stover**, A.K. Murthy, S.P. Gourisankar, M. Martinez, A. Issac, T. Truskett, K. Sokolov, K.P. Johnston

Section C

Marriott City Center Denver
Colorado C/D

Metallic Nanostructures for Optical & Electrochemical Sensing & Alternative Energy Conversion

Biosensing, Energy Conversion & Catalysts

Cosponsored by PRES

Financially supported by Sigma-Aldrich

J. Zheng, *Organizer*
S. Pan, *Organizer, Presiding*
C. Yang, *Presiding*

8:30 COLL **327.** Metallic nanocomposites of carbon nanotube and their bioconjugates: effective antimicrobials? **A. Chaudhari**, S. Singh, S. Pillai

9:00 COLL **328.** Au/CdS plasmonic photocatalytic nanostructures constructed using P22 virus-like particles for enhanced photoactivity. **A. Gupta**, Z. Zhou, S. Palchoudhury, G. Bedwell, R. Li, P.E. Prevelige

9:30 COLL **329.** Scalable metal-semiconductor nanostructure integration for multimode gas sensing at high temperature. **P. Gao**

10:00 Intermission.

10:10 COLL **330.** Plasmonic enhancement characteristics of multilayered metallic nanostructures. **D.D. Evanoff**, E.R. Butcher, J.P. Cook

10:40 COLL **331.** Exotic Au nanostructures: structure solution, properties, and applications. **Y. Han**

11:10 COLL **332.** Ultrasensitive detection using SERS and SEHRS: From nonlinear optical properties to nuclear forensics. **J.P. Camden**

Section D

Marriott City Center Denver
Denver III

Biomembrane Synthesis, Structure, Mechanics, & Dynamics

Structure and Interactions

S. Muralidharan, M. Nieh, A. N. Parikh, N. Srividya, *Organizers*
F. Gai, *Presiding*

9:00 COLL **333.** Conformation and dynamics of endogenous cannabinoid ligand 2-AG in a lipid matrix and its interaction with cannabinoid type II receptor. T. Kimura, M. Mihailescu, D.L. Lynch, P.H. Reggio, A.A. Yeliseev, **K. Gawrisch**

9:30 COLL **334.** Studying the mechanism of coiled coil mediated membrane fusion. **A. Kros**

10:00 COLL **335.** Exploring the interactions of ions with supported lipid membranes. **P.S. Cremer**

10:30 Intermission.

10:40 COLL **336.** Dynamic reorganization and correlation among lipid raft components probed by imaging mass spectrometry. **S.G. Boxer**

11:10 COLL **337.** Functionalized lipid–nucleic acid nanoparticles for delivery applications. **C.R. Safinya**, R.N. Majzoub, K.K. Ewert

11:40 COLL **338.** Nanometric gap structure between substrate-supported model membrane and silicone elastomer. **K. Morigaki**

Section E

Marriott City Center Denver
Colorado G

Plasmonic Catalysis and Sensing

Cosponsored by PRES

C. Matranga, *Organizer*
E. Borguet, *Organizer, Presiding*

8:30 COLL **339.** Super-resolution imaging of plasmonic nanostructures. **K.A. Willets**

9:05 COLL **340.** Plasmonic efficiency enhancement for up-hill photocurrent generation at gold electrode modified with self-assembled monolayer. **K. Uosaki**, K. Ikeda

9:40 COLL **341.** Localized surface plasmon (LSPR) based optical detection of ions in aqueous solution. **D. Sil**, K. Gilroy, C. Murphy, S. Sylla, R.A. Hughes, S. Neretina, E. Borguet

10:00 Intermission.

10:15 COLL **342.** Nanogap plasmonic structures for Raman studies of single molecules and heating. **D. Natelson**, Y. Li, P. Zolotavin

10:50 COLL **343.** Ultrabright luminescent metallic nanoparticles. **H. Dai**

11:25 COLL **344.** Hybrid core-shell and coupled nanostructures: Design and applications. **S. Hunyadi Murph**

Section F

Marriott City Center Denver
Colorado I/J

Interfacial Biomolecular Recognition

Cosponsored by BIOL‡

Financially supported by Avanti Polar Lipids, Inc.

J. Ross, *Organizer*
B. E. Bowler, M. Kastantin, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 COLL **345.** Nanoparticle assembly and gelatin binding mediated by collagen mimetic peptide hybridization. **S. Yu**

9:05 COLL **346.** Supercritical angle fluorescence (SAF) microscopy with nanometer resolution investigating the interaction and aggregation of proteins at lipid bilayer. **S. Seeger**

9:35 COLL **347.** Fibrinonectin conformation and integrin binding on crowded surfaces. **M. Kastantin**, N. Grover, D.F. Marruecos, D.K. Schwartz, J. Kaar

10:05 Intermission.

10:20 COLL **348.** Docking model of synaptotagmin 7 C2A via electron paramagnetic resonance. **A. Boo**, J.R. Osterberg, F. Maynard, N.L. Chon, H. Lin, J. Knight

10:45 COLL **349.** Lateral diffusion of synaptotagmin 1 and 7 on supported lipid bilayers: Assessing the frictional additivity of C2A-C2B tandem domains. **D.T. Giardina**, J. Vasquez, J.D. Knight

11:10 COLL **350.** Molecular dynamics simulations of PEGylated dendron-based micelles adsorption on biological membranes. **S. Sen**, P. Kral

11:35 COLL **351.** Xanthan/magnetite scaffolds for neuronal adhesion, proliferation and differentiation of embryonic stem cells. **D. Petri**, T. Glaser, V. Bueno, H. Ulrich

Section G

Marriott City Center Denver
Colorado F

ACS Award in Colloid and Surface Chemistry: Symposium in Honor of Paul S. Weiss

N. Kotov, *Organizer*
A. K. Jen, *Presiding*

9:00 COLL **352.** Programmable atom equivalents from nucleic-acid modified nanostructures: constructing a new "Table of Elements". **C.A. Mirkin**

9:40 COLL **353.** Colloidal nanocrystal buildling blocks for large-area optical metamaterials. **C.R. Kagan**, A.T. Fafarman, S. Hong, W. Chen, X. Ye, T. Paik, H. Caglayan, C.B. Murray, N. Engheta

10:20 COLL **354.** Surface chemistry of DNA at the single molecule level: Plenty of room at the bottom? **T. Ye**

10:50 COLL **355.** Molecular photonics for materials science, energy and healthcare. **Y. Zheng**

Molecular-Scale Processes Controlling Reactivity at Mineral-Water Interfaces

Sponsored by GEOC, Cosponsored by COLL

TUESDAY AFTERNOON

Section G

Marriott City Center Denver
Colorado F

ACS Award in Colloid and Surface Chemistry: Symposium in Honor of Paul S. Weiss

N. Kotov, *Organizer*
M. Hersam, *Presiding*

2:00 COLL **356.** Surface chemistry in solar energy harvesting materials. **E. Sargent**

2:40 COLL **357.** Anomalous nanocolloids defying the likes dissolves likes rule. **N. Kotov**, J. Bang, B. Yeom

3:10 COLL **358.** Dimensional control of chemical interfaces using polymerizable amphiphiles. **S.A. Claridge**

3:40 COLL **359. Award Address** (ACS Award in Colloid and Surface Chemistry sponsored by Colgate-Palmolive Company). Assembly and measurements of isolated and coupled functional molecules. **P.S. Weiss**

Molecular-Scale Processes Controlling Reactivity at Mineral-Water Interfaces

Sponsored by GEOC, Cosponsored by COLL

WEDNESDAY MORNING

Section A

Marriott City Center Denver
Colorado A

Natural Resource Capture, Storage & Energy Conversion

Theory, Synthesis, Hybrid/Soft Materials, Catalysts, MOFs and Related Application (TSHSCMA)

S. Bashir, *Organizer*
J. Liu, *Organizer, Presiding*
J. Uddin, *Presiding*

8:30 COLL **360.** Light-activated multicomponent materials for tandem catalysis. **M.R. Knecht**, E.M. Zahran, M.A. Nguyen, N. Bedford, Y. Chang, B.S. Guiton, R.R. Naik, L. Bachas

9:00 COLL **361.** Zn-MOFs with pyridine-based organic linkers and their carburized, N-doped carbons analogues as CO_2 capture adsorbents. **J. Kim**, A.G. Oliver, G.T. Neumann, J.C. Hicks

9:25 COLL **362.** Synthesis of VTMS(X)-HMS-3 mesoporous ordered silica for hydrogen storage. **Y. Mao**, D. Owens, A. Han, L. Sun

9:50 COLL **363.** Insights in sol-gel matrix diffusion methodology in the synthesis of soft materials from second group (Ca^{2+}, Ba^{2+}, Mg^{2+}) earth alkaline metals. **T. Chavez-Gil**

10:15 COLL **364.** Synthesis of Pt-based catalysts for DMFCs by microfluidic reactors. D. Zhang, F. Wu, **X. Wang**, D. Xia, J.L. Liu, G. Guo

10:40 COLL **365.** Design of polymeric solid acid catalyst for efficient biofuel production. **X. Sun**, X. Qian

11:05 COLL **366.** Metal-organic frameworks for on-board storage of hydrogen and natural gas. J.A. Mason, E.D. Bloch, M.T. Kapelewski, M.K. Taylor, J. Oktawiec, K. Sumida, M.I. Gonzalez, D. Gygi, W. Queen, **J.R. Long**

Section B

Marriott City Center Denver
Colorado I/J

Interfacial Biomolecular Recognition

Cosponsored by BIOL‡

Financially supported by Avanti Polar Lipids, Inc.

J. Ross, *Organizer*
B. E. Bowler, M. Kastantin, *Organizers, Presiding*

8:30 COLL **367.** Detecting biomolecular interactions and photodynamics in solution by suppression of Brownian motion. **W.E. Moerner**, Q. Wang, G. Schlau-Cohen, H. Yang

‡ *Cooperative Cosponsorship*

9:00 COLL 368. Super-resolution imaging and reaction mapping of P450 3A4 and P450 reductase in heterogeneous biomimetics: Starry night. **J.A. Brozik**, S.C. Humphreys, C. Barnaba, A.O. Barden, J.P. Jones

9:30 COLL 369. Stimuli-responsive chymotrypsin conjugates synthesized using polymer-based protein engineering. **C.S. Cummings**, H. Murata, A.J. Russell

10:00 Intermission.

10:15 COLL 370. Cytochrome c: An electrostatically bound peripheral membrane protein. **P.K. Kinnunen**

10:45 COLL 371. Interfacial exposure, recognition, and signaling by nitochondrial cardiolipins. **V. Kagan**

11:15 COLL 372. Conformational diversity of cytochrome c on cardiolipin containing liposomes probed by fluorescence and circular dichroism spectroscopy. **R. Schweitzer-Stenner**, L.A. Pandiscia, L. Serpas, D. Malyshka

Section C

Marriott City Center Denver
Colorado C/D

Metallic Nanostructures for Optical & Electrochemical Sensing & Alternative Energy Conversion

Biosensing, Catalysts, & Electrochemistry

Cosponsored by PRES

Financially supported by Sigma-Aldrich

S. Pan, *Organizer*
J. Zheng, *Organizer, Presiding*
B. Nelson, *Presiding*

8:30 COLL 373. Template free fabrication of vertically aligned Ag nanorods for surface plasmon enhanced photocatalytic reactions and Raman spectroscopy. **J. Wang**, S. Pan

8:50 COLL 374. Copper plasmonics and catalysis: Role of electron-phonon interactions in dephasing localized surface plasmon. **Q. Sun**, Y. Ding, S.M. Goodman, H.H. Funke, P. Nagpal

9:10 COLL 375. Electrodeposited alloy thin films for catalysis applications. M. Gira, M. Milliken, K. Tkacz, **J.R. Hampton**

9:30 COLL 376. Block copolymer template-directed synthesis of mono- and bimetallic nanoparticle catalysts. **D.A. Rider**, K. Mikkelsen, A. Taylor, D.S. Perez

9:50 Intermission.

10:00 COLL 377. Rational design of nanocatalysts for oxygen reduction reaction. **S. Guo**

10:20 COLL 378. Tunable plasmonic nanoparticles for enhancing photocatalytic reactions. **C. Li**, T. Lee, T. Lee

10:40 COLL 379. Enhanced photocatalytic activities of chemical vapor deposited hematite films for solar water splitting by Au NPs in embedded configuration. **A. Panikar**, N. Pachauri, Z. Shan, S. Pan, A. Gupta

11:00 COLL 380. Electrochemical investigation of nanoparticles modified glassy carbon electrode and its application for ketoconazole determination. **M. Alshalalfeh**, **K. Alaqad**, **T.A. Saleh**

Section D

Marriott City Center Denver
Denver III

Biomembrane Synthesis, Structure, Mechanics, & Dynamics

Structure and Modeling

S. Muralidharan, A. N. Parikh, N. Srividya, *Organizers*
M. Nieh, *Organizer, Presiding*

9:00 COLL 381. Biomembrane structure using neutron scattering and molecular labeling. J.D. Nickels, S. Chatterjee, J.G. Elkins, F.A. Heberle, R.F. Standaert, D.A. Myles, **J. Katsaras**

9:30 COLL 382. Experiment and simulation reveal the bending properties of nanoscopic lipid domains. **J. Nickels**, M. Ohl, X. Cheng, F. Heberle, C.B. Stanley, M. Feygenson, J. Neuefeind, P. Zolnierczuk, B. Mostofian, B. Linder, R.F. Standaert, J. Katsaras

10:00 COLL 383. Shear flow-induced de-registration of compositional domains in supported lipid bilayer membranes. **M. Haataja**

10:30 Intermission.

10:40 COLL 384. Determination of membrane bending moduli from fully atomistic simulations. **F.L. Brown**

11:10 COLL 385. Nanoscale structure of sphingolipid containing liquid-ordered phases. **E. Lyman**, A. Sodt, R. Pastor

11:40 COLL 386. Withdrawn.

Section E

Marriott City Center Denver
Colorado G

Plasmonic Catalysis and Sensing

Cosponsored by PRES

E. Borguet, *Organizer*
C. Matranga, *Organizer, Presiding*

8:30 COLL 387. Enhancing catalytic efficiency of hollow palladium nanoparticles by photothermal heating of added gold nanoparticles to their cavity: palladium-gold nanorattles. **M.A. Mahmoud**, M.A. El-Sayed

9:05 COLL 388. Plasmon resonant enhancement of photocatalytic processes. **S. Cronin**, J. Qiu, G. Zeng

9:40 COLL 389. Visible-light, plasmonic, heating for catalytic CO_2 conversion applications. **C. Matranga**

10:00 Intermission.

10:15 COLL 390. Photochemical reactions on plasmonic metal nanostructures. **S. Linic**

10:50 COLL 391. Active control of surface chemistry on plasmonic nanomaterials. **C.F. Landes**

11:25 COLL 392. Plasmon-driven CO oxidation in Au-$SrTiO_3$ nanostructures at room temperature. **B.C. Sweeny**, K. Qian, J.S. DuChene, J. Qiu, A.C. Johnston-Peck, D. Su, E.A. Stach, W.D. Wei

Section F

Marriott City Center Denver
Colorado H

Elucidation of Mechanisms & Kinetics on Surfaces

Cosponsored by CATL and ENVR

A. Savara, *Organizer, Presiding*

9:00 Introductory Remarks.

9:10 COLL 393. Elucidation of reaction mechanisms in complex catalytic networks. **T. Bligaard**

9:30 COLL 394. Isolated metal active site concentration controls catalytic CO_2 reduction selectivity. **J. Matsubu**, P. Christopher, V. Yang

9:50 COLL 395. Mechanism and kinetics of surface limitations in MFI ezolite catalysts. A.R. Teixeira, C. Chang, W. Conner, W. Fan, **P.J. Dauenhauer**

10:10 Discussion.

10:20 COLL 396. Hydrogenation of butadiene on Pt in realistic hydrogen pressure: mechanistic insights from DFT. **P. Sautet**, S. Gautier

10:40 COLL 397. Kinetics and mechanisms of oxidation reactions on metal oxide surfaces. **S.L. Scott**, D.H. Coller

11:00 COLL 398. Differences in the reaction mechanisms of hydrodeoxygenation (HDO) of m-cresol on platinum and ruthenium catalysts. **D.E. Resasco**, Q. Tan, G. Wang, L. Nie

11:20 COLL 399. Theoretical studies of oxygenates derivatives by metallic heterogeneous catalysts. A micro-solvation approach. **C. Michel**, P. Sautet

11:40 Discussion.

11:50 COLL 400. Thermodynamics and kinetics of oxygen induced chain-like reconstructions on the Pt(111) surface. **L. Herder**, W.F. Schneider

12:10 COLL 401. Adsorbate-adsorbate interaction model for microkinetic trend studies and catalyst screening. **B. Yang**, T. Khan, Y. Xu, A. Lausche, J.K. Norskov, T. Bligaard

12:30 Discussion.

Section G

Marriott City Center Denver
Colorado B

Basic Research in Colloids, Surfactants & Nanomaterials

Amphiphilic Systems

Cosponsored by PRES

R. Nagarajan, *Organizer, Presiding*

8:30 COLL 402. Long chain alkylimidazole switchable surfactants. **W. Qiao**, M. Chai

8:50 COLL 403. Interfacial characterization of chemically modified sophorolipid derivatives. **A. Koh**, R.A. Gross

9:10 COLL 404. Bilayer self-assembly from single-chain amphiphiles during the origins of life. **S.E. Maurer**

9:30 COLL 405. Monitoring the effect of surfactant type and process condition on sebum removal from CNF/PET surfaces in an aqueous solution using QCM/SPR technique. **A.H.M. Tayeb**, O.J. Rojas, C.L. Salas, K. Ghosh, M.A. Quddus

9:50 COLL 406. Study of surfactant influence on the low-pH stability of polyolefin dispersions. **Q. Wan**, M. Crimmins, S.L. Jordan, R. Yan, M. Hus

10:10 COLL 407. Solutes stabilized by brush amphiphiles: A study of solutes induced morphlogical transitions of brush amphiphile micelles. **H. Luo**, M. Herrera-Alonso

10:30 COLL 408. Aqueous delivery of π-π conjugated polymer solutions through a network formed by a fungal Janus-like surfactant. **C. Rosu**, N. Kleinheinz, D. Choi, P.S. Russo, E. Reichmanis

10:50 COLL 409. Self-assembly of novel fluorosurfactants with polyoxometalates (POMs) as polar component in acetonitrile/water solution. **B. Zhang**

11:10 COLL 410. Characterization of a chelating surfactant: Solution behavior and application prospects in ion flotation. I. Svanedal, **M. Norgren**, H. Edlund

11:30 COLL 411. Properties of novel bioinspired glycolipid surfactants: Tailoring function by disaccharide headgroup and alkyl tail length. **L. Kegel**, L. Szabo, R. Polt, J.**E. Pemberton**

11:50 COLL 412. CO_2-reactive surfactant ionic liquids for reversible control of colloidal morphology and DNA compaction. **P. Brown**, T. Hatton

Molecular-Scale Processes Controlling Reactivity at Mineral-Water Interfaces

Sponsored by GEOC, Cosponsored by COLL

WEDNESDAY AFTERNOON

Section A

Marriott City Center Denver
Colorado A

Natural Resource Capture, Storage & Energy Conversion

Theory, Synthesis, Hybrid/Soft Materials, Catalysts, MOFs and Related Application (TSHSCMA)

J. Liu, *Organizer*
S. Bashir, *Organizer, Presiding*
X. Wang, *Presiding*

2:00 COLL 413. Vapor-assisted crystallization synthesis of a microporous (Ti) MIL-125 exhibiting significant mesoporosity. **N.D. McNamara**, J.C. Hicks

2:30 COLL 414. Synthesis and electromagnetic absorption properties of core-multishell MWCNT/Fe3O4/PANI/Au hybrids. **Y. Xu**, C. Liu, Z. Wang

2:55 COLL 415. Computational discovery of metal-organic frameworks gas capture and storage. **D. Siegel**

3:20 COLL 416. Enhancement of optical absorptions in oxide nanostructures: Insight from a TDDFT study. **M. Huda**

3:45 COLL 417. Selective reduction of CO_2 to formate by a homogeneous Iron electrocatalyst in water between pH 5 and 13. **L.A. Berben**, A. Taheri

4:10 COLL 418. Nanoparticles and nanomaterials for electrochemical conversion of oxygen and carbon cioxide. **A.A. Gewirth**, C. Tse, T. Hoang, K.G. Schmitt

4:35 COLL 419. Optical response of molecule — semiconducting nanoparticle hybrids. **A. Keller**, V. Mujica

Section B

Marriott City Center Denver
Colorado H

Interfacial Biomolecular Recognition

Cosponsored by BIOL‡

Financially supported by Avanti Polar Lipids, Inc.

J. Ross, *Organizer*
B. E. Bowler, M. Kastantin, *Organizers, Presiding*

2:00 COLL 420. Cytochrome *c* unfolding at cardiolipin-rich membrane surfaces. **E.V. Pletneva**

2:30 COLL 421. Conformational dynamics of cytochrome *c* related to peroxidase activity during apoptosis. L. McClelland, S. Bandi, T. Mou, S.R. Sprang, **B.E. Bowler**

3:00 COLL 422. Artificial virus nanoparticles to control cellular processes at the virus-host interface. **B.M. Reinhard**, X. Yu, S. Gummuluru

3:25 Intermission.

3:40 COLL 423. Tracking amyloids with fluorescent oligo(*p*-phenyleneethynylene) electrolytes. **P. Donabedian**, T. Pham, D.G. Whitten, E.Y. Chi

4:05 COLL 424. Super-resolving the dynamics of a membrane-bound virulence regulator in *Vibrio cholerae*. **J.S. Biteen**

4:35 COLL 425. Proximity energies and their consequences in living systems. **T. Laue**

5:05 COLL 426. Molecular basis of high-affinity membrane binding by the C2A domain of granuphilin. A. Watson-Siriboe, T. Lyakhova, **J. Knight**

Section C

Marriott City Center Denver
Colorado C/D

Metallic Nanostructures for Optical & Electrochemical Sensing & Alternative Energy Conversion

Fabrication for Biosensing, Energy Conversion & Catalysts

Cosponsored by PRES

Financially supported by Sigma-Aldrich

S. Pan, J. Zheng, *Organizers, Presiding*

2:00 COLL 427. Gold nanoparticle assembly for selective two photon scattering imaging of cancer cell. **P.C. Ray**

2:20 COLL 428. Size selective SERS analysis using nanorattles with porous polymer shell and entrapped gold nanoparticles. **Y. Jia**, S. Shmakov, E. Pinkhassik

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2:40 COLL **429.** Ultrafast laser induced synthesis of narrowly distributed sub-5 nm surfactant-free Au-Pd nanoparticles. **D. Sil**, K. Moore Tibbetts, J.H. Odhner, R.J. Levis, E. Borguet

3:00 COLL **430.** Fabrication of plasmonic nanoantenna arrays on flexible substrates via colloidal lithography for biosensing. **A. Bohloul**, V.L. Colvin

3:20 Intermission.

3:30 COLL **431.** Withdrawn.

3:50 COLL **432.** Enhancement of enzymatic colorimetric response by silver island films on high throughput screening microplates. **B. Abel**, K. Aslan

4:10 COLL **433.** Development of polymer-metal colloid hybrid platforms for bioassays with improved dynamic range. E. Bonyi, **K. Aslan**

4:30 COLL **434.** Surface plasmon enhanced photoelectrochemical performance of core-shell Ag@Ag_2S nanoparticles decorated Ti@TiO_2 nanowire electrodes. **Z. Shan**, S. Pan, A. Panikar, A. Gupta

4:50 Concluding Remarks.

Section D

Marriott City Center Denver

Denver III

Biomembrane Synthesis, Structure, Mechanics, & Dynamics

Structure and Mechanics

S. Muralidharan, M. Nieh, N. Srividya, *Organizers*

A. N. Parikh, *Organizer, Presiding*

2:00 COLL **435.** Probing cellular mechano-sensitivity using biomembrane-mimicking cell substrates of adjustable stiffness. **C. Naumann**, Y. Lin, L. Lautscham, Y. Ge, W. Goldmann, B. Fabry

2:30 COLL **436.** Evaluation of drug mediated changes in rhythmic contractile activity of cardiomyocytes. **S. Zou**

3:00 Intermission.

3:10 COLL **437.** Changes in the cell surface during progression to cancer of human cervical epithelial cells. **I. Sokolov**, M. Dokukin, N. Guz, C. Woodworth

3:40 COLL **438.** Probing the coupling between polybasic peptides and PIP_2 lipids in asymmetric supported lipid bilayers. **A.W. Smith**, X. Shi, X. Li

4:10 COLL **439.** Oncogene induced stiffening of living cells. **N. Nordgren**, L.Z. Rathje, T. Pettersson, D. Rönnlund, J. Widengren, P. Aspenström, A.K. Gad

Section E

Marriott City Center Denver

Colorado G

Plasmonic Catalysis and Sensing

Cosponsored by PRES

C. Matranga, *Organizer*

E. Borguet, *Organizer, Presiding*

2:00 COLL **440.** Electronic structure models of plasmon-enhanced processes. **G.C. Schatz**

2:35 COLL **441.** Ultrafast size-dependent electronic interactions in metal clusters. **N. Del Fatti**, T. Stoll, P. Maioli, A. Crut, F. Vallee

3:10 COLL **442.** Plasmon-driven growth of gold nanoprisms with implications for photocatalysis. **Y. Zhai**, J.S. DuChene, Y. Wang, A.C. Johnston-Peck, B. DiCiaccio, K. Qian, E.W. Zhao, J. Qiu, F. Ooi, D. Hu, D. Su, E. Stach, Z. Zhu, W.D. Wei

3:30 Intermission.

3:45 COLL **443.** Plasmon enhanced sensing and catalysis. **P.J. Nordlander**

4:20 COLL **444.** Unique properties of metal nanocrystals for driving photocatalysis. **P. Christopher**

4:55 COLL **445.** Analysis of 2- and 3D plasmon coupling between nanoparticles on cellular and viral surfaces. **B.M. Reinhard**, X. Yu, A. Feizpour

Section F

Marriott City Center Denver

Colorado H

Elucidation of Mechanisms & Kinetics on Surfaces

Cosponsored by CATL and ENVR

A. Savara, *Organizer, Presiding*

2:00 COLL **446.** Impact of self-assembled monolayers on (oxidized) cobalt for Si-based molecular electronic junctions. **C.A. Hacker**, S. Pookpanratana

2:20 COLL **447.** Dynamics of self-assembled monolayers on Au(111) studied by time-resolved scanning tunneling microscopy. **H. Wu**, K. Sotthewes, P.M. Schön, G.J. Vancso, H. Zandvliet

2:40 COLL **448.** Polyurethane degradation and characterization of aerospace coatings. **J.H. Wynne**, N.K. Weise, A.E. Mera, D. Bellevou

3:00 COLL **449.** Cyclic azasilanes: A kinetic approach to rapid silane surface modification. **A.F. Maddox**, J.G. Matisons, M.P. Singh, J. Zazyczny, B. Arkles

3:20 Discussion.

3:30 Intermission.

3:40 COLL **450.** Pyridinium as the electrocatalyst in carbon dioxide reduction on polycrystalline gold electrodes. **A.J. Lucio**, S.K. Shaw

4:00 COLL **451.** Rapid formation of reactive initiator monolayers for conjugated polymer brushes using electrochemical reduction of Ni(II). **A. Roy**, J.J. Locklin

4:20 COLL **452.** Vibrational sum frequency generation studies for elucidating mechanisms and kinetics at surfaces. **F. Geiger**

4:40 Discussion.

4:50 COLL **453.** Advancements in the determination of membrane zeta potential at high ionic strengths: Specific application to semipermeable polymeric membrane. **B.D. Coday**, T. Luxbacher, A. Childress, N. Almaraz, T.Y. Cath

5:10 COLL **454.** Nucleation and crystallization kinetics of initial apatite nanocrystal formation within biological templates. **D. Kim**, B. Lee, S. Thomopoulos, Y. Jun

5:30 COLL **455.** Three column series approach to investigate role of desorption rates in colloid-facilitated transport of americium, cesium, and plutonium: Experiments and modeling. **T.M. Dittrich**, H. Boukhalfa, P.W. Reimus

5:50 Discussion.

Molecular-Scale Processes Controlling Reactivity at Mineral-Water Interfaces

Sponsored by GEOC, Cosponsored by COLL

THURSDAY MORNING

Section A

Marriott City Center Denver

Colorado A

Natural Resource Capture, Storage & Energy Conversion

Biofuels, Fuel Cells, Membranes, Electrolytes, & Batteries (BFCMEB)

S. Bashir, *Organizer*

J. Liu, *Organizer, Presiding*

J. Uddin, *Presiding*

8:30 COLL **456.** Structure-function relationships into layered solid oxide fuel cell cathode material. **S. McIntosh**

9:00 COLL **457.** Tailoring the structure of active materials for solar thermochemical fuel production through templating. **A. Stein**, C. Malonzo, S. Rudisill, N. Petkovich, J. Davidson, R. DeSmith, L. Venstrom

9:25 COLL **458.** Reducing cracks in photoanode of dye-sensitized solar cells based on binder-free TiO_2 nanoparticles by 1D electrospun metal oxide nanofibers. **X. Wang**, M. Xi, H. Fong, Z. Zhu

9:50 COLL **459.** Metabolic characterization of nonmodel microalgae for sustainable biofuel production. **G. Atilla-Gokcumen**, E. Matich, E. Camgoz, M. Ghafari, B.A. Pfeifer, B.Z. Haznedaroglu

10:15 COLL **460.** Pore collapse and regrowth in silicon electrodes for rechargeable batteries. **S. DeCaluwe**, B. Dhar, J. Dura, H. Wang

10:40 COLL **461.** Fast charging of dual lithium-ion-insertion cells. **R. Chandrasekaran**

Section B

Marriott City Center Denver

Colorado I/J

Interfacial Biomolecular Recognition

Cosponsored by BIOL‡

Financially supported by Avanti Polar Lipids, Inc.

J. Ross, *Organizer*

B. E. Bowler, M. Kastantin, *Organizers, Presiding*

8:30 COLL **462.** Hierarchical view of DNA based recognition, and the role of flexibility and shape. **J.J. De Pablo**

9:00 COLL **463.** Withdrawn.

9:30 COLL **464.** Entropic and electrostatic effects on the folding free energy of a surface-attached biomolecule: An experimental and theoretical study. **K. Plaxco**, H. Watkins

10:00 Intermission.

10:15 COLL **465.** Surface-mediated DNA hybridization. J. Monserud, **D.K. Schwartz**

10:45 COLL **466.** Single molecule view of conformational changes and hybridization of DNA on dynamic surfaces. **T. Ye**

11:10 COLL **467.** Quantitative single-molecule imaging of DNA hybridization at capture surfaces with sequence specificity. **E.M. Peterson**, M.W. Manhart, D. Kriech, J.M. Harris

11:35 COLL **468.** Using nonlinear optical spectroscopy to monitor DNA molecular recognition and structure at the buried silica/aqueous interface. **J. Gibbs-Davis**

Section C

Marriott City Center Denver

Colorado C/D

Basic Research in Colloids, Surfactants & Nanomaterials

Polymeric Materials

Cosponsored by PRES

R. Nagarajan, *Organizer*

J. Jahnke, *Presiding*

8:30 COLL **469.** Rapid synthesis of faujasite/polyethersulfone composite membrane and application for CO_2/N_2 separation. **B. Wang**, L. Zhao, W. Ho, P.K. Dutta

8:50 COLL **470.** Relationship between polyelectrolyte bulk complexation and kinetics of their layer-by-layer assembly. **P.S. Desai**, A. Salehi, J. Li, R.G. Larson

9:10 COLL **471.** Adsorption of bacteria into electrospun cellulose nanofiber mats: Development of a dynamic model. **K. Rieger**, R. Thyagarajan, M. Hoen, D.M. Ford, J.D. Schiffman

9:30 COLL **472.** Multilayer chromorphore thin film fabrication via layer by layer deposition technique. **M. Zhu**, G.H. Aryal, H. Zhang, J. Jayawickramarajah

9:50 COLL **473.** Modulating the uptake of dextran coated SPIONs in stem cells: The effect of surface charge. **M. Barrow**

10:10 COLL **474.** Effect of membrane structural dopants on charge transport through conjugated oligoelectrolyte modified phospholipid bilayers. **J. Jahnke**, G. Bazan, J. Sumner

10:30 COLL **475.** Uniform cross-linked cellulase aggregates prepared in millifluidic reactors. **L. Nguyen**, K. Yang

10:50 COLL **476.** Self-healing and disruption of arboreol fibrils. **G. Parkinson**, J. Sun, P.S. Russo

11:10 COLL **477.** Two-photon absorption properties of chromophores in polyelectrolytes. **M. Hatshan**, R. Guda

Section D

Marriott City Center Denver

Denver III

Basic Research in Colloids, Surfactants & Nanomaterials

Biomolecular Materials

Cosponsored by PRES

R. Nagarajan, *Organizer, Presiding*

8:30 COLL **478.** Substrate mediated stability of DNA origami at elevated temperatures and in diverse solvent environments. **M.A. Pillers**, M. Lieberman

8:50 COLL **479.** Exploring biomedical applications of nanoparticles by their surface functionalization. K. Rashwan, G. Sereda, **P. Jampani**, B. Burum, D. Christianson, E. Brakke, K. Kaufman, C. Pap

9:10 COLL **480.** DNA nanotubes and nanotapes via self-assembly of ssDNA-amphiphiles. T.R. Pearce, B. Waybrant, **E. Kokkoli**

9:30 COLL **481.** Connections between nanoparticle (NP) surface chemistry and protein corona formation: Influence of the corona on small (d_{core} < 5.0 nm) NP- supported lipid bilayer interactions. **S.E. Lohse**, E. Melby, J. Park, B. Putans, R.J. Hamers, J.A. Pedersen, C.J. Murphy

9:50 COLL **482.** New generation of well-defined lipid-based magnetic nanoparticles for theranostics. **S. Biswas**, J.A. Kulkarni, Y.C. Tam, P.R. Cullis

10:10 COLL **483.** Robust and tailored wet adhesion in biopolymer thin film with wet adhesion and toughness superior to wet adhesion in bone. **T. Pettersson**, S. Pendergraph, S. Utsel, A. Marais, E. Gustafsson, L. Wagberg

10:30 COLL **484.** Chiral recognition and selection during the self-assembly process of protein-mimic macroanions: The effect of long-range electrostatic interactions. **P. Yin**, T. Liu

10:50 COLL **485.** Synergetic DNA delivery with pyridinium amphiphiles with different packing parameters – toward composite DNA delivery systems. **M.A. Ilies**, A. Kizewski

11:10 COLL **486.** Distinct Adsorption Configurations and Self-assembly characteristics of elongated proteins on chemically uniform and alternating surfaces. **S. Song**, J. Hahm

Section E

Marriott City Center Denver

Colorado G

Basic Research in Colloids, Surfactants & Nanomaterials

Basic Research on Surfaces and Interfaces

Cosponsored by PRES

R. Nagarajan, *Organizer, Presiding*

8:30 COLL **487.** Superhydrophobicity and oleophobicity via increased modified surface topography. **K.T. Flynn**, M.D. Tustison, C. Zhou, K. Jiao

8:50 COLL **488.** Reconfigurable anisotropic coatings via magnetic field-directed assembly and translocation of locking magnetic chains. **A. Tokarev**, Y. Gu, A. Zakharchenko, O. Trotsenko, I.A. Luzinov, K. Kornev, S. Minko

9:10 COLL **489.** Assembly of surface-anchored metal-organic frameworks: Controlling deposition conditions to tune film morphology. M.L. Ohnsorg, B. Bowser, L. Gentry, **M.E. Anderson**

9:30 COLL **490.** Estimating sorption kinetics from the transient shape of a pendant drop. **A.R. White**, T. Ward

9:50 COLL **491.** Probing the effect of the HC–FC dipole on the properties of thin films formed from hydrocarbon-terminated perfluorinated alkanethiols. **O. Zenasni**, M.D. Marquez, T. Lee

10:10 COLL **492.** Synthesis and characterization of partially fluorinated self-assembled monolayers having an inverted surface dipole. **M.D. Marquez**, O. Zenasni, T. Lee

‡ *Cooperative Cosponsorship*

10:30 COLL **493.** Analysis of interactions at fluid-solid interface: Exploring the complete slip boundary condition. **S.L. Nania**, S.K. Shaw

10:50 COLL **494.** Multilayered metallic nanostructures with an embedded internal standard as surface enhanced Raman substrates. **E.R. Butcher**, D.D. Evanoff

11:10 COLL **495.** X-ray photoelectron spectroscopy at the liquid-nanoparticle interface: Opportunities for colloidal science. **M.A. Brown**

11:30 COLL **496.** Interfacial liquids, Most soft surfactants probed by AFM. **H. Onishi**

11:50 COLL **497.** Selenium: The better anchor group for self-assembled monolayers (SAMs) on gold? **A. Terfort**, M. Zharnikov, P. Cyganik

12:10 COLL **498.** Withdrawn.

Section F

Marriott City Center Denver
Colorado H

Basic Research in Colloids, Surfactants & Nanomaterials

Basic Research on Colloids

Cosponsored by PRES

R. Nagarajan, *Organizer, Presiding*

8:30 COLL **499.** Dynamic adhesion forces between microparticles and substrates in water. **Q. Xu**, Z. Xia, M. Li, L. Zhang, J. Niu

8:50 COLL **500.** Formation of luminescent inorganic precipitation tubes. P.J. Fryfogle, E.J. Nelson, **J.J. Pagano**

9:10 COLL **501.** Incorporation of nanoparticles into tunable, highly-ordered, porous silica films. **Y. Vasquez**, M. Kolle, L.A. Mishchenko, B.D. Hatton, J. Aizenberg

9:30 COLL **502.** Ionic and molecular modifiers of calcium oxalate crystallization: Tailoring interfacial interactions. **B.G. Alamani**, J. Chung, J.D. Rimer

9:50 COLL **503.** Colloidal particle dispersions for the synthesis of full color electrophoretic inks. **K. Belsey**, C. Topping, L. Farrand, S.J. Holder

10:10 COLL **504.** Selecting the swimming mechanisms of colloidal particles: Bubble propulsion vs. self-diffusiophoresis. **S. Wang**, N. Wu

10:30 COLL **505.** Characterization and dispersion behavior of quaternary ammonium encapsulated polyoxometalates in polyurethane. **J. Lundin**, S.L. Giles, P. Fulmer, R.F. Cozzens, J.H. Wynne

10:50 COLL **506.** Janus particles for probing and manipulating immune functions. **Y. Yu**, Y. Gao, L. Sanchez, Y. Jia

11:10 COLL **507.** Intra-phase mixing in binary drops translating through corrugated microchannels. **T. Ward**

11:30 COLL **508.** Molecular dynamics simulations of colloidal nanoparticles solvation. **S. Sen**, P. Kral

11:50 COLL **509.** Theoretical description of architectures of nanoparticles. **N. Almora Barrios**, N. Lopez

THURSDAY AFTERNOON

Section A

Marriott City Center Denver
Colorado A

Natural Resource Capture, Storage & Energy Conversion

Biofuels, Fuel Cells, Membranes, Electrolytes, & Batteries (BFCMEB)

J. Liu, *Organizer*
S. Bashir, *Organizer, Presiding*
X. Wang, *Presiding*

2:00 COLL **510.** Understanding abiotic:biotic interface: Molecular-level insights into the behavior of enzymes covalently immobilized on surfaces. T. Ogorzalek, Y. Liu, S. Wei, C.L. Brooks, Z. Chen, **N. Marsh**

2:30 COLL **511.** Direct synthesis of single layer layered double hydroxide nanosheets. **J. Yu**, B.R. Martin, J.E. Sims, L. Sun

2:55 COLL **512.** Silyl electrolytes for lithium-ion battery applications. **L.J. Lyons**

3:20 COLL **513.** Withdrawn.

3:45 COLL **514.** Creation of natural dye sensitized solar cell by using nanostructured titanium oxide. **J. Uddin**, S.S. Jenny, A. Ahmed, S. Yadav, M. Jiru

4:10 COLL **515.** Amphiphilic functionalization of cathode catalyst to advance electrochemical reactivity of fuel cells. **D. Gaona**, S. Bashir, J.L. Liu

Section B

Marriott City Center Denver
Colorado I/J

Interfacial Biomolecular Recognition

Cosponsored by BIOL‡

Financially supported by Avanti Polar Lipids, Inc.

J. Ross, *Organizer*
B. E. Bowler, M. Kastantin, *Organizers, Presiding*

2:00 COLL **516.** Aiding developments of single-molecule force spectroscopy for biosensing via molecular simulation. **Z.E. Hughes**, K.L. Drew, T. Walsh

2:25 COLL **517.** Use of surface-specific spectroscopy techniques to unravel molecular recognition in biosensing. **O.N. Oliveira**

2:50 COLL **518.** New roles for antifreeze proteins in recognizing non-ice surfaces. **X. Wen**

3:15 Intermission.

3:30 COLL **519.** Studying receptor-mediated liposome fusion kinetics at aqueous/liquid crystal interfaces. **K. Macri**, P. Noonan, D.K. Schwartz

3:55 COLL **520.** Effect of nanoparticle surface chemistry and salt concentration on binding to RNA and DNA. **J.A. Nash**, A. Singh, N.K. Li, Y.G. Yingling

4:20 COLL **521.** Ultrasound biosensing techniques based on biomolecule-induced aggregation of nanodroplets. **R. Chattaraj**, P. Mohan, J.D. Besmer, C.M. Livingston, A.P. Goodwin

4:45 COLL **522.** Impedimetric biosensors for detecting VEGF based on PEDOT carboxylic acid/PEDOT copolymer. **M. Kim**, R. Iezzi, D.C. Martin

Section C

Marriott City Center Denver
Colorado C/D

Basic Research in Colloids, Surfactants & Nanomaterials

Carbon and Organic Materials

Cosponsored by PRES

R. Nagarajan, *Organizer, Presiding*

2:00 COLL **310.** Artificial light harvesting system composed of organic dyes and clay minerals. **S. Takagi**, Y. Ishida, T. Shimada

2:20 COLL **523.** SiC porous materials derived from apple for high-performance electromagnetic interference shielding. **Z. Wang**, C. Liu, Y. Xu

2:40 COLL **524.** Modeling fullerene aggregation in electrolyte solutions: A combined deterministic-stochastic framework. S. Mortuza, **S. Banerjee**

3:00 COLL **525.** Synthesis of carbon-based nanoscale composite particles for imaging applications. **M.J. Meziani**, **M.A. Mottaleb**, B. Yoo, Y. Sun

3:20 COLL **526.** Label-free two photon imaging of live cells using graphene dots. **P.C. Ray**

3:40 COLL **527.** Developing carbenes as surface modifiers. **M. Macleod**, J.A. Johnson

4:00 COLL **528.** Carbon dots preparation and effect on protein fibrillation. **S. Li**, R.M. Leblanc

4:20 COLL **529.** Conductance and rectification through asymmetric biphenyl molecule systems. **J.E. Meany**, S.A. Woski

4:40 COLL **530.** Electron transfer and molecular binding to nanostructured carbon for supercapacitor materials. D. Banks, J. Mitchell, I. Shcherbakov, **J.C. Poler**

Section D

Marriott City Center Denver
Denver III

Basic Research in Colloids, Surfactants & Nanomaterials

Functionalized Nanoparticles

Cosponsored by PRES

R. Nagarajan, *Organizer, Presiding*

2:00 COLL **531.** Withdrawn.

2:20 COLL **532.** Withdrawn.

2:40 COLL **533.** Phase transport of citrate stabilized gold nanoparticles using nonspecifically adsorbed polymers. **L.B. Thompson**, A.M. Alkilany, A. Caravana

3:00 COLL **534.** Highly efficient poly-lysine functionalization of gold surfaces by dual click reactions utilizing dithiol adsorbates. **A. Shakiba**, A.C. Jamison, T. Lee

3:20 COLL **535.** Toward understanding electronic and optical properties of colloidal germanium nanocrystals as a function of size and surface ligand. **A.L. Holmes**, J. Hütges, A. Reckmann, E. Muthuswamy, K. Meerholz, S. Kauzlarich

3:40 COLL **536.** Withdrawn.

4:00 COLL **537.** Orthogonal functionalization of patchy particles. **X. Zheng**, Y. Wang, Y. Wang, D. Pine, M. Weck

4:20 COLL **538.** Strong hydrophobizer: Laterally chemisorbed low-molecular-weight polydimethylsiloxane. **T. Lee**, S. Chae

4:40 COLL **539.** Elucidating structure/property relationships of peptide-decorated Au nanoparticles using advanced molecular simulations. **Z.E. Hughes**, T. Walsh

Section E

Marriott City Center Denver
Colorado G

Basic Research in Colloids, Surfactants & Nanomaterials

Semiconductor Materials

Cosponsored by PRES

R. Nagarajan, *Organizer, Presiding*

2:00 COLL **540.** Optical signatures of crystal phase in semiconductor nanocrystals. **S. Lim**, A. Schleife, A. Smith

2:20 COLL **541.** Shape controlled narrow-gap tin chalocogenide nanostructures. **S. Guo**

2:40 COLL **542.** Colloidal synthesis and photocatalytic properties of orthorhombic $AgGaS_2$ nanocrystals. **C. Fan**, M. Regulacio, M. Han, A. Xu

3:00 COLL **543.** Careful control of confinement potential and interfacial lattice strain in colloidal quantum dots to improve radiative recombination and fluorescence blinking. **C.D. Heyes**

3:20 COLL **544.** Size characterization and alternative synthesis of monolayer-protected quantum dots. A.E. Conner, L.R. Tinoco, W.L. Wright, S.C. Francone, E.V. Aguilar, F.E. Acosta, **D.T. Miles**

3:40 COLL **545.** Excited state dynamics in doped quantum dots. **C. Tuinenga**, P.V. Kamat

4:00 COLL **546.** Withdrawn.

4:20 COLL **547.** Characterization of the transformation of collodial CdSe quantum dots into ferroelectric particles. **T. Wrenn**, J. McBride, J. Mares

4:40 COLL **548.** Formation of 1D-nanostructures using surface-directed vapor-liquid-solid growth process. **B. Nikoobakht**, A. Herzing

Section F

Marriott City Center Denver
Colorado H

Basic Research in Colloids, Surfactants & Nanomaterials

Colloidal Assembly and Gels

Cosponsored by PRES

R. Nagarajan, *Organizer, Presiding*

2:00 COLL **549.** Electric field-directed nanowire assembly. **S.J. Boehm**, L. Lin, C.D. Keating, T.S. Mayer

2:20 COLL **550.** Designing a super-assembly using mixed biological and synthetic nanostructures. **J. Reyes**, R. Balaraman, N.D. Becerra-Mora, J.B. Fiske, P. Kohli

2:40 COLL **551.** Bifurcation in the equilibrium height of colloidal particles near an electrode in oscillatory electric fields. **T. Woehl**, B. Chen, K. Heatley, N. Talken, C. Dutcher, S. Bukosky, W. Ristenpart

3:00 COLL **552.** Self-assembly of colloidal nanoparticles into chiral ribbons and hollow capsules. **P. Kral**

3:20 COLL **553.** Self-assembly of nanometer scaled macroions in dilute solution. **J. Zhou**, T. Liu

3:40 COLL **554.** Direct nanoscale visualization of the kinetics of colloidal gold nanoparticle chain assembly. **T. Woeh**l, T. Prozorov

4:00 COLL **555.** Withdrawn.

4:20 COLL **556.** Magnetoactive hydrogels for dynamic modulation of pro-angiogenic signaling from mesenchymal stem cells. **K.A. Kilian**, A. Abdeen

4:40 COLL **557.** Monodisperse polymeric ionic liquid microgels by post modifications and their versatile biomedical applications. **N. Sahiner**, A.O. Yasar, S. Yildiz, S. Demirci, **N. Aktas**

5:00 COLL **558.** Supercooled water in nanoconfinement: Molecular simulation study of single-molecule and collective dynamics. N.J. Kuon, **A.A. Milischuk**, B.M. Ladanyi

5:20 COLL **559.** Ionic liquids and water: the surprising connection. **M.A. Gebbie**, H.A. Dobbs, M. Valtiner, J.N. Israelachvili

COMP

Division of Computers in Chemistry

E. Esposito and S. Wildman, *Program Chairs*

BUSINESS MEETINGS:
Business Meeting, 3:00 PM: Sat

SUNDAY MORNING

Section B

Colorado Convention Center
Mile High Ballroom 1E

Computational Design, Discovery and Optimization of Organic Semiconductor Materials

Cosponsored by PHYS

M. Halls, *Organizer*
G. B. Fitzgerald, *Organizer, Presiding*

8:30 COMP **1.** Using Gaussian to aid in π-conjugated semiconducting polymer design for organic photovoltaics. **C.K. Luscombe**

9:00 COMP **2.** Computational description of donor-acceptor pi-conjugated materials for organic photovoltaics applications. **J.E. Bredas**

9:30 Intermission.

9:45 COMP **3.** High-throughput computational design of semiconducting polymers: Predictions and rational guidance from DFT calculations. **B.M. Wong**

10:15 COMP **4.** Application of density functional theory in the design of organic molecules for intramolecular singlet fission. Q. Wu, **E. Busby**, J. Xia, J. Low, R. Song, J.R. Miller, X. Zhu, L.M. Campos, M. Sfeir

10:45 COMP **5.** Atomistic simulations of donor-acceptor polymer morphologies for high-efficiency organic photovoltaic. **T.W. Kemper**, R.E. Larsen, D.C. Olson

Section C

Colorado Convention Center

Mile High Ballroom 1F

Electronic Structure Methods for Highly Polarizable Systems

Dynamics

Cosponsored by PHYS

D. Lambrecht, J. Parkhill, *Organizers, Presiding*

8:30 COMP **6.** Nonadiabatic molecular dynamics of singlet fission and charge separation. **O.V. Prezhdo**

9:00 COMP **7.** First principles ultrafast charge transfer dynamics in solution: A time-domain TDDFT approach coupled with dielectric relaxation. **F. Ding**, D. Lingerfelt, B. Mennucci, X. Li

9:30 COMP **8.** Modeling inter-domain electron tunneling in copper monooxygenases. **A. Migliore**, D.N. Beratan

10:00 Intermission.

10:15 COMP **9.** Time-dependent two-component electronic structure methods for modeling spin dynamics. **X. Li**, F. Ding, J. Goings

10:45 COMP **10.** Pseudopotential approach to electronic structure of anionic species on metallic surfaces. **A.F. Izmaylov**

Section D

Colorado Convention Center

Mile High Ballroom 4E

Drug Discovery

Structural Informatics & Target Based: Structure-Based

Cosponsored by MEDI

Y. Tseng, S. A. Wildman, *Organizers, Presiding*

8:30 COMP **11.** Structural informatics modeling of Daclatasvir and analogs reveals asymmetric binding to HCV-NS5A: Dual mechanisms responsible for picomolar activity and acquired resistance. **J.H. Nettles**, R. Stanton, J. Broyde, F. Amblard, H. Zhang, L. Zhou, J. Shi, T. McBrayer, T. Whitaker, S.J. Coats, J.J. Kohler, R.F. Schinazi

9:00 COMP **12.** Structure-based discovery and de novo design of HIV fusion inhibitors. **W.J. Allen**, R.C. Rizzo

9:30 COMP **13.** Dual layer QM/MM binding study of antimicrobial oligomer-viral capsid complexes. **T. Martin**, E.H. Hill, D.G. Whitten, E.Y. Chi, D.G. Evans

10:00 Intermission.

10:00 COMP **14.** Fungicides and exploration of chemical spaces: Homology modeling of lanosterol 14-alpha-demethylase. **L. Nitsch** Velasquez

10:30 COMP **15.** Identification and characterization of allosteric site(s) for dihydrogambogic acid (DHGA) and trans-β-caryophyllene (TBC) as cannabinoid CB_2 allosteric modulators. **P. Pandey**, K.K. Roy, R.J. Doerksen

Technical program information known at press time.
The official technical program for the 249th ACS National Meeting is available at:
www.acs.org/denver2015

11:00 COMP **16.** Molecular docking screens for the discovery of novel A_2A adenosine receptor agonists: Are there any in chemical libraries? **D. Rodriguez**, Z. Gao, S.M. Moss, K.A. Jacobson, J. Carlsson

Section E

Colorado Convention Center

Mile High Ballroom 4F

Molecular Mechanics

Proteins

E. X. Esposito, S. A. Wildman, *Organizers, Presiding*

8:30 COMP **17.** Computational approach to enzyme design. S. Sirin, **W. Sherman**

9:00 COMP **18.** Molecular dynamics simulations on the periplasmic-open state lactose permease. **X. Zhuang**, J.B. Klauda

9:30 COMP **19.** Investigating the structure and dynamics of the PIK3CA wild-type and H1047R oncogenic mutant for potential allosteric modulation. P. Gkeka, A. Papafotika, S. Christoforidis, **Z. Cournia**

10:00 Intermission.

10:15 COMP **20.** Structural insight into ROS1/ALK kinase conformational dynamics. **N.A. Vellore**, J. Wagner, C.A. Edie, M.W. Deininger, B.J. Druker, T. O'Hare, M.A. Davare

10:45 COMP **21.** Computational study of pH-dependent conformational changes in proteins. **N. Di Russo**, A.E. Roitberg

11:15 COMP **22.** cAMP modulation of the hyperpolarization-activated cyclic nucleotide-gated 2 ion channels. **F. Tofoleanu**, B. Brooks

Computational Chemical Dynamics: Advancing our Understanding of Chemical Processes in Gas-Phase, Biomolecular & Condensed-Phase Systems: A Symposium in Honor of Donald Truhlar

Accurate Energies for Dynamics

Sponsored by PHYS, Cosponsored by COMP

Role of Membrane in Amyloid-Formation & the Pathogenicity of Amyloid Disease

Amyloid β: Structures and Molecular Interactions

Sponsored by PHYS, Cosponsored by COLL and COMP

Modeling Complex Biomolecules: From Structure to Dynamics & Function

Advances in Simulation Methodology

Sponsored by PHYS, Cosponsored by COMP

Modeling Excited States of Complex Systems

Complex Materials and Molecules

Sponsored by PHYS, Cosponsored by COMP

SUNDAY AFTERNOON

Section A

Colorado Convention Center

Mile High Ballroom 1D

Molecular Mechanics

Methodology

E. X. Esposito, S. A. Wildman, *Organizers, Presiding*

1:30 COMP **23.** Correcting for the free energy costs of bond or angle constraints in molecular dynamics simulations. **G. Koenig**, B. Brooks

2:00 COMP **24.** Importance of sugar pucker correction to QM/MM simulation of RNA systems. **M. Huang**, D.M. York

2:30 COMP **25.** Improving efficiency in SMD simulations through a hybrid differential relaxation algorithm. **C.L. Ramirez**, A. Zeida, G.E. Jara, A.E. Roitberg, M.A. Marti

3:00 Intermission.

3:15 COMP **26.** Enhancing constant-pH simulation in explicit solvent with a two-dimensional replica exchange method. **J. Lee**, B. Miller, A. Damjanovic, B. Brooks

3:45 COMP **27.** Toward a virtual chemist: Application to asymmetric catalyst discovery. **J. Pottel**, M. Bezanson, N. Moitessier

4:15 COMP **28.** Computer-aided molecular design of neutral lanthanide extractants. **B.W. McCann**

Section B

Colorado Convention Center

Mile High Ballroom 1E

Computational Design, Discovery and Optimization of Organic Semiconductor Materials

Cosponsored by PHYS

G. B. Fitzgerald, *Organizer*

M. Halls, *Organizer, Presiding*

1:30 COMP **29.** Finding polymorphs of organic semiconductors. **P. Clancy**, K.M. Lenn, P. Frazier

2:00 COMP **30.** Coarse-grained simulations of benzodithiophene-thienopyrrolodione copolymer film structure for organic photovoltaics. **E. Jankowski**, D.C. Olson

2:30 COMP **31.** Molecular dynamics of prototypical organic photovoltaic materials. S. Yerusu, **V.K. Kuppa**

3:00 Intermission.

3:15 COMP **32.** High throughput computational approaches to materials discovery and development for organic electronics. **M.E. Thompson**, P. Saris, P.I. Djurovich, L. Martin

3:45 COMP **33.** Efficient knowledge discovery of optoelectronic materials using evolutionary strategies. **T.F. Hughes**, Y. Cao, J. Gavartin, D.J. Giesen, A. Goldberg, M.D. Halls, S. Kwak

4:15 COMP **34.** Charge percolation in non-crystalline molecular materials. **N. Jackson**, L.X. Chen, M.A. Ratner

Section C

Colorado Convention Center

Mile High Ballroom 1F

Electronic Structure Methods for Highly Polarizable Systems

Embedding: QM/QM and QM/MM

Cosponsored by PHYS

D. Lambrecht, J. Parkhill, *Organizers, Presiding*

1:30 COMP **36.** Embedded descriptions of condensed phases. **G.K. Chan**

2:00 COMP **35.** Embedding from multiscale chemical problems to crystal energetics. **F.R. Manby**

2:30 COMP **37.** Embedded correlated wavefunction theory: Advances and applications. **E.A. Carter**

3:00 Intermission.

3:15 COMP **38.** Molecular fragments as a tool for electronic structure. **T.A. Van Voorhis**

3:45 COMP **39.** High-level QM/MM free energy simulations at affordable computational costs. P.S. Hudson, G. Koenig, F.L. Kearns, S. Boresch, **H.L. Woodcock**

4:15 COMP **40.** MoD-QM/MM structural refinement method: Characterization of hydrogen bonding in the Oxytricha nova G-quadruplex. J. Ho, C.M. Ragain, J. Gascon, E.R. Batista, J. Loria, **V.S. Batista**

Section D

Colorado Convention Center

Mile High Ballroom 4E

Drug Discovery

Structural Informatics & Target Based: Structure-Based

Cosponsored by MEDI

Y. Tseng, S. A. Wildman, *Organizers, Presiding*

1:30 COMP **41.** Structure-focused modeling approach to identify family-specific kinase inhibitors. S. Ravichandran, B.T. Luke, J.R. Collins

2:00 COMP **42.** Computational analysis of the binding specificity of DMH1 to Alk2, Alk5, and VEGFR2 kinases. A. Alsamarah, J. Hao, Y.L. Luo

2:30 COMP **43.** Chemical fragments positively interact with protein side chains: An analysis of PDB and CSDB database. **M. Tu**

3:00 Intermission.

3:15 COMP **44.** Knowledge based conformation sampling algorithms and its application in Foldit drug design game. S.K. Kothiwale, J. Mendenhall, S. Combs, J. Meiler

3:45 COMP **45.** X-ray fragment screening for allosteric sites. M. Verdonk

4:15 COMP **46.** Withdrawn.

Section E

Colorado Convention Center

Mile High Ballroom 4F

Quantum Chemistry

Methodology

Cosponsored by PHYS

E. V. Patterson, *Organizer, Presiding*

1:30 COMP **47.** Fast calculation of two-electron integrals. A numerical approach. **P.E. Lopes**

2:00 COMP **48.** Advances in local RI methods for SCF calculations. S. Manzer, E. Epifanovsky, M.P. Head-Gordon

2:30 COMP **49.** Exploiting sparsity to enable petascale applications in material science and quantum chemistry. **M. Keceli**, H. Zhang, P. Zapol, D.A. Dixon, A.F. Wagner

3:00 Intermission.

3:15 COMP **50.** Accurate and efficient propagator methods for calculating electron binding energies of large molecules: Applications to fullerenes and other large acceptors. **J.V. Ortiz**

3:45 COMP **51.** Learning non-local kinetic energy functionals for hydrocarbons with computers. **J. Parkhill**, K. Yao

4:15 COMP **52.** Simulating plasmon-molecule interactions in the time domain. **A.E. DePrince**

Computational Chemical Dynamics: Advancing our Understanding of Chemical Processes in Gas-Phase, Biomolecular & Condensed-Phase Systems: A Symposium in Honor of Donald Truhlar

Gas-phase Kinetics and Dynamics

Sponsored by PHYS, Cosponsored by COMP

Role of Membrane in Amyloid-Formation & the Pathogenicity of Amyloid Disease

Amyloid Precursor Protein, Origin of Amyloid β

Sponsored by PHYS, Cosponsored by COLL and COMP

Modeling Complex Biomolecules: From Structure to Dynamics & Function

Classical and Quantum Descriptions of Protein Function

Sponsored by PHYS, Cosponsored by COMP

Modeling Excited States of Complex Systems

Complex Materials and Molecules

Sponsored by PHYS, Cosponsored by COMP

MONDAY MORNING

Section A

Colorado Convention Center

Mile High Ballroom 1D

Molecular Mechanics

Force Field Development

Cosponsored by PHYS

E. X. Esposito, S. A. Wildman, *Organizers, Presiding*

8:30 COMP **53.** Multistate reweighting as an effective tool for force field parameterization. **M.R. Shirts**, L. Naden, B. Zimmerman, H. Paliwal

9:00 COMP **54.** Wolf$_2$Pack: A scientific workflow and molecular database for force-field optimization. **K.N. Kirschner**, O. Krämer-Fuhrmann, M. Hülsmann, D. Reith

9:30 COMP **55.** Residue-specific force fields based on protein coil library and their applications. **F. Jiang**, C. Zhou, S. Xun, Y. Wu

‡ *Cooperative Cosponsorship*

10:00 COMP **56.** Development of a tuned interfacial force field for the simulation of protein adsorption to poly(methyl methacrylate). **J.A. Yancey**, T.M. Abramyan, J.A. Snyder, S.J. Stuart, R.A. Latour

10:30 Intermission.

10:45 COMP **57.** Accurate parameterization of ionic surfactants at high concentration. **G.B. Goh**, D.M. Eike, B.P. Murch, C.L. Brooks III

11:15 COMP **58.** Development of an accurate multipolar-polarizable force field for ionic liquids. **H. Torabifard**, G.A. Cisneros

11:45 COMP **59.** Concentration effect on the hydrogen-bond strength between small molecules at the oil/water interface. **V.K. Yadav**

Section B

Colorado Convention Center
Mile High Ballroom 1E

Computational Design, Discovery and Optimization of Organic Semiconductor Materials

Cosponsored by PHYS

G. B. Fitzgerald, M. Halls, *Organizers*
M. Thompson, *Presiding*

8:30 COMP **60.** Modeling of organic light emitting diodes: From molecular to device properties. P. Kordt, J. van der Holst, M. Al Helwi, W. Kowalsky, F. May, A.B. Badinksi, C. Lennartz, **D. Andrienko**

9:00 COMP **61.** Theoretical investigation of organic light-emitting diode materials. **O. Kwon**

9:30 COMP **62.** Molecular design for high efficiency thermally activated delayed fluorescence aimed for OLED application. K. Shizu, **Q. Zhang**, S. Huang, H. Kaji, **C. Adachi**

10:00 Intermission.

10:15 COMP **63.** Computational screening of organic light-emitting diodes. **A. Aspuru-Guzik**

10:45 COMP **64.** Quantum chemical view on OLEDs: designing charge transport materials and phosphorescent emitters. **C. Lennartz**, F. May, D. Andrienko

11:15 COMP **65.** Tunable charge transport in donor-acceptor charge transfer complexes. K.P. Goetz, **O.D. Jurchescu**

Section C

Colorado Convention Center
Mile High Ballroom 1F

Electronic Structure Methods for Highly Polarizable Systems

Correlation Methods & DFT

Cosponsored by PHYS

D. Lambrecht, J. Parkhill, *Organizers, Presiding*

8:30 COMP **67.** Many-body dispersion interactions in molecular crystals. **N. Marom**

9:00 COMP **68.** Electronic structure of pi-conjugated materials for organic electronics applications. **J.E. Bredas**

9:30 COMP **69.** Systematically Improvable multi-scale methods for correlated electron systems. **D. Zgid**

10:00 Intermission.

10:15 COMP **66.** Scaling coupled-cluster theory to nanoclusters using molecular cluster perturbation theory. **J.N. Byrd**, N. Jindal, B. Sanders, R.J. Bartlett

10:45 COMP **70.** Improving electronic excitation energies and couplings. **J.E. Subotnik**, E.C. Alguire, X. Liu, Q. Ou

11:15 COMP **71.** Ab initio characterization of the electrochemical stability and solvation properties of condensed-phase ethylene carbonate and dimethyl carbonate mixtures. T. Barnes, J. Kaminski, O. Borodin, **T.F. Miller**

Section D

Colorado Convention Center
Mile High Ballroom 4E

Drug Discovery

Structural Informatics & Target Based: Structure-Based

Cosponsored by MEDI

Y. Tseng, S. A. Wildman, *Organizers, Presiding*

8:30 COMP **72.** Fragment-based free energy perturbation. T. Steinbrecher, **W. Sherman**

9:00 COMP **73.** Binding specificity of bone morphogenetic protein (BMP) receptors: Insight from free energy simulations. **Y.L. Luo**, A. Alsamarah, W. Jiang, J. Hao

9:30 COMP **74.** Quantifying key determinants of molecular recognition: Significance of pi interactions and charged hydrogen bonds in protein-ligand binding. **B.K. Rai**, G.A. Bakken

10:00 Intermission.

10:15 COMP **75.** Design of peptides for improved binding to radiation-inducible targets in cancer therapy. **S.A. Wildman**

10:45 COMP **76.** Toward structure prediction of cyclic peptides. H. Yu, **Y. Lin**

11:15 COMP **77.** Benchmark of ensemble docking against crystal docking for use in kinases drug discovery projects. **T.L. Claiborne**, R.V. Swift, R.E. Amaro

Section E

Colorado Convention Center
Mile High Ballroom 4F

Molecular Mechanics

Proteins

E. X. Esposito, S. A. Wildman, *Organizers, Presiding*

8:30 COMP **78.** Structural and energetic insight into the cross-seeding amyloid assemblies of human IAPP and rat IAPP. **M. Zhang**, R. Hu, H. Chen, Q. Wang, C. Zhao, J. Zheng

9:00 COMP **79.** NS3 helicase translocation along ssRNA. **A. Perez-Villa**, M. Darvas, G. Bussi

9:30 COMP **80.** Binding studies of a *Saccharomyces cerevisiae* peripheral protein Osh4. **V. Monje-Galvan**, J.B. Klauda

10:00 Intermission.

10:15 COMP **81.** Stabilization effects of disulfide bonds and dimerization on CXCL7. **C. Singer**, C. Herring, E. Ermakova, D.J. Jacobs, I. Nesmelova

10:45 COMP **82.** All-atom simulation of the folding and binding of an intrinsically disordered protein. **R.E. Ithuralde**, A.E. Roitberg, A.G. Turjanski

11:15 COMP **83.** Possible mechanism for redox control of human neuroglobin activity revealed by crystallography and simulation. **D.C. Chatfield**, O. Morozov, J.P. Roach

Computational Chemical Dynamics: Advancing our Understanding of Chemical Processes in Gas-Phase, Biomolecular & Condensed-Phase Systems: A Symposium in Honor of Donald Truhlar

Enzyme Kinetics and Dynamics

Sponsored by PHYS, Cosponsored by COMP

Role of Membrane in Amyloid-Formation & the Pathogenicity of Amyloid Disease

α-Synuclein, the Parkinson's Protein

Sponsored by PHYS, Cosponsored by COLL and COMP

Modeling Complex Biomolecules: From Structure to Dynamics & Function

Membrane Proteins

Sponsored by PHYS, Cosponsored by COMP

Modeling Excited States of Complex Systems

Excited States in Biology

Sponsored by PHYS, Cosponsored by COMP

MONDAY AFTERNOON

Section A

Colorado Convention Center
Mile High Ballroom 1D

ACS Award for Computers in Chemical and Pharmaceutical Research: Symposium in Honor of David A. Case

Cosponsored by PHYS

K. Merz, A. E. Roitberg, *Organizers*
D. M. York, *Organizer, Presiding*

1:30 COMP **84.** Proteins are the easy part: Chemical diversity in the PDB archive. **H.M. Berman**

2:00 COMP **85.** Origins of Species: The evolutionary biology of computer agents. **I. Kuntz**

2:30 COMP **86.** How well can a force field match the Born-Oppenheimer surface? The water dimer as an example. **T. Darden**

3:00 Intermission.

3:15 COMP **87.** Collagen triple helix interactions with the integrin receptor: Highlighting the role of conformational fluctuations. **J. Baum**

3:45 COMP **88.** Structure of disorder. **J. Holton**, P. Janowski, D.A. Case, D.S. Cerutti

4:15 COMP **89.** Simulation of pH-dependent unfolding and target-inhibitor interactions. **D. Bashford**

Section B

Colorado Convention Center
Mile High Ballroom 1E

ACS Award for Research at an Undergraduate Institution: Symposium in Honor of George C. Shields

G. C. Shields, *Organizer*
E. C. Sherer, *Organizer, Presiding*

1:30 Introductory Remarks.

1:40 COMP **90.** Concertedness and synchronicity—from arynes to electrochemistry. **C.J. Cramer**

2:10 COMP **91.** Molecular simulations in conjunction with experimental studies illustrate internal protein logic controlled by conformation and dynamic structural change. **T.E. Morrell**, I.U. Rafalska-Metcalf, J. Chu, H. Yang

2:30 COMP **92.** Predicting permeability and target binding of complex macrocycles. **K.W. Lexa**, M.P. Jacobson

3:00 Intermission.

3:20 COMP **93.** Molecular studies of halogen bonding, protein folding and combustion. **C.A. Parish**

3:50 COMP **94.** Anharmonic effects in vibrational spectra of protonated water clusters. **K.A. Archer**, T. Odbadrakh, J.A. Fournier, M.A. Johnson, K.D. Jordan

4:10 COMP **95.** Insight Into hydrazone-based dye fluorescence from density functional theory. **M.D. Liptak**, E.H. Horak

4:40 COMP **96.** Recent developments in high accuracy nonbonded interactions in the CHARMM simulation package. **F.C. Pickard**, A.C. Simmonett, B. Brooks

5:10 COMP **97.** Examining the interface: Simulations exploring the effect of solid substrates on thin liquid films. **K.E. Anderson**, S. Wenzel, H.M. Nemec, J. Lee, S. Watkins, T. Stoneham, J.I. Siepmann

Section C

Colorado Convention Center
Mile High Ballroom 1F

Electronic Structure Methods for Highly Polarizable Systems

Excitons

Cosponsored by PHYS

D. Lambrecht, J. Parkhill, *Organizers, Presiding*

1:30 COMP **98.** Toward new materials for singlet fission. J. Wen, M. Jovanovic, Z. Havlas, **J. Michl**

2:00 COMP **99.** Exciton delocalization in disordered conjugated polymer films. **A. Willard**

2:30 COMP **100.** Numerical simulations of the optical response and energy transfer coupled exciton-plasmon systems. M. Sukharev, **A. Nitzan**

3:00 Intermission.

3:15 COMP **101.** Understanding the coupling between molecular excited states and plasmons. **L. Jensen**

3:45 COMP **373.** Ab initio implementation of the Frenkel-Davydov exciton model. **J. Herbert**, A. Morrison

4:15 COMP **102.** Effect of shape, size, and heterojunction on excitonic interactions in semiconductor nanoparticles. J. Scher, **A. Chakraborty**

4:45 COMP **103.** Chiroptical properties and excitation data with local coupled cluster methods. **H. McAlexander**, T. Crawford

Section D

Colorado Convention Center
Mile High Ballroom 4E

Drug Discovery

ADME & Informatics

Cosponsored by CINF and MEDI

Y. Tseng, S. A. Wildman, *Organizers, Presiding*

1:30 COMP **104.** Methodology for machine learning in chemical design. **S. Chonde**, J. Storer, K.T. Mueller, S. Kumara

2:00 COMP **105.** PubChem and big data. **S. Kim**, G. Fu, L. Han, B. Yu, L. Geer, A. Gindulyte, S. He, P. Thiessen, E.E. Bolton, S.H. Bryant

2:30 COMP **106.** Toward the ubiquitous use of cheminformatics: From the development of reliability boosters for structure-based molecular docking to the analysis and modeling of hyperdimensional HTS data. **D. Fourches**

3:00 Intermission.

3:15 COMP **107.** Evaluating structural toxicity alerts with metabolism and reactivity models. **T. Hughes**, G.P. Miller, S. Swamidass

3:35 COMP **108.** Predicting regioselectivity and lability of cytochrome P450 metabolism using quantum mechanical simulations. M.D. Segall, **J. Tyzack**, P. Hunt

4:15 COMP **109.** In silico approaches to CYP P450 site-of-metabolism (SOM) and microsomal stability prediction. **J.H. Voigt**, U. Schmitz

Section E

Colorado Convention Center
Mile High Ballroom 4F

Quantum Chemistry

Methodology

Cosponsored by PHYS

E. V. Patterson, *Organizer, Presiding*

1:30 COMP **110.** Combining active-space coupled-cluster approaches with moment energy corrections via the CC(*P*;*Q*) methodology: Ground and excited states. **P. Piecuch**, J. Shen, N.P. Bauman

2:00 COMP **111.** Calculation of two-photon absorption cross-sections within EOM-EE-CCSD formalism: Theory and examples. **K. Nanda**, A. Krylov

2:30 COMP **112.** Systematic expansion of active spaces beyond the CASSCF limit: A GASSCF/SplitGAS benchmark study. **K.D. Vogiatzis**, G. Li Manni, S. Stoneburner, D. Ma, L. Gagliardi

3:00 Intermission.

3:15 COMP **113.** Time-dependent projected Hartree-Fock for degenerate excited states. **T. Tsuchimochi**, T.A. Van Voorhis

3:45 COMP **114.** Variational state specific solvent models for excited states from time dependent self-consistent field methods. **J. Bjorgaard**, K. Velizhanin, S. Tretiak

4:15 COMP **115.** Accurate ab initio potential energy curves and spectroscopic properties of C_2 singlet states. **J. Boschen**, D. Theis, K. Ruedenberg, T.L. Windus

Computational Chemical Dynamics: Advancing our Understanding of Chemical Processes in Gas-Phase, Biomolecular & Condensed-Phase Systems: A Symposium in Honor of Donald Truhlar

Catalysis

Sponsored by PHYS, Cosponsored by COMP

Role of Membrane in Amyloid-Formation & the Pathogenicity of Amyloid Disease

Islet Amyloid Polypeptide (IAPP) at the Water/Lipid Interface

Sponsored by PHYS, Cosponsored by COLL and COMP

Modeling Complex Biomolecules: From Structure to Dynamics & Function

Molecular Machines

Sponsored by PHYS, Cosponsored by COMP

Modeling Excited States of Complex Systems

Multiple Chromophores

Sponsored by PHYS, Cosponsored by COMP

MONDAY EVENING

Section A

Colorado Convention Center
Halls C/D

Sci-Mix

E. X. Esposito and S. A. Wildman, *Organizers*

8:00 - 10:00
180, 182-183, 222, 235, 259, 261-262, 264, 265, 275, 280, 291. See subsequent listings.

TUESDAY MORNING

Section A

Colorado Convention Center
Mile High Ballroom 1D

ACS Award for Computers in Chemical and Pharmaceutical Research: Symposium in Honor of David A. Case

Cosponsored by PHYS

A. E. Roitberg, D. M. York, *Organizers*
K. Merz, *Organizer, Presiding*

8:30 COMP **116.** Molecular understanding of hydrophobic association in ethanol-water mixtures. **T. Ichiye**

9:00 COMP **117.** Quantum mechanical force fields: A breakthrough in multiscale modeling tools. **D.M. York**

9:30 Intermission.

9:45 COMP **118.** Decoding the dynamics properties of protein loops by the combination of NMR and molecular dynamics simulations. Y. Gu, D. Li, **R. Bruschweiler**

10:15 COMP **119.** Reproducibilty and convergence in the assessment, validation and improvement of force fields for RNA. **T.E. Cheatham**

10:45 COMP **120.** Thermodynamic estimates from molecular dynamics. **C.B. Post**

Section B

Colorado Convention Center
Mile High Ballroom 1E

ACS Award for Research at an Undergraduate Institution: Symposium in Honor of George C. Shields

E. C. Sherer, G. C. Shields, *Organizers, Presiding*

8:30 COMP **121.** Thermodynamic quantities and structural information from a molecular printing press. **K.M. Merz**

9:00 COMP **122.** Addressing problems at the interface of chemistry and medicine: Computational and chemical biology approaches. **K. Alser**, G.C. Shields, D.G. McCafferty

9:20 COMP **123.** From the atmosphere to the interstellar medium: Long-range molecular interactions. **M.A. Allodi**, S. Ioppolo, B.A. McGuire, G.A. Blake

9:40 Intermission.

10:00 COMP **124.** Comparison of diffusion Monte Carlo and CCSD(T) methods on model systems. **K.D. Jordan**, M.J. Deible

10:30 COMP **125.** From the computational chemistry lab to treating cancer: Inspiration for drug development in our time. **K. Larkin**

10:50 COMP **126.** Evolution of methods for modeling hydrogen-bonded systems accurately and efficiently. **B. Temelso**, G.C. Shields

11:20 COMP **127.** Role of water in arginine-rich motif peptide-RNA recognition. L. Michael, B. Miller, S. Bernard, M. Hoffman, W. Hodges, Z. Fallon, **M.C. Nagan**

Section C

Colorado Convention Center
Mile High Ballroom 1F

Materials Science

Quantum Materials

E. X. Esposito, *Organizer, Presiding*

8:30 COMP **128.** Self-consistent projector constrained density functional theory in ONETEP. **G. Teobaldi**, D.D. O'Regan, N.D. Hine, A.A. Mostofi

9:00 COMP **129.** Stopping powers from time-dependent density functional theory. **R.J. Magyar**

9:30 COMP **130.** Hybrid functional study of stability and electronic structure of $Cu_2ZnSn(S,Se)_4$ polytypes. **J. Park**, I. Repins, S. Wei

10:00 Intermission.

10:15 COMP **131.** Enhanced oxygen vacancy formation in cation doped bulk Cr_2O_3. **M. Nolan**, M. Legesse, A. Van Veen

10:45 COMP **132.** CO_2 adsorption in M-IRMOF10 (M=Mg, Ca, Fe, Cu, Zn, Ge, Sr, Cd, Sn, Ba). **J.D. Borycz**, D. Tiana, E. Haldoupis, L. Gagliardi, J.I. Siepmann

11:15 COMP **133.** AIMing toward better prediction of corrosion inhibitor prediction. **R.L. Cook**

Section D

Colorado Convention Center
Mile High Ballroom 4E

Drug Discovery

Methodology

Cosponsored by CINF and MEDI

Y. Tseng, S. A. Wildman, *Organizers, Presiding*

8:30 COMP **134.** Flexible CDOCKER: Development and application of a docking method incorporating non-rigid receptors within CHARMM. **J. Gagnon**, S. Law, C.L. Brooks

9:00 COMP **135.** Small molecule design using single step free energy perturbation (SSFEP): Blinded validation against the relative binding affinities of inhibitors of p38 and ACK1 kinases. E. Raman, A.D. Mackerell, **R.A. Denny**

9:30 COMP **136.** Expert system for predicting different local structure-activity relationship environments using the concept of emerging chemical patterns. **V. Namasivayam**, D. Gupta-Ostermann, J. Balfer, J. Bajorath

10:00 Intermission.

10:15 COMP **137.** Scoring doesn't work — or does it? **C. Detering**

10:45 COMP **138.** ProBiS-ligands: A web server for prediction of ligands by examination of protein binding sites. **D. Janezic**, J. Konc

11:15 COMP **139.** Movable type method applied to the biomolecules study. **Z. Zheng**, M. Ucisik, K.M. Merz

Section E

Colorado Convention Center
Mile High Ballroom 4F

Computational Study of Water

D. J. Sindhikara, *Organizer, Presiding*

8:30 COMP **140.** Water's role in compound design for drug discovery. **H. Zhu**

9:00 COMP **141.** Quantitative prediction of water thermodynamics and applications to drug design. **W. Sherman**

9:30 COMP **142.** Insights into hydration propensity from systematic analyses of water in crystal structures. **S. Vyas**, C. Groom, S. Ward, I. Bruno

10:00 Intermission.

10:15 COMP **143.** Water-biomolecule interaction studied by 3D-RISM and X-ray scattering. **H.T. Nguyen**, D.A. Case

10:45 COMP **144.** Water dynamics in aqueous solutions of hydrophilic and amphiphilic peptides: Molecular simulation study of polarizability anisotropy response. **B.M. Ladanyi**, A.A. Milischuk

11:15 COMP **145.** Study of the protonation states of the curcumin molecule and their visible absorption spectra in aqueous solution using M06, SMD, and TDDFT and compared to experiment. **J.D. Alia**, P. Braegelmann, T. Roettgen, H. Goemann

TUESDAY AFTERNOON

Section A

Colorado Convention Center
Mile High Ballroom 1D

ACS Award for Computers in Chemical and Pharmaceutical Research: Symposium in Honor of David A. Case

Cosponsored by PHYS

K. Merz, D. M. York, *Organizers*
A. E. Roitberg, *Organizer, Presiding*

1:30 COMP **146.** Role of functional disorder in large protein complexes. **H. Dyson**, S. Sue, S. Mukerjee

2:00 COMP **147.** Mechanistic strategies in the HDV ribozyme: Metal ion identity controls the reaction pathway. **S. Hammes-Schiffer**, P.C. Bevilacqua

2:30 COMP **148.** Development of the ff14SB force field and application to protein folding simulations. **C.L. Simmerling**, J. Maier, H. Nguyen

3:00 Intermission.

3:15 COMP **149.** Withdrawn.

3:45 COMP **150. Award Address** (ACS Award for Computers in Chemical and Pharmaceutical Research sponsored by the ACS Division of Computers in Chemistry). Simulating biomolecules with implicit solvent models: GB, PB and 3D-RISM. **D.A. Case**

Section B

Colorado Convention Center
Mile High Ballroom 1E

ACS Award for Research at an Undergraduate Institution: Symposium in Honor of George C. Shields

E. C. Sherer, G. C. Shields, *Organizers, Presiding*

1:30 COMP **151.** On things that move. Protons, electrons, and other beasts in molecular modeling. **A.E. Roitberg**

2:00 COMP **152.** Highlights of a science career that began with undergraduate research. **H. McCuen**

2:20 COMP **153.** Computational chemistry's impact beyond discovery chemistry: Spectroscopy, cheminformatics and application of density functional theory in support of process/analytical chemistry. **E.C. Sherer**

2:50 Intermission.

3:10 COMP **154.** It's all about the fundamentals. **K. Kirschner**

3:40 COMP **155.** Conformation of retinal controls the pKa of protonated Schiff base during rhodopsin activation. **S. Feller**

4:10 COMP **156.** Role of quantum chemistry, PM3 and magic water clusters in unlocking Rodin's "Gates of Hell". **M. Jurema**

4:30 COMP **157. Award Address** (ACS Award for Research at an Undergraduate Institution sponsored by Research Corporation for Science Advancement). Research with undergraduates — a fabulous career. **G.C. Shields**

Section C

Colorado Convention Center
Mile High Ballroom 1F

Materials Science

Application and Movement

E. X. Esposito, *Organizer, Presiding*

1:30 COMP **158.** Low-temperature removal of crystallized fats: Investigation of nanodiamond adsorption on the disruption of the aqueous tristearin interface. **Z.E. Hughes**, T. Walsh

2:00 COMP **159.** Using crystal structures to understand pharmaceutical materials. S. Vyas, **C. Groom**, S. Ward, N. Feeder, I. Bruno

2:30 COMP **160.** Molecular dynamics simulations of biomolecules adsorbed on colloidal nanoparticles. **P. Samanta**, S. Wu, S. Sen, P. Kral

3:00 Intermission.

3:15 COMP **161.** Molecular dynamics simulation of CO_2 transport in hydrated Zeolite X. **S. Chakraborty**, S.J. Singer, P.K. Dutta

3:45 COMP **162.** Assessing and predicting flexibility in framework materials with molecular simulation: MOFs, zeolites, and molecular frameworks. A. Ortiz, A. Boutin, **F. Coudert**

4:15 COMP **163.** Zooming in on the solid-to-solid polymorphic transitions in DL-norleucine. **H. Cuppen**, J.A. Van Den Ende, M.M. Smets, D.T. de Jong, S.J. Brugman, H. Meekes

Section D

Colorado Convention Center
Mile High Ballroom 4E

Drug Discovery

Methodology

Cosponsored by CINF and MEDI

Y. Tseng, S. A. Wildman, *Organizers, Presiding*

1:30 COMP **164.** Predicting melting points of drug-like molecules using free energy perturbation. **R.A. Denny**, S. Jayaraman, R.J. Unwalla, M.E. Bunnage

2:00 COMP **165.** Biasing potential replica exchange multisite λ-dynamics: Toward scalable and simultaneous free energy calculations of more than 1000 compounds. **G.B. Goh**, K.A. Armacost, C.L. Brooks III

2:30 COMP **166.** Thermodynamics of ligand binding — consequences of local environment for drug optimization. **J. Ulander**

3:00 Intermission.

3:15 COMP **167.** Toward a complete, fully knowledge-driven pseudo force field for protein-ligand interactions. **M. Verdonk**

3:45 COMP **168.** Hierarchy of density functional theory-based benchmarks for a chemical space relevant to drug discovery applications. **A.D. Bochevarov**

4:15 COMP **169.** Rational design of potent factor VIIa inhibitors using quantum chemical methods. **D.L. Cheney**, I. Delucca, P.W. Glunz, W. Jiang, V. Ladziata, B. Parkhurst, Y. Zhang, Y. Zou, J.M. Bozarth, J.M. Luettgen, A.R. Rendina, L. Mueller, A. Wei, J.A. Newitt, J.K. Tamura, D. Seiffert, P.C. Wong, R.R. Wexler, E.S. Priestley

Section E

Colorado Convention Center
Mile High Ballroom 4F

Quantum Chemistry

Applications

Cosponsored by PHYS

E. V. Patterson, *Organizer, Presiding*

1:30 COMP **170.** Theoretical studies of the synchronization of the catalytic cycles in the second half-reaction step of nitric oxide synthase. **I. Shamovsky**, G. Belfield, F. Narjes, L. Ripa, C. Tyrchan, L. Öberg, P. Sjö

2:00 COMP **171.** Insight into the catalytic reaction mechanism of CO oxidation on reducible oxide-supported Au catalysis by AIMD simulation. **Y. Wang**, J. Li, R. Rousseau

2:30 Intermission.

‡ *Cooperative Cosponsorship*

2:45 COMP **172.** Tunable luminescence in CdSe quantum dots doped by Mn impurities. **Y. Dahnovsky**, V. Proshchenbko

3:15 COMP **173.** Highly-reduced corannulene: The influence of alkali metals on the structure and formation of aggregates. **A.Y. Rogachev**

3:45 COMP **174.** Quantum mechanical study of structural and electronic dilution effects in paramagnetic chemical exchange saturation transfer agents. **W.A. Miller**, P.B. Moore

Role of Membrane in Amyloid-Formation & the Pathogenicity of Amyloid Disease

Prions and Beyond

Sponsored by PHYS, Cosponsored by COLL and COMP

Modeling Excited States of Complex Systems

Electronic Structure

Sponsored by PHYS, Cosponsored by COMP

TUESDAY EVENING

Section A

Colorado Convention Center

Hall B2

NVIDIA GPU Award

M. E. Berger, R. Gomperts, *Organizers*

6:00 - 8:00

COMP **175.** Ligand-specific conformational changes in CCR7 coupled to signaling pathway selection. **Z. Gaieb**, D.D. Lo, D. Morikis

COMP **176.** Theoretical view of the C3d-CR2 binding controversy. **R. Mohan**, R.D. Gorham, D. Morikis

COMP **177.** Entropically driven CK-ASB9 interaction: How GPU-enabled computing provided unique insight into an intrinsically disordered 116 kDa protein complex. **J. Schiffer**, J. Parnell, E.A. Komives, R.E. Amaro

COMP **178.** GPU-enabled real-time electron dynamics of large light-harvesting systems in explicit solvent. **B.M. Wong**, M. Oviedo

COMP **179.** GPU-accelerated implementations of advanced electronic structure methods in Q-Chem. **K. Nanda**, E. Epifanovsky, A. Krylov

Section A

Colorado Convention Center

Hall B2

Poster Session

E. X. Esposito, S. A. Wildman, *Organizers*

6:00 - 8:00

COMP **180.** Possible mechanisms for interconversion of polar forms for the ferroelectric diisopropylammonim halides. **K.R. Cousins**

COMP **181.** Numerical modeling of carbon condensation in detonation products. **C. Mader**

COMP **182.** Identification of a new class of potential antimalaria agents using in-silico methodology. **R. Richardson**

COMP **183.** DFT and MP2 analysis of ligand selectivity in the catechol-O-methyltransferase enzyme. **A.K. Hatstat**, M. Morris, L. Peterson, M.L. Cafiero

COMP **184.** Effects of implicit solvation, relaxed amino acid side chains, and point mutations on the MP2 and DFT calculations of ligand-protein structure and interaction energies of dopaminergic ligands in the SULT1A3 enzyme active site. D. Bigler, L. Peterson, **M.L. Cafiero**

COMP **185.** MP2 and DFT analysis of the ligand selectivity of a sulfotransferase enzyme: SULT 1A. **A.H. Weems**, M.L. Cafiero, L.W. Peterson

COMP **186.** Study of the translocation of chloride ions through *Escherichia coli* transporters using the combined QM/MM method. **C. Davis**, S. Pezeshki, C. Garza, H. Lin

COMP **187.** Weighing energetics against best fit in development of RNA structure prediction models. **D. Bell**, Z. Xia, P. Ren

COMP **188.** Interactions between amino acid and graphene oxide: Experiments and theoretical calculations. **L. Huang**, K.E. Gubbins

COMP **189.** Applying intelligent design to biocatalyst engineering. **J. Pottel**, A. Tomberg, C. Bendell, N. Moitessier

COMP **190.** Interfacial force field parameterization in CHARMM for the accurate representation of peptide adsorption free energy on high-density polyethylene. **T. Abramyan**, J. Snyder, J.A. Yancey, S. Stuart, R.A. Latour

COMP **191.** Anions and computation: A match made in chemical heaven. **R.C. Fortenberry**

COMP **192.** Multiscale approach to decipher enzymatic processing and selectivity of lipids. **L. Riccardi**, J. Arencibia, A. Armirotti, M. Devivo

COMP **193.** In silico discovery of FKBP52 inhibitors as a prospective therapy for prostate cancer. **H. Li**, N. Guy, M.B. Cox, A. Cherkasov

COMP **194.** Withdrawn.

COMP **195.** Identification of 'dynamic hotspots' for lead discovery using MD simulation and spatiotemporal cluster analysis. **A. Arakawa**, O. Ichikawa, K. Yamazaki, K. Fujimoto, M. Okada, A. Yamada, S. Okazaki

COMP **196.** Density-based energy decomposition analysis. **Q. Wu**

COMP **197.** Prioritizing high throughput screening hits using a filtering workflow implemented in KNIME and QSAR models for antimalarial drug discovery. **S. Capuzzi**, D. Fourches, A. Tropsha

COMP **198.** Simulating X-ray, UV, and VIS absorption spectra with orthogonality constrained density functional theory. **F.A. Evangelista**, W.D. Derricotte

COMP **199.** Fast and reliable first principles approaches for the prediction of electro-mechanical properties in organic "smart" materials. K. Werling, B. Albrecht, **D. Lambrecht**

COMP **200.** Towards accurate parameterization for pyrrolidinium-based ionic liquids in lithium-ion batteries. **H. Torabifard**, G.A. Cisneros

COMP **201.** Withdrawn.

COMP **202.** Investigation of the effects of water in the binding site on protein-ligand interaction energy. **H. Sato**, A. Matsuura

COMP **203.** Insights into cobalt oxide water oxidation catalysts: A theoretical perspective from model dimer and cubane complexes. **A. Fernando**, C.M. Aikens

COMP **204.** Molecular modeling of dielectric constant of EC/DMC mixtures. **I. Daniels**, Z. Wang, B. Laird

COMP **205.** Site of reactivity models predict molecular reactivity of diverse chemicals. **T.B. Hughes**, G.P. Miller, S. Swamidass

COMP **206.** Molecular dynamics study of the confinement of alkane guests in an octa-acid dimer. **J. Barnett**, H. Ashbaugh, B.C. Gibb

COMP **207.** Robust and efficient coupled cluster-polarizable solvation methods for electronic molecular properties in the condensed phase. **M. Caricato**

COMP **208.** Pharmacophore-based similarity scoring method for DOCK. **L. Jiang**, R.C. Rizzo

COMP **209.** Mechanistic analysis of water oxidation catalyzed by a mononuclear copper(II) polypeptide in aqueous solutions. **W.C. Isley**, C.J. Cramer

COMP **210.** Development and in silico evaluation of large-scale metabolite identifcation methods using functional group detection for metabolomics. **J.M. Mitchell**, T.W. Fan, A.N. Lane, H.N. Moseley

COMP **211.** Nanoscale structure and dynamics of the liquid ordered phase of lipid bilayers. **E. Lyman**

COMP **212.** Strength, not depth: An exploration of differential membrane binding kinetics of Synaptotagmin-1 and Synaptotagmin-7 C2 domains. **J. Vermaas**, E. Tajkhorshid

COMP **213.** Withdrawn.

COMP **214.** Tolerance-dependent algorithm for core-constrained ligand docking with glide. **I. Tubert-Brohman**, J.L. Banks, M.P. Repasky

COMP **215.** Quartic force fields for electronically excited states: Theoretical ro-vibronic spectra. **W.J. Morgan**, R.C. Fortenberry

COMP **216.** Comparison of local correlation methods applied to chiroptical properties and excited states. **H. McAlexander**, T. Crawford

COMP **217.** Bond length alternation of conjugated oligomers: Performance of recent double-hybrid functionals. **M. Wykes**, N.Q. Su, X. Xu, C. Adamo, J.C. Sancho-Garcia

COMP **218.** Supramolecular engineering via fragment-based design. **B.P. Hay**, B. McCann

COMP **219.** Molecular mechanism of gated ligand binding. **Y. Li**, Z. Dong

COMP **220.** Validation of a tuned interfacial parameter set using dual-force-field CHARMM for the accurate simulation of protein adsorption on a silica glass surface. **J. Snyder**, T. Abramyan, J.A. Yancey, S. Stuart, R.A. Latour

COMP **221.** Implementation of the generalized internal coordinates for molecular geometry, energy gradients, and force constants. **A.V. Marenich**, H.P. Hratchian, J.L. Sonnenberg, M.J. Frisch

COMP **222.** Price of admission: Exploring the transition from straight chain to first cycle in sesquiterpene biosynthesis using quantum chemical calculations. **C.S. Hamann**, M.W. Lodewyk, D.J. Tantillo

COMP **223.** Photoionization of water in gas phase and in bulk: Insight from equation-of-motion coupled-cluster Dyson orbitals. **S. Gozem**, A. Krylov

COMP **224.** Exploring rovibrational states of floppy molecules using diffusion Monte Carlo. **J. Ford**, A.B. McCoy

COMP **225.** Scientific and technological advances in the quantum chemistry package Jaguar. **A.D. Bochevarov**, T.F. Hughes, L.D. Jacobson, D.M. Philipp, M.A. Watson

COMP **226.** DFT study of structural evolution of gold clusters.Au^-_n with n= 40-50. S. Pande, **X.C. Zeng**

COMP **227.** Quantum chemistry for X-ray photoelectron spectroscopy: Computation of XPS chemical shifts in amino acids and simple polypeptides. **I. Tolbatov**, D.M. Chipman

COMP **228.** In silico prediction of charge carrier mobility in organic semiconductors. **S. Kwak**, A. Goldberg, D. Giesen, M. Halls

COMP **229.** Withdrawn.

COMP **230.** Distinguishing the protonation states of the histidine ligands of the Rieske iron-sulfur cluster by ^{15}N isotopic substitution and vibrational frequency shifts. **B.R. Jagger**, A.M. Koval, R.A. Wheeler

COMP **231.** Nucleation mechanisms of γD-crystallin protein aggregates found in cataracts. **S.A. Richards**, R.A. Wheeler

COMP **232.** Computed chemical properties for the functional sorting of the haloacid dehalogenase superfamily. **E.M. Mozur**, M. Touch, M.J. Ondrechen

COMP **233.** Gold nanoparticle-nucleic acid modeling using GPU-accelerated molecular dynamics. **J.A. Nash**, A.L. Kwansa, Y.G. Yingling

COMP **234.** Withdrawn.

COMP **235.** Development of OPLS-AA Force Field Parameters for Ionic Liquids. **S.M. Gathiaka**, B. Li, O. Acevedo

COMP **236.** Accelerating DFT and hybrid DFT in VASP Using GPUs. **P. Fleurat-Lessard**, M. Hutchinson, M. Widom, A. Anciaux-Sedrakian, T. Guignon, D. Stosic, j. Bedorf, S. Tariq

COMP **237.** Simulations of fluorescence solvatochromisms in substituted *p*<-phenylene vinylene oligomer derivatives: Excited state molecular dynamics with implicit solvent. **J. Bjorgaard**, K. Velizhanin, S. Tretiak

COMP **238.** First-principle study of the structural and electronic properties of graphene on Zn(II) phthalocyanine tetrasulfonic acid adsorption. **R. Li**, D. Nicholls, M.R. Hoffmann, N. Oncel

COMP **239.** Quantum mechanical molecular interactions for calculating excitation energy in molecular environments: A first-order interacting space approach. **K. Yanai**, K. Ishimura, J. Hasegawa

COMP **240.** Nitrogen dopants and vacancy defects in graphene nanoflakes: Theoretical study of size-dependent electronic excitation properties. **C. Lin**

COMP **241.** Free energy study of small molecules to RNA with multiple binding poses. **Y. Tanida**, A. Matsuura

COMP **242.** Uncovering topological signatures of instability and metastability. **J. Miorelli**

COMP **243.** Molecular dynamics of metallodiporphyrins. **J. Coda**, W.M. Ames

COMP **244.** Computational insights into intramolecular hydrogen migration via agostic-type interactions. **J. Duchimaza**, K. Yan, A. Ellern, A.D. Sadow, M.S. Gordon

COMP **245.** Predictive methods for CO_2 solubilities in reactive ionic liquids. **Q. Sheridan**, T. Lee, E. Maginn, W.F. Schneider

COMP **246.** Theoretical study of (hetero) aromatic fluorination catalyzed by palladium. P. Fleurat-Lessard, **J. Roger**, C. Testa, J. Hierso

COMP **247.** Computer simulations of forward osmosis for desalination. **O. Lee**

COMP **248.** Withdrawn.

COMP **249.** Computational insight into origins of *Z*-selectivity and enantioselectivity of asymmetric ring-opening/cross-metathesis catalyzed by a stereogenic-at-Ru complex. **J.W. Nelson**, H.D. Pham, X. Wang

COMP **250.** Coordination number and molecular geometry influences on methanethiol binding strength and acidity in $[(Imidazole)_{4-x}Zinc(II)–S(H)CH_3]$ complexes. **D.P. Linder,** K.R. Rodgers

COMP **251.** DFT study of the rate determining steps of carbon chain growth on Co. **D. Petersen**, L. Arnadottir

COMP **252.** Theoretical study on the fluorescent spectrum of enhanced green fluorescent protein. **Y. Uchida**, M. Higashi, S. Hayashi

COMP **253.** Identification of a pKa-regulating motif stabilizing imidazole modified double stranded DNA. **D. Buyst**, V. Gheeraardijn, J. van den Begin, A. Madder, J.C. Martins

COMP **254.** Alpha-hydrogen bonding stereochemical consequences in alpha,beta-unsaturated aldehydes complexed with chiral menthoxyaluminum dichloride Lewis acid catalysts in Diels-Alder reactions. **B. Vernier**, A.N. Ahmed, J. Rohde, J.D. Evanseck

COMP **255.** Calculation of the association trajectories of oseltamivir and sialic acid to wild type and H274Y viral neuraminidase. **R.W. Wenner**, L.M. Krause, J.F. Graziadei, P.F. Marris, A.W. Van Wynsberghe

COMP **256.** Effect of surface defects on the optical properties of silicon quantum dots. **N.K. Dandu**

COMP **257.** Targeted delivery of peptidoglycan immunomodulators using liposomal carriers: MD study of the lipid encapsulation. **K. Feher**

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COMP **258.** Semantic web and computational chemistry. **N.S. Ostlund**, B. Wang

COMP **259.** Reparameterization of gold thiolate ReaxFF. **B.M. Barngrover**, E.M. Kinder, T.J. Manges, T.J. Cobb, C.M. Aikens

COMP **260.** Online parameter and property database for the TraPPE force field. **A. Sunnarborg**, A. Bliss, H. Stern, B.L. Eggimann, J.I. Siepmann

COMP **261.** Elucidating a chemical defense mechanism of Antarctic sponges. S.K. Vankayala, **F.L. Kearns**, B.J. Baker, H.L. Woodcock

COMP **262.** Characterization of fullerene structure and electronic properties using DFT and EPR parameters: Charge localization in polymer-fullerene composite solar cells. **J.N. Webb**, J. Niklas, O. Poluektov, K. Mardis

COMP **263.** Quantum chemical studies of gas hydrates. **P. Warrier**, C.A. Koh

COMP **264.** Nature of the β-cyclodextrin-graphene interface: A quantum chemical analysis. **P. Jaiyong**, R.A. Bryce

COMP **265.** Investigation of different binding kinetics among the neuraminidase inhibitors. **G. Kang**, D.J. Mermelstein, R.B. Clayton, A.W. Van Wynsberghe

COMP **266.** Interaction of aqueous ammonium chloride with *Helicobacter pylori* urease. **M. Minkara**, M.N. Weaver, K.M. Merz

COMP **267.** Iron pyridine-2,6-diimine (PDI) scaffolds: A new model with MRMP2. **J. McNeely**, A.Y. Rogachev

COMP **268.** Density functional analysis of donor-acceptor complexes formed between ethers and sulfur trioxide or sulfur dioxide. **G. Van Den Driessche**

COMP **269.** Human pepsin 3A hydrolysis reaction mechanism. **A.N. Mascarenas**, E. Cowles, J.J. Stewart, S.B. Braun-Sand

COMP **270.** Substrate binding of human MTH1 protein. **H.E. Ryan**, M. Carter, J.J. Stewart, S.B. Braun-Sand, P. Stenmark

COMP **271.** Ab initio computations of nuclear quadrupolar coupling constants: Why they don't work, and how to fix them. **G.S. Harbison**

COMP **272.** Characterization of carbene intramolecular reactivity with various substituents through computer modeling. **M. Roth**, W.M. Ames

COMP **273.** Withdrawn.

COMP **274.** Using TD-DFT and NTOs to model photocatalysis. **C.M. Midkiff**, A.K. Rappe

COMP **275.** First principle study on optimizing conditions for charge transfer in quantum dots through dye functionalization. **P. Cui**, S. Kilina

COMP **276.** SO2 – yet another two-faced ligand. **J. Li**, A.Y. Rogachev

COMP **277.** Impact of substituent size and electronegativity on the band gap of TiO_2 polymorphs. **A.J. Glaid**, M.N. Srnec, J.A. Aitken, J.D. Madura

COMP **278.** Enrichment of computational chemistry data with the semantic web. **B. Wang**, L. Nardozi, S.J. Chalk, M. Sopek, N.S. Ostlund

COMP **279.** HK propagator uniformized along a 1D manifold. **L. Kocia**, E.J. Heller

COMP **280.** Structural determinants of promiscuous and specific binding in protein - protein complexes using component analysis techniques. **A. Sherani**, Y.Y. Zhang, M.L. Radhakrishnan

Technical program information known at press time.
The official technical program for the 249th ACS National Meeting is available at: www.acs.org/denver2015

COMP **281.** Q-Chem: An engine for innovation. Z. Gan, E. Epifanovsky, **Y. Shao**

COMP **282.** Adsorption of O_2 on neutral/charged Au_n (n = 1-3) clusters: A comparative study between DFT and coupled cluster calculations. Y. Zhao, **N.S. Khetrapal**, H. Li, Y. Gao, X.C. Zeng

COMP **283.** Exploring the mechanisms of enantioselective organocatalytic reactions: A DFT study. **K.E. Blise**, D.L. Kohen, G.E. Hofmeister, D.G. Alberg, M. Cvitkovic

COMP **284.** Molecular simulations of fluorescent sensors with amyloid-β protein aggregates. **J. Thompson**, E.H. Hill, E.Y. Chi, D.G. Whitten, D.G. Evans

COMP **285.** Constrained heuristic optimization of NLO chromophores. **C.B. Rinderspacher**, J. Elward

COMP **286.** Modeling of a bench-scale biomass pyrolyze: An experimentalist's viewpoint. **R.J. French**

COMP **287.** Modeling some features of the reaction mechanism of chymotrypsin using semiempirical methods. **W.C. Kelly**, S.B. Braun-Sand, J.J. Stewart, **B.M. Guerrero**

COMP **288.** Visualizing the interplay of delocalization and strong correlation in catalysis. **B.G. Janesko**

COMP **289.** Ab initio dynamics of the unfolding and decarboxylation of pseudo-chair carboxyphosphate in aqueous solution. **E. Jesikiewicz**, S. Boesch, S.M. Firestine, J.D. Evanseck

COMP **290.** Carboxyphosphate formation from the reaction of bicarbonate and ATP in ATP-dependent carboxylases. **S.E. Kochanek**, T. Clymer, V. Pakkala, S.M. Firestine, J.D. Evanseck

COMP **291.** Analysis of the components of halogen bonding. **M. Billman**, A.K. Rappe

COMP **292.** GPU-accelerated stochastic evaluation of second-order many-body perturbation energies. **R. Brewster**, S. Willow, S. Hirata

COMP **293.** Molecular modeling of the binding interaction of RGD-functionalized poly(ethylene glycol) hydrogels with lipid bilayer surface. **Y. Lin**, G. Chen, F. Ryvkin

COMP **294.** Ab initio study of halocarbons. **K.R. Jorgensen**

COMP **295.** Computational study of activation energies in 1,3-dipolar cycloadditions. **P. Esempio**, H.A. Trujillo

COMP **296.** Microscale multiphysics simulations of intra-particle transport phenomena and pyrolytic conversion using biomass particle models with realistic morphology and resolved microstructure. **P. Ciesielski**, M.F. Crowley, B. Donohoe, M.R. Nimlos, T. Foust

COMP **297.** Theoretically determined mechanism for the formation of guanine C8 adducts from arylamine derived carcinogens. **A.S. Dutton**, J. Bautista, S. Shrestha

COMP **298.** Feedstocks thermal and compositional effects on pyrolysis yields. **D. Robichaud**

COMP **299.** Theoretical study of criegee biradical molecule in the atmosphere. **S. Alhowity**

COMP **300.** Modeling non-covalent interactions in biomolecules: An ab initio based fragmentation approach. **D. Kosenkov**

COMP **301.** Exploring novel energetic materials: A constrained search approach. **J.M. Elward**, C.B. Rinderspacher

COMP **302.** Withdrawn.

COMP **303.** Chemist view on reaction pathways. N. Chéron, R. Ramozzi, R. Grüber, **P. Fleurat-Lessard**

Section A

Colorado Convention Center
Hall B2

The Chemical Computing Group Excellence Award for Graduate Students

Financially supported by Chemical Computing Group

C. L. Simmerling, *Organizer*

6:00 - 8:00

COMP **304.** Time-dependent nonequilibrium dynamics in QM/continuum approaches. **F. Ding**, D. Lingerfelt, B. Mennucci, X. Li

COMP **305.** MD-generated volume profiles as a tool for probing transition states of conformational changes. **H. Wiebe**, N. Weinberg

COMP **306.** Theoretical investigations of the fumarate addition reaction: Implications for the biological stability of future fuels and opportunities for bioremediation of hydrocarbon contaminated areas. **V.S. Bharadwaj**, C.M. Maupin, A.M. Dean

COMP **307.** Simulations of the self-assembly of polyelectrolyte block copolymers using dissipative particle dynamics with an implicit solvent ionic strength (ISIS) method. **N.K. Li**, W.H. Fuss, Y.G. Yingling

COMP **308.** Sum frequency generation spectra of the air/water interface from first principles-based models. **G.R. Medders**, F. Paesani

Section A

Colorado Convention Center
Hall B2

The OpenEye Outstanding Junior Faculty Award

Financially supported by OpenEye Scientific Software

C. L. Simmerling, *Organizer*

6:00 - 8:00

COMP **309.** Physically-motivated first-principles force fields for molecular simulation: Theory and applications. **J.R. Schmidt**, J.G. McDaniel

COMP **310.** RNA design rules through internet-scale social computing and high-throughput chemistry. E. Participants, J. Lee, W. Kladwang, M. Lee, D. Cantu, M. Azizyan, H. Kim, L. Alex, S. Yoon, A. Treuille, **R. Das**

COMP **311.** Development of electron-hole explicitly correlated wave function based method with pseudopotential theory for investigation of optical properties of quantum dot-protein complexes. **A. Chakraborty**

COMP **312.** Benchmarking the adsorption energies on carbon nanotubes. D.G. Smith, **K. Patkowski**

WEDNESDAY MORNING

Section A

Colorado Convention Center
Mile High Ballroom 1D

Molecular Mechanics

Applications

E. X. Esposito, S. A. Wildman, *Organizers, Presiding*

8:30 COMP **313.** Temperature effects on the spatial distribution of electrolyte mixtures at the aqueous liquid-vapor interface. **B.L. Eggimann**, A. Sunnarborg, J.I. Siepmann

9:00 COMP **314.** Molecular simulation of surface density effects on heterogeneous DNA hybridization. **J.M. Stubbs**, S. Cooper, W. Scamman, M. van den Berg

9:30 COMP **315.** Structural properties of DNA basepair mismatches. A. Kingsland, **L. Maibaum**

10:00 Intermission.

10:15 COMP **316.** Quantam mechanical molecular mechanical calculations using amoeba force fields. **Y. Shao**, A.C. Simmonett, Y. Mao, F.C. Pickard, G. Koenig, B. Brooks, J. Herbert, T.L. Head-Gordon, M.P. Head-Gordon

10:45 COMP **317.** Molecular dynamics by flexible-boundary QM/MM: On-the-fly partial charge transfer between QM and MM subsystems. S. Pezeshki, **H. Lin**

11:15 COMP **318.** Quantum Drude oscillator model for linear scale atomistic simulation – a coarse grained electronic structure allowing for high environmental transferability. **G.J. Martyna**

Section B

Colorado Convention Center
Mile High Ballroom 1E

Quantum Chemistry

Quantum Dynamics & Monte Carlo Simulations

Cosponsored by PHYS

E. V. Patterson, *Organizer, Presiding*

8:30 COMP **319.** Second-quantized surface hopping. **A.V. Akimov**, O.V. Prezhdo

9:00 COMP **320.** Systematically improvable models in excited-state dynamics calculations. **A. Molina**, A. Chien, T.G. Goodson, P.M. Zimmerman

9:30 COMP **321.** Real-time electron transport from parity-time symmetric quantum mechanics. J. Elenewski, **H. Chen**

10:00 Intermission.

10:00 COMP **322.** Ring polymer molecular dynamics: New quantum dynamical method for calculating chemical reaction rates. **Y. Suleymanov**

10:30 COMP **323.** Direct dynamics simulations of steroidal ring-closing events. **R.P. Pemberton**, D.J. Tantillo

Section C

Colorado Convention Center
Mile High Ballroom 1F

Computational Pyrolysis & Upgrading of Bio-Oils

Bonding and Kinetics

Cosponsored by MPPG

D. Robichaud, *Organizer*
R. Surendran Assary, R. S. Weber, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 COMP **324.** Molecular-level kinetic modeling in biomass thermochemical conversions: Software tools and their applications. **M.T. Klein**

9:20 COMP **325.** Toward automated mechanism generation of lignin pyrolysis models: Development of group additivity parameters for aromatic species. **H.H. Carstensen**, A. Ince, M. Reyniers, G.B. Marin

9:50 COMP **326.** First-principles study of phenol hydrogenation on Pt and Ni catalysts in aqueous phase. **R. Rousseau**, D. Mei, Y. Yoon, R.S. Weber, J.A. Lercher

10:20 Intermission.

10:35 COMP **327.** Charting elementary steps in the cellulose pyrolysis reaction network. **H. Mayes**, X. Zhou, G. Beckham, L.J. Broadbelt

11:05 COMP **328.** In silico zeolite catalyzed carbon-carbon coupling reactions for furan upgrading. **C. Liu**, L. Cheng, R. Surendran Assary, L.A. Curtiss

11:35 COMP **329.** Mechanistic study of furan formation in HZSM-5 using quantum mechanical modeling. **S. Kim**, D. Robichaud, C. Mukarakate, L. Bu, T. Evans, G. Beckham, R.S. Paton, M.R. Nimlos

12:05 Concluding Remarks.

Section D

Colorado Convention Center
Mile High Ballroom 4E

Drug Discovery

Ligand-Based

Cosponsored by CINF and MEDI

Y. Tseng, S. A. Wildman, *Organizers, Presiding*

8:30 COMP **330.** Halogen bonds in drug design. **S. Sirimulla**

9:00 COMP **331.** Highly visual workflow for designing, selecting and enumerating new compounds for assay. **J.W. Sager**, T.E. Mansley, P. Mounteney

9:30 Intermission.

‡ *Cooperative Cosponsorship*

9:45 COMP **332.** Discovery of new and diverse TLR9 receptor antagonists for regulating innate immune reactions. **A. Goldblum**, A. Burger-Kentischer, A. Mattes, M. Zatsepin

10:15 COMP **333.** In silico design, synthesis, and assays of specific substrates and peptidomimetic inhibitors for proteinase 3. S. Narawane, C. Grauffel, A. Schillinger, B. Haug, **N. Reuter**

10:45 COMP **334.** Ligand based drug design of novel pyrimidine derivatives as Tankyrase inhibitors for the treatment of colorectal cancer. **A.P. Patel**, H.G. Bhatt

Section E

Colorado Convention Center
Mile High Ballroom 4F

Computational Study of Water

D. J. Sindhikara, *Organizer, Presiding*

8:30 COMP **335.** Advanced potential energy surfaces for water simulations. **T.L. Head-Gordon**

9:00 COMP **336.** Development and implementation of an advanced density based potential for water. R.E. Duke, O.N. Starovoytov, J.A. Piquemal, **G.A. Cisneros**

9:30 COMP **337.** Effects of three-body nonadditive exchange and induction forces in liquid water. **O. Akin-Ojo**, K. Szalewicz

10:00 Intermission.

10:15 COMP **338.** Microscopic structure, equilibrium density, and local environment in liquid water: A highly accurate ab initio path-integral molecular dynamics study. **R.A. Distasio**, B. Santra, H. Ko, F. Martelli, M. Ceriotti, R. Car

10:45 COMP **339.** Ice nucleation on graphene surface supports the classical theory of heterogeneous nucleation. **R. Cabriolu**, T. Li

11:15 COMP **340.** Direct calculation of the rate of homogeneous nucleation of ice for TIP4P/ICE from massively parallel molecular simulations. **A. Haji-Akbari**, P.G. Debenedetti

Computational Chemical Dynamics: Advancing our Understanding of Chemical Processes in Gas-Phase, Biomolecular & Condensed-Phase Systems: A Symposium in Honor of Donald Truhlar

Properties and Processes in Solvated Systems

Sponsored by PHYS, Cosponsored by COMP

Modeling Complex Biomolecules: From Structure to Dynamics & Function

Modeling of Macromolecular Structure and Function

Sponsored by PHYS, Cosponsored by COMP

Modeling Excited States of Complex Systems

Electronic Structure

Sponsored by PHYS, Cosponsored by COMP

WEDNESDAY AFTERNOON

Section A

Colorado Convention Center
Mile High Ballroom 1D

Symposium Organizer Selections

SOS

E. X. Esposito, S. A. Wildman, *Organizers, Presiding*

1:30 COMP **341.** Multi-scale computational investigations of the cAMP activation-mechanism of Protein Kinase A RI_{α} using Brownian Dynamics and Molecular Dynamics simulations. **S.P. Hirakis**, R. Malmstrom, R.E. Amaro

2:00 COMP **342.** Water dynamics at protein-protein interfaces: A molecular dynamics study of virus-host receptor complexes. **P. Dutta**, M. Botlani, S. Varma

2:30 COMP **343.** Homology modeling and molecular dynamics study of ALKBH1 enzyme. **P. Silvestrov**, T. Müller, K. Clark, R. Hausinger, G.A. Cisneros

3:00 Intermission.

3:15 COMP **344.** Partitioning of nitroaromatic compounds through lipid bilayer. **A. Golius**, O. Isayev, L. Gorb, F. Hill, J.R. Leszczynski

3:45 COMP **345.** Bondalyzer: A tool for the discovery of charge density property relationships. **T.R. Wilson**, M. Eberhart, T. Jones

4:15 COMP **346.** Field-dependent peak shift in real-time time-dependent density functional theory. **M. Provorse**, B. Habenicht, C. Isborn

Section B

Colorado Convention Center
Mile High Ballroom 1E

Membranes

S. A. Wildman, *Organizer, Presiding*

1:30 COMP **347.** Surface-functionalized nanoparticle permeation triggers lipid displacement and water and ion leakage. **P.A. Oroskar**, S. Murad, C. Jameson

2:00 COMP **348.** Investigating the forces governing the peripheral membrane association and dissociation of a bacterial phospholipase C (*Bt*PI-PLC). H.M. Khan, C. Grauffel, B. Yang, T. He, R. Mary, A. Gershenson, **N. Reuter**

2:30 COMP **349.** Partitioning of anionic nanoparticles in cholesterol-containing membranes occurs via local disordering and cholesterol depletion. P. Gkeka, P. Angelikopoulos, L. Sarkisov, **Z. Cournia**

3:00 Intermission.

3:15 COMP **350.** Lateral organization and transverse coupling in asymmetric biomembranes. **X. Cheng**, J. Nickels, F. Heberle, J. Katsaras

3:45 COMP **351.** Investigating lipid phase changes from liquid crystalline to ripple to gel phases with all-atom molecular dynamics simulations. **P. Khakbaz**, J.B. Klauda

4:15 COMP **352.** Spatial organization of cellular membranes. K. Sapp, S. He, **L. Maibaum**

Section C

Colorado Convention Center
Mile High Ballroom 1F

Computational Pyrolysis & Upgrading of Bio-Oils

Reaction Engineering

Cosponsored by ENFL‡ and MPPG

R. S. Weber, *Organizer*
D. Robichaud, R. Surendran Assary, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 COMP **353.** Impact of H_2 addition on formation of PAH during anisole pyrolysis. **Y. Koirala**, S. Villano, A.M. Dean, H.H. Carstensen, M. Reyniers, G.B. Marin

2:20 COMP **354.** Insights into the hydrodeoxygenation mechanisms for lignin upgrade. **D.G. Vlachos**

2:50 COMP **355.** Role of solid, liquid, and gaseous phases during pyrolysis of biomass. **R.C. Brown**

3:20 Intermission.

3:35 COMP **356.** Strike a happy medium: Identifying appropriate reaction conditions for upgrading bio-oil. **M.R. Nimlos**, R.S. Weber

4:05 COMP **357.** Reactor simulations for catalytic upgrading of pyrolysis vapors. **J. Ziegler**, S. Pannala, T. Foust, M.R. Nimlos, D. Robichaud

4:35 COMP **358.** Multiscale/multiphysics modeling of biomass fast pyrolysis and vapor phase upgrading reactors. S. Pannala, E. Ramirez, J. Ziegler, D. Robichaud, M.R. Nimlos, T. Foust, C. Daw

5:05 Panel Discussion: What is Needed to Advance the State of the Art in Biomass Conversion and Upgrading?

5:35 COMP **359.** Thermal properties of pine, poplar, and fir blocks from room temperature to 500°C. **D.M. Stevens**, T.L. Westover, C.L. Williams

6:05 Concluding Remarks.

Section D

Colorado Convention Center
Mile High Ballroom 4E

Drug Discovery

Ligand-Based

Cosponsored by CINF and MEDI

Y. Tseng, S. A. Wildman, *Organizers, Presiding*

1:30 COMP **360.** Small molecule crystal structures in drug discovery and development. **C. Groom**, S. Ward, S. Vyas, I. Bruno

2:00 COMP **361.** QSAR modeling independent of input tautomers. M. Waldman, **R. Fraczkiewicz**, R. Clark

2:30 COMP **362.** General applicability of template CoMFA to prospective bioactivity prediction. R.D. Cramer

3:00 COMP **363.** Exploring conformational search protocols for ligand-based virtual screening and 3D QSAR modeling. D. Cappel, S. Dixon, **W. Sherman**, J. Duan

3:30 Intermission.

3:45 COMP **364.** Experimentally derived interaction fields as a basis for ligand-based virtual screening. **C. Groom**, J. Cole, I. Giangreco, O. Korb, S. Gothe, I. Bruno

4:15 COMP **365.** Alignment of diverse ligands for a protein: a solved problem? **T. Cheeseright**, P. Tosco, M. Mackey

4:45 COMP **366.** Exhaustive pairwise overlays: the gold standard for molecular alignment? **P.C. Hawkins**, R.W. Tolbert

Section E

Colorado Convention Center
Mile High Ballroom 4F

Quantum Chemistry

Applications

Cosponsored by PHYS

E. V. Patterson, *Organizer, Presiding*

1:30 COMP **367.** Importance of a nonlocal description of electron–electron interactions in modeling the dissociative adsorption of H_2 on Cu(100). **F. Goeltl**, C. Houriez, M. Guitou, G. Chambaud, P. Sautet

2:00 COMP **368.** Density functional investigation of 2-alkyl-anthraquinone hydrogenation on a palladium cluster. **E. Yuan**, L. Wang, F. Ren

2:30 COMP **369.** Theoretical prediction of the effects of substitution on the efficacies of ruthenium water oxidation catalysts. **A.B. League**, M. Ertem, P. Miro Ramirez, C.J. Cramer

3:00 Intermission.

3:15 COMP **370.** DFT study of dehydrogenation of ethanol on alkaline earth metal oxides. **Y. Izumi**, H. Kamata, H. Ushiyama

3:45 COMP **371.** Stereospecific zirconium catalyzed cycloamination of 4-penteneamine. **W.C. Everett**, T.L. Windus, A.D. Sadow

4:15 COMP **372.** Reversible olefin binding to nickel dithiolenes and a variety of related complexes. **E.N. Brothers**, M.B. Hall

Computational Chemical Dynamics: Advancing our Understanding of Chemical Processes in Gas-Phase, Biomolecular & Condensed-Phase Systems: A Symposium in Honor of Donald Truhlar

Nonadiabatic Dynamics

Sponsored by PHYS, Cosponsored by COMP

Modeling Complex Biomolecules: From Structure to Dynamics & Function

Folding and Aggregation

Sponsored by PHYS, Cosponsored by COMP

Modeling Excited States of Complex Systems

Electronic Structure

Sponsored by PHYS, Cosponsored by COMP

ENFL

Division of Energy and Fuels

A. Park, *Program Chair*

OTHER SYMPOSIA OF INTEREST:

Computational Pyrolysis and Upgrading of Bio-Oils *(see COMP, Wed)*

Catalytic Materials and Technologies for Upgrading of COx and Natural Gas Oxidation *(see CATL, Tue, Wed, Thu)*

SOCIAL EVENTS:

Dinner, 7:30 PM: Tue

SUNDAY MORNING

Section A

Colorado Convention Center
Mile High Ballroom 4A

Nanomaterials for Solar Energy Conversion & Storage

Cosponsored by MPPG‡

R. T. Koodali, Y. H. Ng, N. Wu, *Organizers*
Y. H. Hu, Y. Wu, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENFL **1.** Nanocarbons for optoelectronic applications. **D. Guldi**

8:45 ENFL **2.** Plasmonic metal-semiconductor nanostructures for solar fuel generation. **N. Wu**

9:15 ENFL **3.** Uniform doping of metal oxide nanowires using solid state diffusion for photoelectrochemical water oxidation. **J. Resasco**, N.P. Dasgupta, J. Roque-Rosell, J. Guo, P. Yang

9:35 ENFL **4.** Impact of humidity in the preparation of $CoTiO_3$ perovskites: Effective ABO_3 type catalysts for O_2 evolution. **S. Rasalingam**, R.T. Koodali

9:55 Intermission.

10:00 ENFL **5.** Chalcogenide nanostructured precursors in fabrication of polycrystalline absorber layers in thin-film photovoltaics. **D.R. Radu**

10:30 ENFL **6.** Light management in extremely thin photoelectrode architectures. **I. Thomann**

11:00 ENFL **7.** Sustainable inorganic nanocrystals for solar energy conversion and storage applications. **K. Ramasamy**, R. Gupta, H. Sims, S. Ivanov, A. Gupta

11:20 ENFL **8.** Tailoring zinc oxide nanostructures for solar cell applications. K. Sakar, E.V. Braden, L. Song, M. Rawolle, S.V. Roth, **P. Mueller-Buschbaum**

11:40 ENFL **9.** Structural studies of solution-grown iron pyrite (FeS_2) nanoparticles via synchrotron and neutron diffraction. **R.C. Miller**, D. Agocs, S. Fredrick, J.R. Neilson, A.L. Prieto

Section B

Colorado Convention Center
Mile High Ballroom 4B

Materials & Interfaces in Lithium Batteries & Beyond

New Materials/Systems

A. A. Gewirth, A. Manivannan, *Organizers*
Y. Shao, D. Wang, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENFL **10.** From nanomaterials to energy storage systems. **J. Liu**

8:35 ENFL **11.** Flexible high-energy Li-ion batteries with fast-charging capability. **J. Cho**

9:05 ENFL **12.** Enable high energy-density lithium-ion battery conversion cathodes based on iron fluorides using integrated in situ experimental and computational approaches. **S. Jin**, L. Li

9:35 ENFL **13.** Chalcogen elements' electrochemistry for lithium batteries and beyond systems. **Y. Guo**

10:05 Intermission.

10:15 ENFL **14.** Recent progress on high-energy density batteries with aqueous electrolytes. **P. Liu**

10:45 ENFL **15.** Redox flow lithium battery. **Q. Wang**, Q. Huang, C. Jia, F. Pan, Y. Zhu

11:15 ENFL **16.** Suppressing manganese dissolution form lithium manganate via graphene coatings. **M. Hersam**

11:45 ENFL **17.** $LiMn_2O_4$ cathodes for Li-ion batteries: Effect of Mn in electrolyte on anode and Au coating to minimize dissolution. **J. Esbenshade**, M. Fox, A.A. Gewirth

12:05 Concluding Remarks.

Section C

Colorado Convention Center
Mile High Ballroom 3C

Chemistry of Energy & Fuels

A. Park, *Organizer*
G. Gadikota, X. Wang, *Organizers, Presiding*

8:00 ENFL **18.** Ionic conduction in doped ceria-carbonate composite electrolytes. **Z. Yicheng**, Y. Li

8:20 ENFL **19.** Enhanced butanol production from starch by *Clostridium* species. T. Li, Y. Yan, **J. He**

8:40 ENFL **20.** Research work conducted on the fuels, renewable energy, and poverty reduction with sustainable development in the developing countries of the world. particularly South Asia. **M. Usman**

9:00 ENFL **21.** Molecular electrocatalysts on a surface: When organometallic chemistry meets surface science. **A.K. Das**, M.H. Engelhard, M. Bullock, A.M. Appel

9:20 ENFL **22.** Noble metal-free Fe-N/C catalyst for highly efficient oxygen reduction reaction under both alkaline and acidic conditions. **L. Lin**, Z. Qing, A. Xu

9:40 Intermission.

9:50 ENFL **23.** Evaluation of carbon nanospheres decorated with nanoparticles for adsorptive desulfurization. **T. Saleh**, **T.D. Shuaib**

10:10 ENFL **24.** Synthesis of ultra large mesostructured cellular foams material with 3D structure using different micelle expanders. **S. Song**, A. Duan, X. Zhou, Z. Zhao, G. Jiang, J. Liu

10:30 ENFL **25.** Silicon parallel process manufacturing techniques for harsh environment chemical gas sensors. **M.R. Mullen**, V.A. Vulcano Rossi, N.A. Karker, Z. Zhao, M.W. Kowarz, M.A. Carpenter, P.K. Dutta

10:50 ENFL **26.** Superadiabaticity in reaction waves as a mechanism for energy concentration. **S.G. Mahajan**, J.T. Abrahamson, S. Birkhimer, E. Friedman, Q. Wang, M. Beck, M. Strano

11:10 ENFL **27.** Interface bonding effect between ternary sulfide solid solution and TiO_2NTs composite by solvothermal synthesis. **Z. Yao**, F. Jia, Z. Yu, Z. Jiang

11:30 ENFL **28.** Fundamental understanding of molecular weight growth kinetics in hydrocarbon conversions. **K. Wang**, S. Villano, A.M. Dean

Section D

Colorado Convention Center
Mile High Ballroom 3B

Catalysis for Un-conventional Energy Sources

Fuel Cell, Solar Cell and Solar Fuel

Cosponsored by CATL and MPPG‡

W. Jang, C. Liu, N. Wu, *Organizers*
R. Glaeser, C. Wang, *Organizers, Presiding*

8:00 ENFL **29.** Bioinspired and biotemplated artificial photosynthetic systems for solar fuels generation. **H. Zhou**, J. Ye, T. Fan, D. Zhang

8:40 ENFL **30.** Carbon-based metal-free catalysts for energy conversion. M. Wang, X. Kong, **L. Dai**

9:20 ENFL **31.** In situ XAS of ceria materials for the thermochemical conversion and storage of concentrated solar thermal power. **M. Rothensteiner**, S. Sala, H. Emerich, J.A. Van Bokhoven

9:40 ENFL **32.** Novel approaches toward solar fuels based on modified graphitic carbon nitride. K. Striegler, **R. Glaeser**

10:00 Intermission.

10:10 ENFL **33.** Sensitized graphene hybrid catalysts and co-catalysts for solar hydrogen generation. **G. Lu**

10:50 ENFL **34.** Investigation of an In-Ni-Ta-O-N overall water splitting photocatalyst. **Y. Li**, Y. Li, X. Zhang, S. Jiang

11:30 ENFL **35.** Sustainability assessment of catalysis for energy storage in hydrogen: Comparative net energy analysis of fuel cell and electrolyzer technologies. **M.A. Pellow**, S. Sridhar, C.J. Emmott, S.M. Benson

Section E

Colorado Convention Center
Mile High Ballroom 4C

Hybrid Functional Porous Materials for Sustainable Energy: Carbon, MOF & Conductive Polymers

Metal Organic Frameworks

J. L. Lutkenhaus, *Organizer*
S. K. Nune, V. Pol, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENFL **36.** Gas separation and ion transport of porous coordination polymers. **S. Kitagawa**

8:45 ENFL **37.** Methane storage in metal-organic frameworks with ultrahigh porosity. **S. Kaskel**

9:15 ENFL **38.** Design principles for electroactive metal-organic frameworks. **C.H. Hendon**, K.T. Butler, A. Walsh

9:45 ENFL **39.** Catalytic metal-organic frameworks (MOFs): Design and preparation. **O.K. Farha**

10:05 Intermission.

10:15 ENFL **40.** Are MOFs *et al.* really the next best thing since sliced bread? A case study for electronic device apps. **M.A. Omary**, A. Cimino, R.M. Almotawa, A. Maspero, C. Giacobbe, G. Palmisano, C. Yang, J.F. Ivy, C. Williams, S. Galli

10:45 ENFL **41.** Withdrawn.

11:15 ENFL **42.** Computational Identification of MOFs suitable for creating conducting materials via ligand infiltration. **D. Sholl**, X. Nie, A. Kulkarni, D. Nazarian, J. Camp

11:45 ENFL **43.** Porous metal-organic frameworks and their sorption property. **W. Sun**

12:05 ENFL **152.** Screening of functionalized or hydrophobic MOFs for capture of ammonia and other toxic compounds. P.Z. Moghadam, K. Kim, D. Fairen-Jimenez, **R. Snurr**

12:25 ENFL **153.** Adsorption of indole vs. naphthalene on F300 MOF by the complementary spectroscopic, kinetic, and DFT studies. J. Dai, M.L. McKee, **A. Samokhvalov**

Section F

Colorado Convention Center
Mile High Ballroom 4D

Negative Carbon Emission Technologies: BECCS (Bio-Energy with Carbon Capture & Storage)

Cosponsored by MPPG‡

M. Kidder, S. M. Mahurin, *Organizers*
D. J. Heldebrant, F. Li, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENFL **44.** What can molecular simulation do for global warming? **D. Jiang**

8:45 ENFL **45.** Molecular modeling of non-aqueous CO_2 capture solvents. **D.C. Cantu**, V. Glezakou, R. Rousseau, D. Malhotra, P.K. Koech, D.J. Heldebrant

9:15 ENFL **46.** Synthesis and characterization of low viscosity carbon dioxide binding organic liquids for flue gas clean up. **P.K. Koech**, D. Malhotra, D.J. Heldebrant, D.C. Cantu, V. Glezakou, R. Rousseau

9:35 ENFL **47.** CO_2 binding employing chelate cooperativity. **S. Hiew**, D.T. Nguyen, M. Kleiman, A. Esser-Kahn

9:55 Intermission.

10:05 ENFL **48.** Post-synthesis modification of nanoporous organic frameworks for enhanced CO_2capture. **T. Islamoglu**, T. Kim, H.M. El-Kaderi

10:25 ENFL **49.** Structure-property relations of cation-exchanged chabazite zeolites for CO_2 adsorption. **T. Pham**, **R.F. Lobo**, **M.R. Hudson**, **C.M. Brown**

10:45 ENFL **50.** Tetraethylenpentamine-functionalized polybenzoxazine aerogel for CO_2 adsorption. **A. Alhwaige**, H. Ishida, S. Qutubuddin

11:05 ENFL **51.** Development of stable Ca-based sorbents for realistic CO_2 capture: Significant stabilizing effect of fly ash. **F. Yan**, J. Jiang, M. Zhao

11:25 ENFL **52.** Review of the post combustion carbon capture technologies with emphasis on polyethylenimine. P. Upadhaya, A. Kadiyala, **R.R. Kommalapati**, Z. Huque

SUNDAY AFTERNOON

Section A

Colorado Convention Center
Mile High Ballroom 4A

Nanomaterials for Solar Energy Conversion & Storage

Cosponsored by MPPG‡

R. T. Koodali, Y. H. Ng, N. Wu, *Organizers*
Y. H. Hu, Y. Wu, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 ENFL **53.** Materials for printed solar cells. **A.B. Holmes**, D.J. Jones, B. Purushothaman, B. Robotham, H. Seyler, J. Subbiah, K. Sun, J. White, Z. Xiao, B. Zhang, W.W. Wong

1:45 ENFL **54.** Air stable A_2MX_6 compounds for large scale processing of solar cells. B. Lee, C. Stoumpos, H. Liao, M.G. Kanatzidis, **R. Chang**

2:15 ENFL **55.** BIAN based π-conjugated polymer as sensitizer for photoelectrochemical water splitting. **R. Vedarajan**, R. Gagan, N. Matsumi

2:35 ENFL **56.** Ratio Influence on morphological and physical properties of P3HT-C_{60} all-conjugated block copolymer systems. **J. Lohrman**, S. Ren

2:55 ENFL **57.** Ru-bipyridyl dye sensitized titania loaded SBA-15 mesoporous materials for visible light induced photocatalytic splitting of water. **H. Naasz**, S. Rasalingam, L.J. Mahoney, K. Mariappan, R.T. Koodali

3:15 Intermission.

3:30 ENFL **58.** Control of nanostructures and interfaces in excitonic solar cells. **G. Cao**

4:10 ENFL **59.** 1D nanostructures design for efficient solar water splitting. **S. Shen**, M. Liu

4:40 ENFL **60.** On the effects of surface and dimensionality of oxide photocatalysts for water splitting. **L. Vayssieres**

5:10 ENFL **61.** Sn_xGe_{1-x} Nanoalloys: Toward new photovoltaic materials. K. Ramasamy, J.M. Pietryga, **S. Ivanov**

Section B

Colorado Convention Center
Mile High Ballroom 4B

Materials & Interfaces in Lithium Batteries & Beyond

Mg Batteries

A. Manivannan, D. Wang, *Organizers*
A. A. Gewirth, Y. Shao, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 ENFL **62.** Materials challenges for multivalent energy storage. **K. Persson**

1:35 ENFL **63.** Hybrid lithium and magnesium ion battery with long-term stability at high current density. **H. Yoo**, Y. Li, Y. Liang, Y. Yao

2:05 ENFL **64.** Activation of MnO_2cathode by water-stimulated Mg^{2+} insertion for magnesium battery. **J. Song**, M. Noked, E. Gillette, J. Duay, S. Lee

2:25 ENFL **65.** Direct observation of magnesium ion intercalation into a spinel-structured λ-manganese oxide at the multilength scale. C. Kim, P. Phillips, **T. Yi**, B. Key, Y. Yu, R. Klie, J. Cabana

2:45 Intermission.

2:55 ENFL **66.** Mg anode interfacial films: Enabling rechargeable Mg batteries. **K.R. Zavadil**, N.T. Hahn

3:25 ENFL **67.** Electrolyte effects on Mg deposition and stripping. **A.A. Gewirth**, C. Barile, E. Miller

3:45 ENFL **68.** Anode/electrolyte interface for magnesium batteries. **T.S. Arthur**, F. Mizuno, R. Mohtadi, J. Guo, P. Glans

4:05 ENFL **69.** Synthetic strategies for magnesium-ion electrolytes. **J.T. Herb**, C. Nist-Lund, C.B. Arnold

4:25 ENFL **70.** Electronic structure at electrode/electrolyte interfaces in Mg based electrochemical systems. **J. Balachandran**, D. Siegel

4:45 ENFL **71.** Promoted Mg ion insertion reversibility with Sn-alloys for Mg ion batteries. **Y. Cheng**, Y. Shao, J. Liu

5:05 ENFL **72.** Amorphous cathodes for magnesium batteries: The V_2O_5:P_2O_5 system. **T.S. Arthur**, K. Kato, J. Germain, F. Mizuno

5:25 Concluding Remarks.

Section C

Colorado Convention Center
Mile High Ballroom 3C

Chemistry of Energy & Fuels

A. Park, *Organizer*
G. Gadikota, X. Wang, *Organizers, Presiding*

1:00 ENFL **73.** Heat of vaporization by measurement using DSC/TGA versus estimation using detailed hydrocarbon analysis. **G. Chupka**, R.L. McCormick, E. Christensen, L. Fouts

1:20 ENFL **74.** Effect of Mg doping on structural properties and optical characterization of NiO. **G. Allaedini**, S. Tasirin, P. Aminayi

1:40 ENFL **75.** Investigations of non-linear polymers as high performance lubricant additives. **J.W. Robinson**, P. Bhattacharya, J. Qu, J. Bays, L. Cosimbescu

2:00 ENFL **76.** Effect of crystalline phases on structural and optical properties of natural ilmenite mineral used for photocatalytic hydrogen production. **A.F. Lopez Vasquez**, R. Lopez-Vasquez, G. Andres Reyes

2:20 ENFL **77.** Hydrogen storage using the formate bicarbonate cycle (FBC). A. Givant, **Y. Sasson**

2:40 ENFL **78.** Design, construction, and experimentation of two components bioclimatic to transport heat solar to rural housing interior environments high Andean Peru. **R. Espinoza Paredas**

3:00 ENFL **79.** Geochemical markers in diagenetic alterations of fracture conductivity of tight sedimentary rocks. A. Olabode, **M. Radonjic**

3:20 Intermission.

3:30 ENFL **80.** Establishment and kinetic analysis of a fourteen-lump model of RFCC process. **K. Xiong**, C. Lu, X. Gao

3:50 ENFL **81.** Reforming of a liquid fuel using a Rh-substituted pyrochlore: A carbon formation study. **M.W. Smith**, D. Shekhawat, D.A. Berry, D. Haynes, D.L. Floyd, J.J. Spivey

Section D

Colorado Convention Center
Mile High Ballroom 3B

Catalysis for Un-conventional Energy Sources

Biofuel and CO_2 Utilization

Cosponsored by CATL and MPPG‡

‡ *Cooperative Cosponsorship*

R. Glaeser, W. Jang, C. Liu, C. Wang, *Organizers*
N. Wu, *Organizer, Presiding*
Y. Li, *Presiding*

1:00 ENFL **82.** In-situ *(trans)*esterification of rice bran oil and co-extraction of bioactive compounds. **A.W. Go**, Y. Ju

1:20 ENFL **83.** Production of synthetic middle-distillates via catalytic dimerization of bio-DME-derived olefins. **M. Behl**, J.A. Schaidle, J. Hensley

1:40 ENFL **84.** In situ X-ray absorbance fine structure (XAFS) of precious metal catalysts during ethanol steam reforming. **S. Crowley**, Y. Li, A. Frenkel, M.J. Castaldi

2:00 ENFL **85.** Development of heterogeneous mesoporous acid catalysts for esterification of oleic acid with methanol. B.S. Chilukuri, **W. Jang**

2:20 ENFL **86.** Nanoparticle catalyst design for electrochemical reduction of carbon dioxide. **D. Kim**, P. Yang

3:00 Intermission.

3:10 ENFL **87.** Alcohol oxidation on TiO_2-based model catalysts and defect engineered MOFs. **Y. Wang**

3:50 ENFL **88.** Biodiesel from used oil under pulse sonication with alcohol mixture solvents. **E. Martinez-Guerra**, **V. Gude**

4:10 ENFL **89.** Effect of microwave and ultrasound irradiations on transesterification of waste vegetable oil. **V. Gude**, **E. Martinez-Guerra**

4:30 ENFL **90.** Selective hydrodeoxygenation of lignin. **I.M. Klein**, T.H. Parsell, M.M. Abu-Omar

4:50 ENFL **91.** Potential of cocoa pod husk as a heterogeneous solid catalyst for the transesterification of non-edible *Azadirachta indica* (neem) seed oil into methyl esters: A case of modeling and optimization studies. A.O. Etim, S.O. Ajala, T.V. Ojumu, **E. Betiku**

Section E

Colorado Convention Center
Mile High Ballroom 4C

Hybrid Functional Porous Materials for Sustainable Energy: Carbon, MOF & Conductive Polymers

Metal Organic Frameworks

J. L. Lutkenhaus, *Organizer*
S. K. Nune, V. Pol, *Organizers, Presiding*

1:00 ENFL **92.** Metal organic frameworks cooperated Si nanorod arrays used for energy storage. Y. Yu, C. Yue, S. Sun, X. He, **J. Li**

1:30 ENFL **93.** Synthesis and characterization of diamine-appended metal-organic frameworks for carbon dioxide capture. **T. McDonald**, J.A. Mason, J.R. Long

2:00 ENFL **94.** Kinetically controlled synthesis of ultrastable metal-organic frameworks. S. Yuan, **H. Zhou**

2:20 ENFL **95.** MOF photoluminescence via metal-ligand tunability. **T.M. Nenoff**, D.F. Sava Gallis, L.E. Rohwer, M.A. Rodriguez

2:40 ENFL **96.** Fabrication of electrically conductive metal-organic framework thin films. A. Talin, F. Leonard, K. Leong, C. SPataru, M. Foster, **V. Stavila**, M. Allendorf

3:00 ENFL **97.** Selective pore sizing for 2D MOFs and 1D MONTs: Implications for guest selectivity. C.R. Murdock, B.C. Hughes, K.M. Nelson, **D.M. Jenkins**

3:20 Intermission.

3:30 ENFL **98.** Topology guided design and syntheses of highly stable mesoporous porphyrinic zirconium MOFs with high surface areas. **T. Liu**

3:50 ENFL **99.** Adsorption characteristics of rare gases (Xe, Kr) in metal-DOBDC from first-principles calculation. **Y. Li,** S. Ghose, P.K. Thallapally

4:10 ENFL **100.** Immobilization of photocatalyst into metal-organic framework. **X. Wang**, W. Lu, Z. Wei, H. Zhou

4:30 ENFL **101.** Conducting metal organic frameworks (MOFs) for electrochemical device applications. **S. Patwardhan**, I. Hod, J.T. Hupp, G.C. Schatz

4:50 ENFL **102.** Nanoporous covalent organic polymers for CO_2 capture. **C.T. Yavuz**, H.A. Patel, D. Thirion, J. Byun, D. Ko

5:10 ENFL **103.** Role of residual H_2O on the adsorption mechanism and kinetics of solid amine-functionalized sorbents for CO_2 capture. M.W. Hahn, M. Steib, E. Berger, **A. Jentys**, J.A. Lercher

5:30 ENFL **154.** Water reaction mechanism in metal organic frameworks with coordinatively unsaturated metal ions: MOF-74. **K. Tan**, S. Zuluaga, Q. Gong, P. Canepa, H. Wang, E. Fuents, J. Li, T. Thonhauser, Y.J. Chabal

Section F

Colorado Convention Center
Mile High Ballroom 4D

Negative Carbon Emission Technologies: BECCS (Bio-Energy with Carbon Capture & Storage)

Cosponsored by MPPG‡

D. J. Heldebrant, F. Li, *Organizers*
M. Kidder, S. M. Mahurin, *Organizers, Presiding*

1:00 ENFL **104.** Mechanism of nanostructure formation and oxygen ion transport in redox reactions of metal oxide alloy materials. L. Qin, Z. Cheng, A. Majumder, N. Deshpande, J. Fan, D. K, **L. Fan**

1:40 ENFL **105.** Novel strategy to reduce sintering, based on polymorphic materials, and application to carbon capture and storage. **M. Zhao**, S. Tian, J. Jiang

2:10 ENFL **106.** Perovskite promoted iron oxide for hybrid water-splitting and syngas generation. **F. Li**, F. He

2:30 ENFL **107.** Abstraction from weak C-H Bond of ortho/para-methylcyclohexadienone isomers critical in improving product distribution in anisole pyrolysis. **Y. Koirala**, S. Villano, A.M. Dean, H.H. Carstensen, M. Reyniers, G.B. Marin

2:50 ENFL **108.** Metal nitrate catalytic graphization of lignin via hydrothermal supporting method. **M. Demir**, B. Aksoy, A. Subramanian, H. El-Kaderi, R. Gupta

3:10 Intermission.

3:20 ENFL **109.** Novel use of low-pH fermentation in bioelectrochemical processes. **V. Gadhamshetty**, J. David

3:25 ENFL **110.** Morphological studies on lignin-anthracite briquettes. **L. Peña Duque**, N. Robitaille Brown

3:55 ENFL **111.** Size tunable hollow nanoporous gold nanoparticles with superior methanol electrooxidation performance. **X. Ling**

4:25 ENFL **112.** Nanostructured metal phosphide catalysts for conversion of biomass to liquid fuels. **S.E. Habas**, F.G. Baddour, D.A. Ruddy, M. Pan, C.P. Nash, M.B. Griffin, J. Wang, J.E. Hensley, J.A. Schaidle

5:10 Concluding Remarks.

Nanotechnology: Delivering on the Promise

Research & Development

Sponsored by PRES, Cosponsored by AGFD, AGRO, ANYL, CARB, CCPA, CCS, CHAS, COLL, COMSCI, CORP, ENFL, HIST, I&EC, IAC, MPPG, PMSE, POLY, SCHB and SOCED

MONDAY MORNING

Section A

Colorado Convention Center
Mile High Ballroom 4A

Nanomaterials for Solar Energy Conversion & Storage

Cosponsored by MPPG‡

Y. H. Hu, N. Wu, Y. Wu, *Organizers*
R. T. Koodali, Y. H. Ng, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENFL **113.** First-principles analysis of the photocatalytic performance of bismuth vanadate. **G.S. Hwang**, K. Kweon

8:35 ENFL **114.** Photovoltaic properties of $CH_3NH_3PbI_3$ perovskites as probed through excited state characterization. **P.V. Kamat**, J.S. Manser

9:15 ENFL **115.** Optical properties and exciton dynamics of organolead halide peroskite quantum dots for solar energy conversion. **J.Z. Zhang**, Y. Pu, Y. Yang, Y. Li

9:45 ENFL **116.** Perovskite solar cells with rutile TiO^2 nanowires as photoanode. **Q. Jiang**

10:05 ENFL **117.** Ab initio modeling of organometallic halide perovskites for photovoltaic applications. **A. Neukirch**, L. Pedesseau, J. Even, C. Katan, S. Tretiak

10:25 Intermission.

10:30 ENFL **118.** High performance organo lead halide perovskite solar cells by incorporating monodisperse upconversion nanocrystals. **Z. Lin**, M. He, X. Pang

11:00 ENFL **119.** Withdrawn.

Section B

Colorado Convention Center
Mile High Ballroom 4B

Materials & Interfaces in Lithium Batteries & Beyond

Li-ion

A. A. Gewirth, D. Wang, *Organizers*
A. Manivannan, Y. Shao, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENFL **120.** Toward high cycle efficiency of high energy density lithium ion batteries. **X. Xiao**

8:35 ENFL **121.** Directing conversion and alloying reactions using multilayer electrodes. **T. Fister**, G. Evmenenko, X. Hu, X. Chen, J. Wu, V. Dravid, M.J. Bedzyk, J. Esbenshade, B. Long, A. Gewirth, B. Shi, P. Fenter

9:05 ENFL **122.** First-principles studies of anode interfacial chemistry for lithium ion battery applications. **J.P. Greeley**, H. Yildirim, M.K. Chan

9:35 ENFL **123.** Strain optimized 3D mesostructured battery electrodes. **P.V. Braun**

10:05 Intermission.

10:15 ENFL **124.** Electrolyte and interphases for Li ion and beyond. C. Wang, **K. Xu**

10:45 ENFL **125.** Near-field optical imaging of the SEI layer on a Sn anode. **R. Kostecki**, M. Ayache, I. Lucas

11:15 ENFL **126.** Hierarchical Sn/C composite as an anode for long-cycle-life lithium-ion batteries. **J. Chen**, X. Huang

11:45 ENFL **127.** Low-cost, pyrolytic carbon black composite anodes for lithium-ion batteries. **M.P. Paranthaman**, A.K. Naskar, Y. Li, S.K. Akato, M. Chi, J. Li, G. Nagasubramanian

12:15 Concluding Remarks.

Section C

Colorado Convention Center
Mile High Ballroom 3C

ENFL Distinguished Researcher Award: Symposium in Honor of James Burrington

E. Delbridge, *Organizer*
A. Sammut, *Presiding*

8:00 Introductory Remarks.

8:10 ENFL **128.** Trends in lubricant additive chemistry: Working under boundary conditions. **J.K. Pudelski**, E. Delbridge

8:40 ENFL **129.** Unified friction theory: A paradigm shift in friction management. **J.K. Pudelski**, E. Delbridge

9:10 ENFL **130.** Seeing is believing: Advanced visualization of surface active chemistry. **D. Jayne**

9:40 Intermission.

9:50 ENFL **131.** Advanced tools for measuring chaotic friction behavior in automotive applications. **O. Smith**

10:20 ENFL **132.** Art and science of lubricant additive formulation chemistry. **E. Delbridge**

10:50 ENFL **133.** Innovative chemical delivery systems for advanced additive formulations. **J.D. Burrington**

11:30 ENFL **134.** Time released technology (TRT®) for lubricant additive delivery via an oil filter. **G. Bilski**

Section D

Colorado Convention Center
Mile High Ballroom 3B

Catalysis for Un-conventional Energy Sources

Novel Catalysts

Cosponsored by CATL and MPPG‡

R. Glaeser, C. Liu, C. Wang, N. Wu, *Organizers*
W. Jang, *Organizer, Presiding*
G. Lu, *Presiding*

8:00 ENFL **135.** Catalytic isomerization and oligomerization of endo-dicyclopentadiene using alkali-treated hierarchical porous HZSM-5. **Q. Deng**, J. Zou, G. Nie, X. Zhang, L. Wang

8:40 ENFL **136.** Tailoring mesoporous cabons and related materials for catalysis. **S. Dai**

9:20 ENFL **137.** Mechanistic studies on catalytically active bimetallic Au/Pd-FAU zeolite for H^2 dissociation: A DFT study. **B. Boekfa**, T. Maihom, M. Ehara, **J. Limtrakul**

9:40 Intermission.

9:50 ENFL **138.** H_2O-functionalized zeolitic Zn(2-methylimidazole)$_2$ framework (ZIF-8) for H_2 storage. P. Cheng, **Y.H. Hu**

10:30 ENFL **139.** Hydrodeoxygenation of anisole over MCM-41 supported Ni_2P catalysts. M. Lu, R. Wei, Q. Guan, **W. Li**

11:10 ENFL **140.** Hydrogenation of CO_2 to methanol over In_2O_3. K. Sun, Z. Fan, N. Rui, J. Ye, Q. Ge, **C. Liu**

11:30 ENFL **141.** New insights on the role of YSZ in a $NiAl_2O_4/Al_2O_3$-YSZ diesel steam reforming catalyst. **E. Achouri**, N. Abatzoglou, N. Braidy

11:50 Concluding Remarks.

Section E

Colorado Convention Center
Mile High Ballroom 4C

Hybrid Functional Porous Materials for Sustainable Energy: Carbon, MOF & Conductive Polymers

Energy Storage

S. K. Nune, *Organizer*
J. L. Lutkenhaus, V. Pol, *Organizers, Presiding*

8:00 ENFL **142.** Role of carbon materials in designing high-energy lithium-ion cells. **D. Abraham**

8:40 ENFL **143.** Transition metal nanoparticles anchored on carbon anodes for advanced Li-ion storage. **V. Etacheri**, C. Hong, V. Pol

9:10 ENFL **144.** Electroactive separators for safer and longer lasting secondary lithium batteries. **G. Chen**, T. Richardson

9:40 ENFL **145.** Mesoscale insights in porous electrodes for energy storage. **P.P. Mukherjee**, Z. Liu, C. Chen, M. Stein IV

10:00 Intermission.

10:10 ENFL **146.** Mesoporous materials in layer-by-layer architectures for sustainable developments. **K. Ariga**

10:40 ENFL **147.** Electric double-layer supercapacitor based on 3D graphitic petals with iongel electrolyte. R. Gupta, K. Saviers, **T. Fisher**, G. Xiong, R. Reifenberger

11:10 ENFL **148.** Bio-inspired synthesis of 3D porous carbons-enhanced electrode materials for high-performane asymmetric supercapacitors. **W. Tian**, Q. Gao

11:40 ENFL **149.** Hybrid redox capacitor with high energy density derived from quinone-functionalized zeolite templated-carbon. **K. Nueangnoraj**, T. Tomai, H. Nishihara, T. Kyotani, I. Honma

12:00 ENFL **150.** Metal-organic frameworks from design strategies to applications. **M. Eddaoudi**

12:20 ENFL **151.** Chemical principles underpinning the performance of HKUST-1. **C.H. Hendon**, A. Walsh

Section F

Colorado Convention Center
Mile High Ballroom 4D

Enhanced Extraction & Utilization of Unconventional Energy Sources: Hydrofracking, EOR and Novel Approaches

Cosponsored by MPPG‡

G. Gadikota, A. G. Stack, *Organizers*
L. Anovitz, M. Kidder, *Organizers, Presiding*

8:00 ENFL **156.** Density functional theory calculations of CO_2 and CH_4 interactions with clay surfaces. M.D. Kilmer, **L. Tribe**

8:20 ENFL **157.** Study of pressure effects on borate cross-linked hydraulic fracturing fluids by small angle X-ray scattering. **R.E. Winans**, S. Lee, T. Li, R.J. Klingler, S. Seifert, R. Hutchins, M. Parris

8:50 ENFL **158.** Phase equilibria and growth phenomena of CO_2 mixed gas hydrates. **Z.T. Ward**, Z.M. Aman, E.F. May, M.L. Johns, C.A. Koh

9:10 ENFL **159.** Shale gas fracturing fluids containing additives of low environmental impact. **M.H. Bell**, A. Viswanath, B.C. Benicewicz

9:30 ENFL **160.** Phase equilibrium and miscibility study of CO_2 and mixed gas in Tensleep oil for enhanced oil recovery. **R. Borgohain**, S. Xie, H. Jiang

9:50 ENFL **161.** Investigation of chemical and morphological changes in shale-supercritical CO_2-water systems for sustainable unconventional hydrocarbon extraction. **G. Gadikota**, S. Yip, A. Park

10:10 Intermission.

10:20 ENFL **162.** Potential microorganisms for enhance oil recovery in a low permeability oil reservoir. **D. Hao**, M. Zhang, H. Dong, S. Sun, Z. Zhang, D. Gao, Z. Song, Z. Zhang

10:40 ENFL **163.** Alcohol-to-jet renewable jet fuel: Characterization, development of a surrogate fuel mixture, and diesel engine combustion. **D.J. Luning Prak**, M.H. Jones, J. Cowart

11:00 ENFL **164.** Evaluating the leachability of residual solids generated from hydraulic fracturing in Marcellus shale. **C. Swann**, G.D. Boardman, J. Parks, R. Hammack

11:20 ENFL **165.** Pyrolysis characteristics of Longkou oil shale under optimized condition. **W. Wang**, S. Li, Q. Shi, S. Liu, J. Wu, Y. Ma

11:40 ENFL **166.** Formulating mixtures of nanoparticles, polymers, and surfactants to stabilize high viscosity high internal phase CO_2-in-water foams. **Z. Xue**, I. Ketchum, S.L. Bryant, C. Huh, M. Prodanovic, K.P. Johnston

12:10 ENFL **167.** Switchable amine surfactants for CO_2 foams in high temperature enhanced oil recovery. **A. Elhag**, Y. Chen, J. Noguera, P. Reddy, G.J. Hirasaki, Q. Nguyen, K.P. Johnston

12:30 ENFL **168.** Biogenic methane production from Bowen Basin coal waste materials using environmental microbial consortium. **H. Zheng**, T. Chen, V. Rudolph, S. Golding

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Nanotechnology: Delivering on the Promise

Opportunities and Challenges for Health, Safety and the Environment

Sponsored by PRES, Cosponsored by AGFD, AGRO, ANYL, CARB, CCPA, CCS, CHAS, COLL, COMSCI, CORP, ENFL, HIST, I&EC, IAC, MPPG, PMSE, POLY, SCHB and SOCED

Biomass to Fuel and Products

Sponsored by SOCED, Cosponsored by CELL, ENFL and MPPG

MONDAY AFTERNOON

Section A

Colorado Convention Center
Mile High Ballroom 4A

Nanomaterials for Solar Energy Conversion & Storage

Cosponsored by MPPG‡

Y. H. Hu, N. Wu, Y. Wu, *Organizers*
R. T. Koodali, Y. H. Ng, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 ENFL **169.** Technical and operational perspective on the DOE Energy Innovation Hub and Fuels from Sunlight, the Joint Center for Artificial Photosynthesis. **N.S. Lewis**

1:45 ENFL **170.** Hybrid nanomaterials for photovoltaics and photocatalysis. **D. Ma**

2:15 ENFL **171.** Surface enhanced Raman spectroscopy for real-time observation of intermediates for photocatalytic reactions. **R. Yan**, P. Yang

2:35 ENFL **172.** Exploration of solar hydrogen evolution using cobalt-doped titanium dioxide. **L.J. Mahoney**, R. Peng, C. Wu, J. Baltrusaitis, R.T. Koodali

2:55 Intermission.

3:00 ENFL **173.** Exploring the role of defects on charge transport in organic semiconductors. K.M. Pelzer, M.K. Chan, S.K. Gray, **S.B. Darling**

3:30 ENFL **174.** Repurposing Blu-ray movie discs as low-cost, quasi-random nanoimprinting templates for photon management. **J. Huang**

4:30 ENFL **175.** Self-adapting layer of robust single-crystal earth-abundant nanoparticles catalyzing oxygen evolution. **H. Chen**

4:00 ENFL **176.** Semiconductor materials for efficient photoelectrochemical water splitting: The PEC working group. **H. Wang**, T.F. Jaramillo, E.L. Miller

5:00 ENFL **177.** Plasmon-enhanced Cu_2O photocathodes for solar water splitting. **J. DuChene**, B. Williams, A.C. Johnston-Peck, J. Qiu, D. Su, E. Stach, W. Wei

Section B

Colorado Convention Center
Mile High Ballroom 4B

Materials & Interfaces in Lithium Batteries & Beyond

Li-O2 & Li-S

A. A. Gewirth, A. Manivannan, D. Wang, *Organizers*
Y. Shao, *Organizer, Presiding*
J. Lu, *Presiding*

1:00 Introductory Remarks.

1:05 ENFL **178.** Water as promoter and catalyst in dioxygen electrochemistry at aqueous and organic electrified interfaces. **N. Markovic**, J. Jirkovsky, D. Strmcnik, L.A. Curtiss, J. Moore, K.R. Zavadil, V. Stamenkovic, K. Harrison, R. Surendran Assary, R. Subbaraman, B. Genorio, C. Diesendruck

1:35 ENFL **179.** In situ fabrication of porous carbon supported α-MnO_2 nanoparticles at room temperature: Application for rechargeable Li-air battery. **J. Lu**, K. Amine

2:05 ENFL **180.** Rechargeable K-Air battery: Principle and mechanism. **Y. Wu**

2:35 ENFL **181.** Li-air battery with ionic liquid based electrolyte flow: Overview and perspectives. **E. Paillard**, S. Passerini

3:05 Intermission.

3:15 ENFL **182.** Computational studies of the stability of lithium superoxide and its role in charge and discharge chemistries in lithium-oxygen batteries. **L.A. Curtiss**, K. Lau, U. Das, R. Surendran Assary, P. Redfern

3:45 ENFL **183.** Li-ion *and* Li-O_2: exploring hybrid electrode/electrocatalyst materials. A. Kinaci, L. Trahey, S. Kirklin, C. Wolverton, M.M. Thackeray, **M.K. Chan**

4:15 ENFL **184.** Modeling the electron transfer reaction at the lithium metal anode-liquid electrolyte interface in lithium-air batteries. S. Kazemiabnavi, P. Dutta, **S. Banerjee**

4:35 ENFL **185.** Establishing the relationship between lithium polysulfides and Li-S cell performance. **R. Xu**, J. Lu, I. Belharouak, K. Amine, Y. Ren, X. Zhang, A. Nie, R. Shahbazian Yassar, J.C. Li

4:55 ENFL **186.** Towards a molecular level understanding of reactions in Li-S electrical energy storage systems. **R. Surendran Assary**

5:15 ENFL **187.** Hierarchical porous carbon materials as electrodes for lithium sulfur batteries. **S. Kaskel**

5:35 Concluding Remarks.

Section C

Colorado Convention Center
Mile High Ballroom 4D

ENFL Distinguished Researcher Award: Symposium in Honor of James Burrington

J. Bradzil, *Organizer, Presiding*

1:00 Introductory Remarks.

1:10 ENFL **188.** Important fundamental principles of selective heterogeneous oxidation catalysis ("7 pillars of oxidation catalysis"). **R. Grasselli**

1:40 ENFL **189.** Mechanism and kinetics of propene oxidation and ammoxidation on bismuth molybdate-based catalysts. **A.T. Bell**

2:10 ENFL **190.** Solid state mechanisms in selective oxidation by metal oxide catalysts. **J.F. Brazdil**

2:40 Intermission.

2:50 ENFL **191.** Mechanism in selective oxidation catalysis by metal oxides. **J.D. Burrington**

3:30 ENFL **192.** Detailed reaction mechanisms for selective transformation of alkanes to oxygenates by heterogeneous transition metal oxide catalysts. **W.A. Goddard**

4:00 ENFL **193.** Compositional inhomogeneity and lattice dynamics in the M1 catalyst: Implications concerning active sites for propane oxidation. **D. Buttrey**, D. Blom, T. Vogt, W. Ueda

4:30 ENFL **194.** Mechanistic insights for propane ammoxidation over Mo-V-Te-Nb-O M1 phase from density functional theory calculations. **Y. Xu**, V.V. Guliants

Section D

Colorado Convention Center
Mile High Ballroom 3B

Two-Dimensional Materials for Energy & Fuel

G. Yu, *Organizer*
L. Hu, Y. Lin, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 ENFL **195.** Intercalation of 2D materials. **L. Hu**

1:35 ENFL **196.** Insights into the solution synthesis of 2D metal chalcogenide nanostructures. D.D. Vaughn, D. Sun, **R.E. Schaak**

2:15 ENFL **197.** Liquid phase exfoliation: A versatile route to materials for energy storage and production. **K. Paton**, J.N. Coleman

2:45 Intermission.

2:55 ENFL **198.** Reversible zero-valent intercalation chemistries for 2D layered materials. **K.J. Koski**

3:15 ENFL **199.** Enhancement of the chemical activity of 2D transition metal dichalcogenides via phase engineering. **M. Chhowalla**

3:55 ENFL **200.** Preparation of new layered and 2D materials with basic science and energy applications. **T. McQueen**

4:25 ENFL **201.** Bioelectrochemical oxidation of graphite drives graphene oxide production and electrosynthesis. **Z. Ren**, L. Lu, C. Zeng, L. Wang, X. Yin, S. Jin, J. Bunch

4:45 ENFL **202.** Withdrawn.

Section E

Colorado Convention Center
Mile High Ballroom 4C

Hybrid Functional Porous Materials for Sustainable Energy: Carbon, MOF & Conductive Polymers

Energy Storage

V. Pol, *Organizer*
J. L. Lutkenhaus, S. K. Nune, *Organizers, Presiding*

1:00 ENFL **203.** Advanced energy-storage devices of high-voltage symmetric supercapcitors fabricated with N-containing carbon materials. **Y. Mei**, Z. Zhou

1:30 ENFL **204.** Peanut shell hybrid sodium ion capacitor with extreme energy: Power rivals lithium ion capacitors. **D. Mitlin**

2:00 ENFL **205.** Nanoscale modifications in quantum dot solar cells. **S. Bhattacharyya**

2:20 ENFL **206.** Energy applications of (photo) electrochemically prepared organic/inorganic hybrid semiconductor assemblies. **C. Janaky**, D. Hursan, G. Samu, C. Visy, K. Rajeshwar

2:40 ENFL **207.** Poly(vinylidene fluoride) nanocomposites with enhanced energy density by filling with a small loading of surface-fluorinated $Ba_{0.6}Sr_{0.4}TiO_3$ nanofibers. **L. Shaohui**, J. Zhai, Z. An

3:00 Intermission.

3:10 ENFL **208.** Block copolymer directed functional ordered mesoporous materials for energy devices: From functional materials to hierarchical materials. **J. Lee**

3:40 ENFL **209.** Die creation and implementation to increase manufacturability in PEM fuel cell electrodes. **K.M. McClung**, S. Mahmoodi, R.S. Besser

4:00 ENFL **210.** Methodology for stable but reactive catalysts (with Å-scale tunability). **S. Das**

4:20 ENFL **211.** Fabrication of energy efficient conductive composites using nonconducting polymeric materials. **R. Gill**, Q. Nadeem, M. Rizwan

4:40 ENFL **212.** Element strategy for new nanomaterials. **H. Kitagawa**

5:00 ENFL **213.** Semitransparent DSSC cathodes based on thin layer tetraaminophthalocyanine polymers. **K.J. Klunder**

5:20 ENFL **214.** Organic-inorganic hybrid materials for gas separation applications: Do MOFs really have any future for practical gas separations? **S.K. Elsaidi**, M.H. Mohamed, P.K. Thallapally, B. Space, M.J. Zaworotko

5:40 ENFL **155.** Method for direct measurement of adsorbed gas redistribution in metal-organic frameworks. **Y. Chen**, H. Zhou

Nanotechnology: Delivering on the Promise

Bridging the Gap to a Thriving US Marketplace

Sponsored by PRES, Cosponsored by AGFD, AGRO, ANYL, CARB, CCPA, CCS, CHAS, COLL, COMSCI, CORP, ENFL, HIST, I&EC, IAC, MPPG, PMSE, POLY, SCHB and SOCED

Sustainability in the 21st Century: Optimizing Complex Interdependent Systems

Sponsored by SOCED, Cosponsored by CELL and ENFL

‡ *Cooperative Cosponsorship*

MONDAY EVENING

Section A

Colorado Convention Center
Halls C/D

Sci-Mix

A. Park, *Organizer*

8:00 - 10:00
19, 31, 54, 83, 106, 124-125, 127, 144, 157, 169, 178, 183, 192, 200. See previous listings.
233, 420, 423, 445, 450, 464, 467, 476, 491-492. See subsequent listings.

TUESDAY MORNING

Section A

Colorado Convention Center
Mile High Ballroom 4A

Nanomaterials for Solar Energy Conversion & Storage

Cosponsored by MPPG‡

Y. H. Hu, R. T. Koodali, Y. Wu, *Organizers*
Y. H. Ng, N. Wu, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENFL **215. Award Address** (ACS Award for Team Innovation sponsored by ACS Corporation Associates). Multidisciplinary approach toward the design, development, and long term performance estimation of the Dow POWERHOUSE™ Building Integrated Photovoltaic (BIPV) product. **A.A. Namjoshi**, R. Gaston, J.R. Keenihan, S.G. Pisklak, J. Reese

8:35 ENFL **216.** Challenge of interfacing the tandem design for water splitting. **I. Chorkendorff**

9:05 ENFL **217.** Tailoring the nature of band gap using passivation of silicon quatum nanostrucutres. **W.M. Hassan**, A. Verma, R. Nekovei, M.M. Khader, M.P. Anantram

9:25 ENFL **218.** Atomic layer deposition for interfacial engineering of solar energy conversion devices. **N.P. Dasgupta**

9:45 Intermission.

10:00 ENFL **219.** 1D core-shell semiconductor nanowire arrays for photoelectrochemical water splitting. **B. Liu**

10:30 ENFL **221.** Role of reduced graphene oxide in promoting the properties of 1D oxide – 0D chalcogenide nanostructures. **V.R. Subramanian**

11:00 ENFL **220.** Photo- and electrochemical water oxidation over mesostructured cobalt oxides. **H. Tuysuz**

11:30 ENFL **222.** Multiscale designing of solar-driven photocatalysts. **G. Liu**, P. Niu, Y. Xie, Y. Yang, C. Zhen, H. Cheng

Section B

Colorado Convention Center
Mile High Ballroom 4B

Materials & Interfaces in Lithium Batteries & Beyond

Li-S & Characterization

A. A. Gewirth, A. Manivannan, D. Wang, *Organizers*
Y. Shao, *Organizer, Presiding*
Y. Cheng, *Presiding*

8:00 Introductory Remarks.

8:05 ENFL **223.** Lithium-sulfur batteries: Novel electrode structures and cell configurations. **A. Manthiram**

8:35 ENFL **224.** X-ray absorption spectroscopy of lithium sulfur battery reaction intermediates. **N.P. Balsara**, K. Wujcik, T. Pascal, D. Prendergast

9:05 ENFL **225.** Li metal anodes and sulfur cathodes through nanomaterial design. **G. Zheng**, Y. Cui

9:35 ENFL **226.** Challenges in high-energy Li-sulfur batteries: Failure mechanism on lithium metal anode. **D. Lv**, Y. Shao, Q. Li, S. Ferrara, W.D. Bennett, G.L. Graff, B. Polzin, J. Zhang, W. Henderson, J. Liu, J. Xiao

9:55 Intermission.

10:05 ENFL **227.** Direct correlation of electrochemical properties with structural and chemical evolution of electrode materials in rechargeable batteries. **C. Wang**

10:35 ENFL **228.** Development of nanoscale planar electrochemical devices and applications. **L. Hu**

11:05 ENFL **229.** In situ/operando XAS studies of electrochemical systems. **F. Jiao**

11:35 ENFL **230.** Thin-film lithiation structural transformations imaged in situ by liquid cell transmission electron microscopy. **A.J. Leenheer**, K.L. Jungjohann, K.R. Zavadil, J.P. Sullivan, C.T. Harris

11:55 Concluding Remarks.

Section C

Colorado Convention Center
Mile High Ballroom 3C

ENFL Distinguished Researcher Award: Symposium in Honor of James Burrington

J. Bradzil, *Organizer, Presiding*

8:00 ENFL **231.** Acid-base and catalytic properties of mixed oxides in heterogeneous selective oxidation reactions: description of active sites. **J.C. Vedrine**

8:30 ENFL **232.** Managing the oxocapacity of catalysts by using adapted reactor. A. Löfberg, P. Sebastien, **E. Bordes-Richard**

9:00 ENFL **233.** Selective oxidation by gold catalysts. **H.H. Kung**, Z. Wang, C. Wu, N. Mashayekhi, X. Hou, M.C. Kung

9:30 ENFL **234.** Vapor-phase cyclohexene epoxidation by H_2O_2 over mesoporous TS-1. S. Kwon, R. Snurr, **P.C. Stair**

10:00 Intermission.

10:10 ENFL **235.** Homogeneous and heterogeneous catalytic selective oxidation of alkanes: Looking backwards and forwards. **J.A. Labinger**

10:40 ENFL **236.** Selective oxidation on a fuel cell anode means going all the way to carbon dioxide. **A.B. Anderson**, H.A. Asiri

11:10 ENFL **237.** Oxidative dehydrogenation of ethane to ethylene. **A.M. Gaffney**

11:40 ENFL **238.** Cationic polymerization using heteropolyacid salt catalysts. **J.R. Johnson**, J.D. Burrington, J.K. Pudelski

Section D

Colorado Convention Center
Mile High Ballroom 3B

Two-Dimensional Materials for Energy & Fuel

V. Barone, Y. Lin, *Organizers*
G. Yu, *Organizer, Presiding*
L. Hu, *Presiding*

8:00 ENFL **239.** Understanding the adsorption on 2D materials with applications to lithium-ion batteries and electrochemical hydrogen production. **Y. Liu**, B.I. Yakobson

8:40 ENFL **240.** Exploring 2D materials for energy storage via combination of computations and experiments. **Z. Zhou**

9:10 ENFL **241.** Theoretical design of MoO3-based nanodevices and high-rate lithium ion battery electrodes. **F. Li**

9:30 Intermission.

9:45 ENFL **242.** Energy storage properties of 2D materials. J. Ko, G. Muller, V. Augustyn, **B. Dunn**

10:25 ENFL **243.** Metal oxide nanosheets for energy applications. **R.D. Robinson**

10:55 ENFL **244.** 2D phenomena in materials for metal-oxygen batteries. **D. Siegel**

11:25 ENFL **245.** Composite of Co_3O_4 hollow nanoparticles and Co organic complexes highly dispersed on N-doped graphene as cathode catalyst for rechargeable Li-O_2 batteries. **Z. Zhang**

Section E

Colorado Convention Center
Mile High Ballroom 4C

C1 Chemistry

Methane Activation

Cosponsored by MPPG‡

N. Kumar, J. J. Spivey, *Organizers, Presiding*

8:00 ENFL **246.** Thermal hydrogen-atom transfer from methane: A mechanistic exercise. **H. Schwarz**, M. Schlangen

8:40 ENFL **247.** Dry reforming of methane on NiO-MgO-ZrO_2 catalyst. J. Titus, T. Roussière, G. Wasserschaff, S. Schunk, A. Milanov, E. Schwab, **R. Glaeser**

9:00 ENFL **248.** Impact of SO_2 and H_2S adsorption on methane steam reforming on Ni-YSZ compared to Ni-alumina. **W.S. Jablonski**, S. Villano, A.M. Dean

9:20 ENFL **249.** Oxidative coupling of methane over microstructured Mn/Na_2WO_4/SiO_2 catalysts. Y. Dusova, A. Leba, A.K. Avci, **R. Yildrim**

9:40 ENFL **250.** Facet-controlled CeO_2 nanocrystals for oxidative coupling of methane. **Y. Zhu**

10:00 Intermission.

10:10 ENFL **251.** Pt on Fecralloy for methane to syngas at high pressure. S. Jazayeri, **D. Boffito**, C. Neagoe, G.S. Patience

10:30 ENFL **252.** First-principles microkinetic modeling of methane oxidation over PdO(101). **M.C. Van den Bossche**, H. Gronbeck

10:50 ENFL **253.** Modeling methane dehydroaromatization (MDA) in catalytic packed-bed membrane reactors. C. Karakaya, **B. Kee**, H. Zhu

11:10 ENFL **254.** Kinetic modeling of methane dehydroaromatization chemistry on Mo/Zeolite catalysts in packed-bed reactors. **C. Karakaya**, H. Zhu, R. Kee

11:30 ENFL **255.** Zeolite-supported indium-molybdenum oxides as efficient catalysts for methane dehydroaromatization. **Y. Zhang**, C.K. Narula

DOE Nanoscience Research Centers

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TUESDAY AFTERNOON

Section A

Colorado Convention Center
Mile High Ballroom 4A

Nanomaterials for Solar Energy Conversion & Storage

Cosponsored by MPPG‡

R. T. Koodali, Y. H. Ng, Y. Wu, *Organizers*
Y. H. Hu, N. Wu, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 ENFL **256.** Semiconductor nanowires for artificial photosynthesis of value-added chemicals. **P. Yang**

1:35 ENFL **257.** Photocatalytic water splitting and CO_2 Fixation over surface-modified semiconductors under visible light. **K. Maeda**

2:05 ENFL **258.** Enhanced photocatalysis on TiO_2-Passivated III-V compounds for water splitting and CO_2 reduction. **S. Cronin**, J. Qiu, G. Zeng

2:35 ENFL **259.** Mesoporous metal oxides prepared by an aerosol-spray-pyrolysis method for photocatalytic hydrogen evolution. **C. Tsung**

3:05 Intermission.

3:05 ENFL **260.** Photo-driven directional assembly of inorganic light absorber-nanocluster catalyst units for CO_2 reduction and H_2O oxidation. W. Kim, **H.M. Frei**

3:35 ENFL **261.** Constructing hybrid photocatalysts for efficient CO_2-to-fuel conversion. C. Liu, T. Jin, M.E. Louis, T. Fenton, **G. Li**

4:05 ENFL **262.** Solar cells, solar fuels, and solar batteries based on dye-sensitized photoelectrodes. **Y. Wu**

4:35 ENFL **263.** Dynamic tuning of molecular optical properties using plasmonic photothermal effects. **H. Gao**

Section B

Colorado Convention Center
Mile High Ballroom 4B

Materials & Interfaces in Lithium Batteries & Beyond

Na-ion & Supercapacitors

A. A. Gewirth, A. Manivannan, D. Wang, *Organizers*
Y. Shao, *Organizer, Presiding*
Y. Cheng, *Presiding*

1:00 Introductory Remarks.

1:05 ENFL **264.** Novel copper-based layered oxide cathode for room-temperature sodium-ion batteries. **Y. Hu**, S. Xu, L. Mu, Y. Li, L. Chen

1:35 ENFL **265.** Investigating the synergetic energy storage mechanism of advanced SnS_2-rGO composite anode for Na-ion batteries. **S. Meng**, C. Ma

2:05 ENFL **266.** Direct conversion of CO_2 to 3D flower-structured graphene for supercapacitors with ultrahigh areal capacitance. **Y.H. Hu**

2:35 ENFL **267.** In situ tem study on sodiation/desodiation cycles of individual ZN_4SB_3 nanowires. **R. Shahbazian Yassar**

3:05 ENFL **268.** Positive impacts of defects and amorphous nature of electrodes for Li-ion and Na-ion batteries. **G. Cao**

3:35 Intermission.

3:45 ENFL **269.** Scalable syntheses of advanced materials for energy storage. C. Bommier, W. Luo, V. Raju, X. Wang, Z. Xing, **X. Ji**

4:15 ENFL **270.** Understanding electric double-layer capacitors. **D. Jiang**

4:45 ENFL **271.** Functional ordered porous materials for high-performance supercapacitors and hybrid supercapacitors. **J. Lee**

5:15 ENFL **272.** Withdrawn.

5:35 ENFL **273.** New platform of porous carbon structure for high energy supercapacitors. **S. Zhang**, N. Pan

5:55 Concluding Remarks.

Section C

Colorado Convention Center
Mile High Ballroom 3C

Advances in the Chemistry of Energy and Fuels

A. Park, X. Wang, *Organizers*

2:00 - 4:00

ENFL **274.** Microwave-assisted synthesis of CZTS nanocrystals. **L. Tamasauskaite-Tamasiunaite**, G. Grinciene, B. Simkunaite-Stanyniene, L. Naruskevicius, A. Matuseviciute, V. Pakstas, A. Selskis, E. Norkus

ENFL **275.** Platform technology for the development of flexible batteries with composite carbon nanotube electrodes. **Z. Wang**, G.D. Benedetto, J.L. Zunino III, S. Mitra

ENFL **276.** Effects of heat treatment on the photocatalytic reduction of carbon dioxide on a TiO_2/functionalized reduced graphite oxide composite. **S.F. Rollins**, A. Castañeda, J.M. Andino

ENFL **277.** Alkyne passivation of aluminum nanoparticles via PIERMEN. **E.M. Lloyd**, B.J. Thomas, P.A. Jelliss, S.W. Buckner

ENFL **278.** Reactivity-structure based rate estimation rules for alkyl radical H-atom shift and alkenyl radical cyclization reactions. **K. Wang**, S. Villano, A.M. Dean

ENFL **279.** Electrochemical reduction of carbon dioxide using clathrate hydrates. **D. DeCiccio**, S. Ahn, S. Sen, F.M. Schunk, Y. Jiao, G.R. Palmore, C. Rose-Petruck

ENFL **280.** Selective oxidation of ethane with O_2 as oxidant on highly dispersed Mo-doped SBA-16 catalysts. **L. Kong**, Z. Zhao

ENFL **281.** Derived measurement of the enthalpy of vaporization of complex fuels using a variable pressure distillation curve approach. **S. Burke**, B. Windom

ENFL **282.** Azeotropic volatility behavior of hydrous ethanol gasoline mixtures. **B. Patz**, B. Windom

ENFL **283.** Enhancement of methane hydrate formation with the presence of tetrahydrofuran and surfactants. A. Siangsai, C. Singer, **P. Rangsunvigit**, B. Kitiyanana, S. Kulprathipanja

ENFL **284.** Effects of surfactants and treatments on co-based nanoparticles in Fischer-Tropsch synthesis reaction. **F. Gou**

ENFL **285.** Nickel sulfides as competent hydrogen evolution catalysts in water. **N. Jiang**, Y. Sun

ENFL **286.** Graphene-semiconductor 3D hybrid nanomaterials for sensitized solar cells. **C. Chaves-Villarreal**, T.M. Terse, A. Hernández-Valle, A.K. Mulchandani

ENFL **287.** Electroless deposition of Co-P-Mo alloys. **E. Norkus**, I. Stankeviciene, A. Jagminiene, B. Sebeka, J. Vaiciuniene, Z. Sukackiene, A. Selskis, L. Tamasauskaite-Tamasiunaite

ENFL **288.** Decoration of fiber structure cobalt with gold nanoparticles for application in fuel cells. A. Zabielaite, L. Tamasauskaite-Tamasiunaite, A. Balciunaite, S. Lichusina, I. Stalnioniene, A. Jagminiene, A. Zieliene, **E. Norkus**

ENFL **289.** Facile synthesis of exfoliated TiS_2 for all-solid-state lithium batteries. **D. Oh**, Y. Nam, K. Park, Y. Jung

ENFL **290.** Effect of fuel evaporation on the gas-phase kinetics in the mixing region of a hydrocarbon reformer. **S. Kim**, A.M. Dean

ENFL **291.** Improved molecular characterization of petroleum vacuum residues by FT-ICR MS analysis of their molecular distillation fractions. D.C. Palacio, J.P. Arenas, X. Ramírez, J.A. Orrego-Ruiz, A. Guzman, R. Cabanzo, **E. Mejía-Ospino**

ENFL **292.** Voltage charging enhances ionic conductivity in gold nanotube membranes. **P. Gao**

ENFL **293.** Withdrawn.

ENFL **295.** Synthesis of Pt@ZSM-5 nanoparticles within hierarchically porous ZSM-5/SBA-15 material with high hydrogenation property. **D. Gao**, X. Dai, Y. Yang, H. Sun, Y. Qin, A. Duan, H. Wang, **X. Zhang**

ENFL **297.** Platinum-cobalt nanocrystals prepared under different atmosphere for high catalytic performance of the methanol electro-oxidation. **Y. Qin**, X. Dai, Y. Yang, H. Sun, D. Gao, H. Wang, **X. Zhang**

ENFL **298.** Single device that converts carbon dioxide to energy via formate. **T. Vo, B. Biggs**, A. Miller, K. Purohit, J. Chanin, J. Haan

ENFL **299.** Multiscale experimental determination of cellulose pyrolysis reaction chemistry and transport phenomena. **C. Krumm**, A. Paulsen, P.J. Dauenhauer

ENFL **300.** Templated growth of multilayer graphene from cellulose for the fabrication of photovoltaic devices. **M. Dasari**

ENFL **301.** Synthesis of amphiphilic copolymers as additive for coal water slurry and their effect on rheology. Y. Chang, C. Cui, K. Huang, K. Meng, **X. Guo**, L. Li

ENFL **302.** How comb-type polymer additives affect the rheology of coal water slurry. C. Cui, J. Huang, T. Wang, J. Xu, L. Li, **X. Guo**

ENFL **303.** Recharge mechanisms of Mg-O_2 batteries. **J. Naruse**, G. Vardar, J. Smith, A.E. Sleightholme, C.W. Monroe, D.J. Siegel

ENFL **304.** Reaction of styrene epoxide with $H_2Os_3(CO)_{10}$. **J.M. Hahn**, M. Thomas, A. Bird

ENFL **305.** Chemical modifications of polybenzimidazoles leading to enhanced properties and performance. **K. Fishel**, G. Qian, B. Benicewicz

ENFL **306.** Investigations on the heat transfer security of endothermic hydrocarbon fuels in a heat-exchanger passage. **L. Yue**, W. Fang

ENFL **307.** Continuing investigations into the photodegradation of poly(methylmethacrylate)-capped aluminum nanoparticles. **W. Zeng**, P.A. Jelliss, S.W. Buckner

ENFL **308.** Withdrawn.

ENFL **309.** Electrochemical investigations of layered double hydroxides for electrocatalysis. **B. Weintraub**

ENFL **310.** Synthesis and evaluation of sustainable construction materials via mineralization of CO_2 from energy production cycles. **G. Gadikota**, X. Zhou, A. Park, S. Jang

ENFL **311.** Novel nanotube-like electrocatalysts of cobalt-tungsten carbonitride with highly active hydrogen evolution reaction. Z. Li, K. Du, **X. Dai**, H. Sun, Y. Yang, Y. Qin, D. Gao, X. Zhang

ENFL **312.** Photoelectrochemical reduction of CO_2 on Cu-Co_3O_4 nanotube arrays. **Q. Shen**, G. Zhao

ENFL **313.** Optical sensor for the detection FAME/biodiesel. R.A. Federico-Perez, J.K. Fong, **Z. Xue**

ENFL **314.** Investigation of nanocrystal heterostructures for photochemical hydrogen production. **A.N. Grennell**, M.B. Wilker, K.A. Brown, P.W. King, G. Dukovic

ENFL **315.** Tunable anatase-brookite TiO_2 bicrystalline for enhanced CO_2 photocatalytic reduction to fuels. **H. Zhao**, L. Liu, Y. Li

ENFL **316.** Catalyzed-cleavage of the bridged bond of coal model compounds over magnetic solid acid. C. Zhao, **W. Zhao**, K. Zhou, J. Fang, Y. Ren, J. Zhao, Q. Lei, Z. Zong, X. Wei

ENFL **317.** Emulsification and performance measurement of pyrolysis oil/diesel. J. Zhao, W. Zhao, Q. Lei, Y. Ren, **C. Zhao**, K. Zhou, J. Fang, Z. Zong, X. Wei

ENFL **318.** Catalytic ethanolysis of wheat stalk over coal cinder. **W. Zhao**, J. Fang, C. Zhao, Q. Lei, K. Zhou, Y. Ren, J. Zhao, Z. Zong, X. Wei

ENFL **319.** Effect of electrolyte anion on charge/discharge rate capability for organic radical battery. **T. Shimoyama**, T. Nishi, S. Iwasa

ENFL **320.** Sequential thermal dissolution of extraction residue from Zaozhuang bituminous coal. **S. Li**, X. Wei, T. Wang, C. Liu, J. Lv, Z. Zong

ENFL **321.** Poplar liquefaction in water-methanol co-solvent. **H. Yan**, Z. Zong, Z. Li, X. Wei

ENFL **322.** Catalytic hydroliquefaction of sawdust into high-value small-molecular chemicals over a novel magnetic solid superbase catalyst. X. Li, **Z. Zong**, W. Ma, X. Wei

ENFL **323.** Fuel properties of heptadecene isomers prepared via tandem isomerization-decarboxylation of oleic acid. **B.R. Moser**, R.E. Murray, K.M. Doll

ENFL **324.** Redox cofactor-aptamer complexes as possible catalysts for biofuel cells. **I. Emahi**, P.R. Gruenke, M.P. Mitchell, D.A. Baum

ENFL **325.** Improving sugar yields and reduce enzyme loadings of DDR (deacetylation and disc refining) process through Szego milling and its techno economic analysis. **X. Chen**, W. Wang, P. Ciesielski, S. Park, O. Trass, M.P. Tucker

ENFL **326.** Production of biodiesel from free fatty acids and triglycerides by reaction with high temperature methanol. **S. Thote**

ENFL **327.** Low-temperature catalytic reforming of volatiles from biomass pyrolysis. **J. Cao**, C. Song, X. Zhao, X. Wei

ENFL **328.** Optimum conditions to produce triacetonamine from fast pyrolysis of sewage sludge. X. Huang, **J. Cao**, **X. Zhao**, **X. Wei**

ENFL **329.** Molecular characteristics of a Chinese subbituminous coal using HPLC/MS. C. You, **X. Fan**, A. Zheng, X. Wei, Y. Zhao, J. Cao, W. Zhao, Z. Zong, J. Zhu, L. Chen

ENFL **330.** Two mass spectrometers for the analysis of high-temperature coal tar. J. Zhu, **X. Fan**, S. Wang, X. Wei, Y. Zhao, J. Cao, W. Zhao, Z. Zong, C. You, L. Chen

ENFL **331.** CO-liquefaction of Shenmu bituminous and white pine sawdust in sub- and supercritical ethanol. Y. Tian, Y. Zhao, H. Yang, S. Chen, **X. Fan**, J. Cao, Z. Zong, X. Wei

ENFL **332.** Electric-field assisted coating of nanoparticles for photon management nanostructures. **J. Gong**, N. Wu

ENFL **333.** From fields to fuels: Setting the target for oxygenates in liquid fuels. **M. Menart**, A. Robinson, R.M. Richards, J.W. Medlin, J. Hensley

ENFL **334.** Re-examination of $Na_3V_2(PO_4)_3$ as novel anode material for sodium-ion batteries. **Z. Jian**, Y. Sun, Y. Hu, X. Ji

ENFL **335.** Thermogravimetric analysis of nitrogen containing material. **A. Hopson**, A.C. Sacco, P. Ponnada, N.P. Rath, R.J. Moser, G.K. Balendiran

ENFL **336.** Aminodiborane: Structure, formation mechanism, and properties. H. Li, N. Ma, **X. Chen**, J. Zhao

ENFL **337.** TiO_2 conformal coating on carbon nanotubes as lithium-ion battery anode. **L. Yan**, M. Zhou, G. Chen, S. Deng, H. Luo

ENFL **338.** Control of methane and carbon dioxide concentrations in the effluent of a catalytic partial oxidation reactor for hydrogen production from natural gas. **A. Al-Musa**, S. Shabunya, M. Al-Johani, V. Martynenko, M. Al-Saleh, A. Al-Zahrani, V. Kalinin

ENFL **339.** Catalytic conversion of monosaccharides into 5-hydroxymethylfurfural using aluminum complexes supported by bidentate phenoxy-amine ligands. **D.S. Saangonyo**, F.T. Ladipo

ENFL **340.** Mechanism of light hydrocarbons adsorption in metal organic framework from direct structural evidence. **A.M. Plonka**, X. Chen, D. Banerjee, W.R. Woerner, J.B. Parise

ENFL **341.** Excess thermopower and the theory of thermopower waves. J.T. Abrahamson, **S.G. Mahajan**, B. Sempere, M. Walsh, J.M. Forman, F. Sen, S. Sen, G.L. Paulus, Q. Wang, W. Choi, M.S. Strano

ENFL **342.** High pressure catalytic conversion of *n*-pentane on H-ZSM-5. **E.P. Schreiner**, S. Teketel, R.F. Lobo

ENFL **343.** Polydopamine-based carbon nanowires for wire-type supercapacitor. **W. Lee**, Y. Oh, Y. Lee, N. Kim

ENFL **344.** Ion mobility and PetroOrg software: Novel techniques for petroleomics investigations. E. Riches, Y. Corilo, R.P. Rodgers, M. O'Leary, **D. Stevens**

ENFL **345.** Cyclic voltammetric studies of the interactions between ferrocene mediators and glucose oxidase. **D. Bamper**, D.T. Glatzhofer

ENFL **346.** Exploring alfalfa hay's potential as an alternative non-food source of biofuel. **J.B. Beloy**, B. Gikonyo

ENFL **347.** Treatment of phenanthrene using sodium persulfate activated by modified diatomite. **C.K. Silva Rackov**, M.M. Vianna, O. Chiavone-Filho, C.A. do Nascimento

ENFL **348.** Organic oxygen transformation during pyrolysis of Baiyinhua lignite. **X. Zhao**, X. Feng, J. Cao, X. Wei

ENFL **349.** Nickel oxide/activated carbon composite electrodes for electrochemical capacitors. **X. Zhao**, S. Huang, **J. Cao**, **X. Wei**

ENFL **350.** Anomalous rising of input current induced in the transformer of inverter. **O. Ide**

ENFL **351.** Consideration of the cause of inverter noise called ringing. **O. Ide**

ENFL **352.** Characterristics of DC power output from an Inverter driven by sharp spike pulse. **O. Ide**

ENFL **353.** Pyrolysis of powdered examination gloves at 340 °C and 440 °C. **N. Hamidi**, M. Marcanikova, M. Ghalili, R. Massoudi

ENFL **354.** What's the "rub" with your salt: A case history of quality assurance for potassium chloride. **A. Evans**, A. Jensen, S. Nguyen, P. Carman, D.A. Castillo, M. Usie

ENFL **355.** What is this "stuff", where did it come from, and how can we get rid of it? Case histories of analytical laboratory methods and instrumental analyses applied to requests for identification of oilfield "unknown material" samples. **A. Evans**, A. Jensen, S. Sun, D. Wang, A. Koch, M. Wilson, D.A. Castillo

ENFL **356.** Temperature and injection gas composition influence on CO_2 miscibility by interfacial tension measurement. **Q. Shang**, S. Xia, M. Shen, P. Ma

ENFL **357.** Treated bio-oils upgraded in a fixed-bed continuous reactor with sulfided CoMo/ γ -Al_2O_3 catalysts. Y. Luo

ENFL **358.** Improved characterization and fractionation of vacuum residues of heavy crude oils using supercritical fluid extraction. **A.Y. Leon Bermudez**, A. Guzman, L.J. Hoyos, E. Mejía, O. Corredor, D. Laverde

ENFL **359.** Arid lands biofuel. **B.P. Neupane**

ENFL **360.** Synthesis of multiwalled carbon nanotubes doped titania for desulfurization of model fuel. T.A. Saleh, **M.N. Siddiqui**

ENFL **361.** Porous membrane assisted-solvent bar microextraction for elemental sulfur in crude oil. I.M. Al-Zahrani, B. Chanbasha, **M.N. Siddiqui**

ENFL **362.** PbS and PbSe quantum dot solar cells: Ion exchange synthesis and metal halide surface passivation for high efficiency devices. R. Crisp, J. Zhang, J. Gao, A. Marshall, D. Kroupa, E. Miller, M.C. Beard, **J. Luther**

ENFL **363.** Hierarchical nanomaterial electrodes for energy storage. **L. Mai**, X. Xu, L. Xu, Q. Wei

ENFL **364.** Nonaqueous all-cobalt redox flow battery using 1,10-phenanthrolinecobalt(II) hexafluorophosphate as the active species. Y. Li, **X. Xing**

ENFL **365.** Photons to formate: Solar driven conversion of CO_2 to solar fuels. **H. Pan**, Y. Zou, M.D. Heagy

ENFL **366.** Ag nanoparticles modified photoelectode for photocatalytic water splitting. **X. Zhang**

ENFL **367.** CdS–mesoporous ZnS core–shell particles of Type I structure for efficient and stable photocatalytic hydrogen evolution under visible light. **Z. Yu**

ENFL **368.** Investigation of the morphology evolution of nanoscale Cu_3Sb electrodes during electrochemical cycling via ex situ electron microscopy. **E. Jackson**, A.L. Prieto

ENFL **369.** $AFePO_4NO_3$ (A = Li, Na): Nitratophosphate as a new family of cathode materials for alkali-metal-ion batteries. **H. Yaghoobnejad Asl**, A. Choudhury

ENFL **370.** Spectroelectrochemical studies of charge transfer processes in stable nitroxyl radical-containing polymers. **B.K. Hughes**, W. Braunecker, J.C. Johnson, A. Ferguson, T. Gennett

ENFL **371.** Molecular level insight into the lithiation mechanism of RuO_2 and the implication for its use as lithium-ion battery electrode material. **A. Hassan**, B.R. Ramachandran, C.D. Wick, A. Navulla, L. Meda

ENFL **372.** Screening of lithium oxygen cathode 3D composite nanonetworks enabled by M13 phage directed synthesis. **L. Tadesse**, J. Ohmura, D. Oh, A.M. Belcher

ENFL **373.** Design and synthesis of direct growth of nanosized nickel oxides on stainless steel substrates as anode in lithium ion battery. L. Meda, A. Navulla, **C. Arnold**

ENFL **374.** Catalytically activated palladium@platinum nanowires for accelerated hydrogen gas detection. **X. Li**, Y. Liu, J.C. Hemminger, R.M. Penner

ENFL **375.** Steam-biogas reforming over a metal-foam-coated (Pd-Rh)/($CeZrO_2$-Al_2O_3) catalyst compared with pellet type alumina-supported Rh, Ru and Ni catalysts. P.S. Roy, C.S. Park, A. Raju, **K. Kim**

ENFL **376.** Water soluble charged nanoparticles featuring core-shell morphology for energy harvesting. **H.P. Rathnayake**, J. Ferguson, A. Braun

ENFL **377.** Co-reaction of methanol and ethylene over MFI and CHA zeolitic catalysts. **Q. Zhu**

ENFL **378.** Product distribution of polyoxymethylene dimethyl ethers from methanol and formaldehyde. **D. Liu**

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Section D

Colorado Convention Center
Mile High Ballroom 3B

Two-Dimensional Materials for Energy & Fuel

L. Hu, Y. Lin, *Organizers*
V. Barone, *Organizer, Presiding*
G. Yu, *Presiding*

1:00 ENFL **379.** Graphene based supercapacitors for integrated energy storage. **R.B. Kaner**

1:40 ENFL **380.** New charge storage mechanism in graphene oxide based solid state capacitors. Q. Zhang, K. Scrafford, M. Li, Z. Cao, Z. Xia, P.M. Ajayan, **B. Wei**

2:20 ENFL **381.** Modified porous graphene and its use in electrode reaction study. **Y. Zhu**, K. Liu, Y. Chen

2:50 ENFL **382.** SnO_2 - graphene dual aerogels as high rate sodium lithium ion battery anodes. **Z. Li**, D. Mitlin

3:10 Intermission.

3:25 ENFL **383.** Carbon nanomaterials in metal oxide based electrodes for supercapacitors. **J. Liu**, Y. Cheng, G. Lee, H. Zhang

4:05 ENFL **384.** Lithium battery applications of graphene materials. **W. Ren**, F. Li, H. Cheng

4:35 ENFL **385.** Lithium adsorption and diffusion in SnS_2 bulk, bilayer, monolayer, and nanoribbon: A computational investigation. **K. Tu**, Z. Chen

Section E

Colorado Convention Center
Mile High Ballroom 4C

C1 Chemistry

Methane Activation

Cosponsored by MPPG‡

N. Kumar, J. J. Spivey, *Organizers, Presiding*

1:00 ENFL **386.** Continuous oxidation of methane to oxygenates under mild reaction conditions using ZSM-5 catalysts. J. Xu, R.D. Armstrong, S.J. Freakley, S.H. Taylor, **G. Hutchings**

1:40 ENFL **387.** Size-and support-dependent electronic and catalytic properties of size selected cluster catalysts on methanation of CO: A combined GIXAS, GISAXS and TPRx study. **S. Lee**, B. Lee, S. Seifert, R.E. Winans, S. Vajda

2:00 ENFL **388.** Structure-performance relationship in the design of Ru/TiO_2 catalyst for CO_2 methanation. **A. Kim**, C. Sanchez, C. Sassoye, D. Debecker

2:20 ENFL **389.** Carbon dioxide hydrogenation into methanol over promoted Cu/Zn-based catalysts. **R.S. Monteiro**, P. Coutinho, J. Miranda, C.J. Mota

2:40 Intermission.

2:50 ENFL **390.** Phase equilibria and characterization of cyclopentane - methane binary hydrates. **P. Warrier**, M. Khan, Z.T. Ward, Y. Yang, C.A. Koh

3:10 ENFL **391.** Gas hydrate phase equilibrium predictions for cyclopentane containing gas mixtures with optimized Kihara parameters. M.N. Khan, **P. Warrier**, C.J. Peters, C.A. Koh

3:30 ENFL **392.** Generation of chemicals from natural gas in a fuel cell. **O.A. Marina**, B. Kirby, C. Coyle, J. Frye, D. Edwards, L. Pederson, C. Freeman, J. Stevenson

3:50 ENFL **393.** Electrocatalytic reduction of CO_2 in water to $CO+H_2$ syngas mixtures. **P. Kang**, Z. Chen, A. Nayak, T.J. Meyer

4:10 ENFL **394.** On the route to commercialization of a CO_2 electrolyzer: Lessons learned from an industry effort to fight climate change. **T.S. Matthews**, M. Kaplun, Z. Liu, Q. Chen, R. Kutz, S. Luopa, K. Lewinski, R. Masel

TUESDAY EVENING

Energy and Materials

Sponsored by POLY, Cosponsored by ENFL‡ and PMSE

WEDNESDAY MORNING

Section A

Colorado Convention Center
Mile High Ballroom 4A

Nanomaterials for Solar Energy Conversion & Storage

Cosponsored by MPPG‡

Y. H. Hu, R. T. Koodali, N. Wu, *Organizers*
Y. H. Ng, Y. Wu, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENFL **395.** Engineered quantum dots for solar energy conversion. **V.I. Klimov**

8:45 ENFL **396.** Withdrawn.

9:05 ENFL **397.** Chemically modifying quantum dot surfaces to improve solar cell performance. **A. Marshall**, A.J. Nozik, M.C. Beard, J. Luther

9:25 ENFL **398.** Resolving carrier multiplication and charge transport in quantum dot solids with ultrafast transient photocurrent. **A.F. Fidler**, J. Gao, G. Chen, W. Koh, V.I. Klimov

9:45 Intermission.

10:00 ENFL **399.** Efficient harvesting of solar energy using quantum-dot luminescent solar concentrators. **J.M. Pietryga**, H. Li, T.A. Baker, J. Lim, H. McDaniel, V.I. Klimov

10:30 ENFL **400.** Field-effect transistors and light-emitting diodes with low-toxicity I-III-VI_2 quantum dots. **H. McDaniel**, S. Draguta, W. Bae, J. Lim, Y. Park, J.M. Pietryga, V.I. Klimov

10:50 ENFL **401.** Auger up-conversion in engineered heterostructured quantum dots for applications in solar energy conversion. **N.S. Makarov**, Q. Lin, K. Velizhanin, V.I. Klimov

11:10 ENFL **402.** Synthesis and analysis of CdTe quantum dot solar cells. K.M. McHenry, E. Kim, **A.L. Asunskis**, D.J. Asunskis

11:30 ENFL **403.** Highly ordered CdTe nanotube arrays for solar cells through patterned electrodeposition. **W.P. Liyanage**, M. Nath

Section B

Colorado Convention Center
Mile High Ballroom 4B

Materials & Interfaces in Lithium Batteries & Beyond

Li-ion

A. A. Gewirth, A. Manivannan, D. Wang, *Organizers*
Y. Shao, *Organizer, Presiding*
J. Esbenshade, *Presiding*

8:00 Introductory Remarks.

8:05 ENFL **404.** All-solid-state polymer electrolyte with plastic crystal materials for secondary lithium-metal batteries. **F. Ding**

8:35 ENFL **405.** High-energy bulk-type all-solid-state lithium batteries using sulfide solid electrolyte. Y. Nam, D. Oh, K. Park, K. Lee, S. Lee, **Y. Jung**

9:05 ENFL **406.** Controllable uniform crystallization towards improved performance in glass-ceramic $Li_{1+x}AlxGe_{2-x}(PO_4)_3$ electrolyte membrane. **A. Vyalikh**, V. Vizgalov, A. Sergeev, L.A. Trusov, E. Brendler, L.V. Yashina, D. M. Itkis

9:25 ENFL **407.** High ionic conductivity of flexible polymer-based electrolyte with low porosity. **W. Zhao**

9:45 Intermission.

9:55 ENFL **408.** High voltage cathodes for advanced lithium-ion batteries. **J. Nanda**, R.E. Ruther, S. Martha, H. Zhou

10:25 ENFL **409.** Investigation of atomic/molecular layer deposition coatings for Li-ion electrodes. **C. Ban**, D. Piper, Y. He, J. Travis, A.M. Wise, J. Weker, S. Son, J. Zhang, M. Toney, C. Wang, S. Lee, S.M. George

10:55 ENFL **410.** Iron borophosphates as novel cathode for alkali-ion battery. **A. Choudhury**, H. Yaghoobnejad Asl

11:15 ENFL **411.** Guiding principles for next-generation batteries from theoretical and experimental studies of $LiMn_2O_4$. **M. Young**, A. Holder, H. Dieter-Schnabel, S.M. George, C. Musgrave

11:35 ENFL **412.** Data-driven review of battery materials: Performance and resource considerations. **L. Ghadbeigi**, J. Harada, T. Sparks

11:55 Concluding Remarks.

Section C

Colorado Convention Center
Mile High Ballroom 3C

12th International Symposium on Heavy Oil Upgrading, Production & Characterization

Fouling and Asphaltenes

Cosponsored by MPPG‡

J. J. Adams, C. Mesters, D. Mitlin, *Organizers*
J. F. Schabron, *Organizer, Presiding*

8:00 ENFL **413.** Thiophene mitigates high temperature fouling of metal surfaces in oil refining. **D. Mitlin**

8:45 ENFL **414.** Protocol for diagnosing and predicting petroleum fouling in upstream and downstream operations. **J.J. Adams**, J.F. Schabron

9:15 ENFL **415.** Influence of acid chemistry on bitumen viscosity. **V. Gonzalez**, A. de Klerk, S. Yang, V. Prasad

9:45 ENFL **416.** Cold flow behavior of waxy crude oil under elevated pressure. T. Wang, J. Xu, H. Zhao, L. Li, **X. Guo**

10:15 Intermission.

10:15 ENFL **417.** Asphaltenes diffusion into catalysts under hydroprocessing conditions. **F. Gaulier**, J. Barbier, B. Guichard, D. Espinat

10:45 ENFL **418.** Role of asphaltenes in oil and water emulsions. **J.J. Adams**, J.F. Schabron

11:15 ENFL **419.** Catalytic cracking of cold lake bitumen and Fischer-Tropsch wax mixtures: Coke suppression and viscosity analysis. **X. Liu**

Section D

Colorado Convention Center
Mile High Ballroom 3B

Two-Dimensional Materials for Energy & Fuel

V. Barone, L. Hu, *Organizers*
G. Yu, *Organizer, Presiding*
Y. Lin, *Presiding*

8:00 ENFL **420.** Efficient photocurrent generation in heterostructures of 2D layered materials. **X. Duan**

8:40 ENFL **421.** Hybrid layer materials for energy conversion and storage. **Y.H. Hu**

9:10 ENFL **422.** Engineering the catalysis at 2D materials for solar water splitting. **L. Cao**

9:40 ENFL **423.** Earth-abundant 2D materials as high performance electrocatalysts for photoelectrochemical energy conversion. **S. Jin**, Q. Ding

10:20 Intermission.

10:35 ENFL **424.** 2D structuring of photocatalytic bismuth-based metal oxides. **T.T. Salguero**, T. Pope, G. Neher, A. Bruning

11:05 ENFL **425.** Theoretical and computational studies of graphene-based materials for use as transparent conducting electrodes in solar cells. **G.J. Martyna**

11:25 ENFL **426.** Atomically thin transition metal disulfides on silicon for high performance water splitting photocathodes. **S. Choi**, K. Kwon, T. Kim, K. Hong, S. Lee, S. Kim, H. Jang

Section E

Colorado Convention Center
Mile High Ballroom 4C

C1 Chemistry

CO_2 Conversion

Cosponsored by MPPG‡

N. Kumar, J. J. Spivey, *Organizers, Presiding*

8:00 ENFL **427.** Utilization of CO_2 as feedstock in C_1 chemistry. **H. Düdder**, L. Chew, M. Muhler

8:40 ENFL **428.** Kinetics of methanol synthesis from carbon dioxide and hydrogen. **K. Kobl**, L. Angelo, Y. Zimmermann, K. Parkhomenko, **A. Roger**

9:00 ENFL **429.** Dihydropteridine/pteridine as a $2H^+/2e^-$ redox mediator for the catalytic reduction of CO_2 to methanol via hydride-proton transfer. **C. Lim**, Y. Kuo, A. Holder, J.T. Hynes, C. Musgrave

9:20 ENFL **430.** Catalysts for the CO_2 recycling into methanol. **L. Angelo**, K. Kobl, Y. Zimmermann, K. Parkhomenko, **A. Roger**

9:40 ENFL **431.** Liquid phase CO_2 hydrogenation to methanol and dimethyl ether using heterogeneous cascade catalysis. **Y. Chen**, S. Choi, L.T. Thompson

10:00 Intermission.

10:10 ENFL **432.** Catalysis for the conversion of CO and CO_2 to fuels and chemicals. **A.T. Bell**

10:50 ENFL **433.** Nanocomposite photocatalysts: Conversion of CO_2 to fuel. **S. Hunyadi Murph**, H. Sessions, Y. Kun, Y. Zhao

11:10 ENFL **434.** High efficient formate production by low temperature hydrogenation of amine captured CO_2 over Pd catalyst. **H. Lin**, J. Su

11:30 ENFL **435.** Modeling the $HCOOH/CO_2$ electrochemical couple: When details are key. **S.N. Steinmann**, C. Michel, P. Sautet

WEDNESDAY AFTERNOON

Section A

Colorado Convention Center
Mile High Ballroom 4A

Nanomaterials for Solar Energy Conversion & Storage

Cosponsored by MPPG‡

Y. H. Hu, R. T. Koodali, Y. H. Ng, *Organizers*
N. Wu, Y. Wu, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 ENFL **436.** Efficiency limiting factors in light-driven H_2 generation using multicomponent semiconductor-metal colloidal nanorod heterostructures. **T. Lian**

1:35 ENFL **437.** Solar energy conversion and electrocatalysis using earth-abundant pyrite nanomaterials. **S. Jin**, M. Caban-Acevedo

2:05 ENFL **438.** Light-induced photoelectrochemical charging and discharging in metal oxide thin silm. **Y. Ng**

2:35 ENFL **439.** Surface optimization strategy for photoelectrochemical H_2 production. **T. Ogitsu**, W. Choi, B. Wood

3:05 Intermission.

3:15 ENFL **440.** Highly efficient visible light photocatalytic production of H2. **Y.H. Hu**, B. Han

3:45 ENFL **441.** Branched nanostructures for photoelectrochemical water splitting. **Y. Mao**

4:15 ENFL **442.** Designing a hybrid multifunctional material for CO_2 capture and photocatalytic conversion. L. Liu, **Y. Li**

4:45 ENFL **443.** Artificial photosystem I and II: Highly selective solar fuels and tandem photocatalysis. **Y. Ding**, I. Castellanos Beltran, V. Singh, P. Nagpal

Section B

Colorado Convention Center
Mile High Ballroom 4B

Materials & Interfaces in Lithium Batteries & Beyond

Li-ion

A. A. Gewirth, A. Manivannan, D. Wang, *Organizers*
Y. Shao, *Organizer, Presiding*
D. Lu, *Presiding*

1:00 Introductory Remarks.

1:05 ENFL **444.** Chemically integrated graphene/inorganic hybrid 2D materials as advanced energy storage electrodes. **G. Yu**

1:35 ENFL **445.** Methods for fabrication of highly conductive $Cu_{2-x}S$ nanoparticle electrode films through room-temperature processing. **R.D. Robinson**, O. Otelaja, D. Ha, T. Ly, H. Zhang

1:55 ENFL **446.** MXene nanosheets as promising anode materials for nonlithium-ion batteries. **Y. Xie**, Y. Dall'Agnese, M. Naguib, Y. Gogotsi, M.W. Barsoum, H.L. Zhuang, P. Kent

2:15 ENFL **447.** Iron fluoride based perovskite type cathode materials for Li/Na-ion batteries. **T. Yi**, W. Chen, L. Cheng, J. Lee, E. Chan, M. Doeff, K. Persson, J. Cabana

2:35 ENFL **448.** Managing the volume fluctuation of iron pyrite cathode in lithium ion batteries using polyacrylonitrile. **T. Yoder**, J.E. Cloud, L. Cain, M. Tussing, X. Li, Y. Yang

2:55 ENFL **449.** Controllably branched 3D electrodes as a test bed for investigating the effect of morphology on the performance of nanostructured V_2O_5 cathodes for Li ion batteries. **E. Gillette**, C. Liu, G. Rubloff, S. Lee

3:15 Intermission.

3:25 ENFL **450.** Electrolyte additives and interfacial mechanisms for high-capacity lithium-ion cells. **D. Abraham**, I. Shkrob

3:55 ENFL **451.** Electrolyte additives for high voltage $LiNi_{0.5}Mn_{1.5}O_4$ batteries. **S. Delp**, T.R. Jow

4:15 ENFL **452.** Novel organophosphine oxide based redox shuttle additives for 4V lithium ion batteries. **J. Huang**, N. Azimi, Z. Zhang, L. Zhang

4:35 ENFL **453.** Accelerating electrolyte discovery by high throughput screening. **L. Cheng**, R. Surendran Assary, X. Qu, A. Jain, S. Ong, N. Rajput, K. Persson, L.A. Curtiss

4:55 ENFL **454.** Catholyte material development for nonaqueous redox flow batteries. **J. Huang**, L. Su, M.S. Ferrandon, F. Brushett, A.K. Burrell, L. Zhang

5:15 ENFL **455.** Exploration of the effective location of surface oxygen defects in graphene-based electrocatalysts for the all-vanadium redox flow batteries. **M. Park**, J. Baek, J. Cho

5:35 Concluding Remarks.

Section C

Colorado Convention Center
Mile High Ballroom 3C

12th International Symposium on Heavy Oil Upgrading, Production & Characterization

Characterization

Cosponsored by MPPG‡

C. Mesters, D. Mitlin, J. F. Schabron, *Organizers*
J. J. Adams, *Organizer, Presiding*

1:00 ENFL **456.** Screening the adsorptive effect of metal oxides nanoparticles loaded activated carbons for sulfur compounds. **T. Saleh**, G.I. Danmaliki

1:30 ENFL **457.** Modifications to a novel method for the isolation of interfacial material from Athabasca bitumen: Characterization by FT-ICR mass spectrometry. **A.C. Clingenpeel**, J.M. Jarvis, W.K. Robbins, R.P. Rodgers

2:00 ENFL **458.** Study on transformation of dissolved organic matter in oilfield produced water during biodegradation using ultrahigh resolution mass spectrometry. **Z. Min**, D. Hao, Y. Hengye, S. Shanshan, Z. Zhongzhi

2:30 ENFL **459.** Molecular reconstruction of vacuum residue from molecular distillation cuts and FT-ICR-MS. **X.X. Ramirez**, **D.C. Palacio**, **J. Arenas**, **A. Guzman**, **J.E. Torres Macias**, **V. Kafarov**

3:00 Intermission.

3:30 ENFL **460.** Compositional model conversion of hydrocracking of vacuum gas oils using molecular reconstruction. **X.X. Ramirez**, **J.E. Torres Macias**, D.D. Perez

4:00 ENFL **461.** Application of an in-line viscometer to study methane hydrate slurry properties. **L. Chen**, C.A. Koh

4:30 ENFL **462.** Molecular characterization of dissolved organic matter in coal gasification waste water by negative ESI FT-ICR MS. **Y. Li**, D. Cui, C. Xu, Q. Shi

Section D

Colorado Convention Center
Mile High Ballroom 3B

Two-Dimensional Materials for Energy & Fuel

L. Hu, G. Yu, *Organizers*
Y. Lin, *Organizer, Presiding*
V. Barone, *Presiding*

1:00 ENFL **463.** Predicting materials for solar energy conversion ab initio spectroscopy of heterogeneous interfaces. **G.A. Galli**

1:40 ENFL **464.** Nanomechanics of bending 2D materials. **T. Dumitrica**

2:10 ENFL **465.** Thermoelectricity layer by layer. **M. Fornari**

2:40 Intermission.

2:40 ENFL **466.** Computational design of 2D nanomaterials toward carbon neutral energy. **Z. Chen**

3:10 ENFL **467.** Materials cartography: Representing and mining material space using structural and electronic fingerprints. **S. Curtarolo**

3:40 ENFL **468.** Interlayer commensurability and sliding in layered materials: The power of the registry index. **O. Hod**

4:10 ENFL **469.** Electronic and adsorption properties of 2D materials by density functional theory calculations. **V. Barone**

Section E

Colorado Convention Center
Mile High Ballroom 4C

C1 Chemistry

Syngas Chemistry

Cosponsored by MPPG‡

N. Kumar, J. J. Spivey, *Organizers, Presiding*

1:00 ENFL **470.** Syngas to fuel and chemicals via FTS: Reaction network and structure-performance for catalyst development. **Y. Sun**, **L. Zhong**, **T. Zhao**

1:40 ENFL **471.** Effect of support pretreatment on the performance of supported Fe Fischer-Tropsch catalysts. K. Keyvanloo, **W. Hecker**

2:00 ENFL **472.** Fe-based Fischer Tropsch synthesis of biomass-derived syngas: Effect of synthesis method. **K. Mai**

2:20 ENFL **473.** Experimental investigation of Fischer-Tropsch synthesis in a microchannel reactor. **X. Ying**, L. Zhang, H. Xu, Q. Luo, H. Zhu

2:40 ENFL **474.** Kinetics of main reaction and deactivation by carbon of cobalt Fischer-Tropsch catalyst. K. Keyvanloo, **W. Hecker**, C.H. Bartholomew

3:00 Intermission.

3:10 ENFL **475.** Supported iron catalyst for the direct conversion of synthesis gas to lower olefins. **K. De Jong**

3:50 ENFL **476.** Direct dimethyl ether synthesis from synthesis gas: The influence of methanol dehydration on methanol synthesis reaction. **F. Dadgar,** R. Myrstad, P. Pfeifer, A. Holmen, H.J. Venvik

4:10 ENFL **477.** Role of lanthanum oxide on cobalt-copper catalyst for the conversion of syngas to ethanol. **Z. Wang**, J.J. Spivey

4:30 ENFL **478.** Gas phase selective oxidation of olefins from a model synthesis gas stream. **S. Wiebe**, S. Villano, A.M. Dean

Computational Pyrolysis & Upgrading of Bio-Oils

Reaction Engineering

Sponsored by COMP, Cosponsored by ENFL‡ and MPPG

THURSDAY MORNING

Section A

Colorado Convention Center
Mile High Ballroom 4A

Nanomaterials for Solar Energy Conversion & Storage

Cosponsored by MPPG‡

Y. H. Hu, N. Wu, Y. Wu, *Organizers*
R. T. Koodali, Y. H. Ng, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENFL **479.** Preparation of Cu-Sb-Se nanoparticles through a hot-injection route. **D. Agocs**, A.L. Prieto

8:25 ENFL **480.** Spectroscopic and solution growth study of co-solvent effects on zinc oxysulfide buffer layers in earth abundant kesterite $Cu_2ZnSnSe_4$ solar cells. X. Steirer, R.L. Garris, J. Li, M. Reinisch, M.J. Dzara, P. Ndione, K. Ramanathan, I. Repins, G. Teeter, **C.L. Perkin**s

8:45 ENFL **481.** Understanding the role of chemical treatments and device architecture on ink-based CdTe solar cells. **R.W. Crisp**, M.G. Panthani, D.V. Talapin, J.M. Luther

9:05 ENFL **482.** Synthesis and characterization of mixed phase anatase TiO_2 and sodium-doped TiO_2(B) thin films by low pressure chemical vapour deposition (LPCVD). **Y. Chimupala**, G. Hyett, R. Simpson, R. Mitchell, R. Douthwaite, S.J. Milne, R.D. Brydson

9:25 ENFL **483.** Tunable nanostructured contact for cSi solar cells. **A.A. Dameron**, W. Nemeth, V.A. LaSalvia, A.G. Norman, D.L. Young, P. Stradins

9:45 Intermission.

9:55 ENFL **484.** Withdrawn.

10:15 ENFL **485.** 1D hematite nanostructures for photoelectrochemical water splitting. **D. Kim**, J. Lee, H. Jang

10:35 ENFL **486.** Enhanced photoelectrochemical water splitting on hematite thin film with ultrathin SiO_2 underlayer. **M. Kang**, Y. Kang

10:55 ENFL **487.** Electrical characterization of nanoscale material interfaces ranging from single nanorods to functional solar cell devices using scanning Kelvin probe microscopy. **S. Nanayakkara**, R. Ihly, M. Law, J. Luther

11:15 ENFL **488.** Systematic strategy to synthesize photoactive titanium metal-organic frameworks (MOFs). **L. Zou**, D. Feng, T. Liu, H. Zhou

Section B

Colorado Convention Center
Mile High Ballroom 4B

Materials & Interfaces in Lithium Batteries & Beyond

Li-ion

A. A. Gewirth, A. Manivannan, D. Wang, *Organizers*
Y. Shao, *Organizer, Presiding*
D. Lu, *Presiding*

8:00 Introductory Remarks.

8:05 ENFL **489.** Fundamental charge transfer processes in stable free-radical organic polymer systems. B.K. Hughes, T. Kemper, W. Braunecker, R. Larsen, D. Bobela, **T. Gennett**

8:25 ENFL **490.** Close packing of radicals in the stable radical polymer, PTMA. **D. Bobela**, B.K. Hughes, W. Braunecker, R.E. Larsen, T. Kemper, T. Gennett

8:45 ENFL **491.** In situ AFM nanoindentation and morphology analysis of mechanically constrained microfabricated silicon anodes. **C. Becker**, K. Strawhecker

9:05 ENFL **492.** Molecular structure and ion transport near electrode-electrolyte interfaces in lithium-ion batteries. **V. Lordi**, M. Ong, O. Verners, A.C. Van Duin, E. Draeger, J. Pask

9:25 ENFL **493.** Mitigating irreversible capacity losses from conducting carbon agents via surface modification. **S. Son**, D. Piper, J. Travis, Y. Lee, S.M. George, S. Lee, C. Ban

9:45 ENFL **494.** Investigating improved capacity retention of $AlPO_4$-coated Cu_2Sb anodes for lithium-ion batteries. **L.A. Kraynak**, E. Jackson, A.L. Prieto

10:05 ENFL **495.** Solvothermal route based in situ carbonization to Fe_3O_4@C as anode material for lithium ion battery. **G. Chen**, M. Zhou, H. Luo

10:25 Intermission.

10:25 ENFL **496.** Lithium-ion battery performance of perfluoropolether-based electrolytes. **D. Wong**, J.M. DeSimone, N.P. Balsara

10:45 ENFL **497.** Spectroscopic investigations of liquid-phase chemistry for advanced battery technologies. **J.L. Wheeler**, J.M. Porter

11:05 ENFL **498.** Computational studies of phosphoranimine electrolytes for Li system. **J.S. McNally**, J.R. Klaehn, E.J. Dufek, H.W. Rollins, M.K. Harrup

11:25 ENFL **499.** Lithium ion solvation and diffusion in bulk organic electrolytes from first principles molecular dynamic. **M. Ong**, V. Lordi, E. Draeger, J. Pask

11:45 Concluding Remarks.

Section C

Colorado Convention Center
Mile High Ballroom 3C

12th International Symposium on Heavy Oil Upgrading, Production & Characterization

Upgrading and Processing

Cosponsored by MPPG‡

J. J. Adams, C. Mesters, J. F. Schabron, *Organizers*
D. Mitlin, *Organizer, Presiding*

8:00 ENFL **500.** Catalytic heavy crude oil upgrading using natural gas. **H. Song**, A. Guo, C. Wu, D. Zhang, Y. Luan, L. Zhao

8:30 ENFL **501.** Visbreaking oils ands bitumen at 300 °C. **L. Yanez Jaramillo**, A. de Klerk

9:00 ENFL **502.** Low CO selectivity of copper-free ZnGaO catalysts used for dimethyl ether reforming to produce H_2. **S. Zhou**, M. Meng

9:30 Intermission.

9:45 ENFL **503.** Electromembrane extraction of sulfur compounds from crude oils. **B. Chanbasha**, I.M. Al-Zahrani, T. Maung

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‡ *Cooperative Cosponsorship*

10:15 ENFL **504.** Visbreaking of Fischer-Tropsch wax mixed with bitumen: Analysis of thermal behavior. **C. Melo Halmenschlager**, A. de Klerk

10:45 ENFL **505.** Effect of hydrogenation and acidity properties of NiMo/Al2O3 catalysts on the hydrodemetallization. **T. Liu**, Y. Zhou, Q. Wei, N. Wang, S. Ding, W. Zhou, L. Ju

Section D

Colorado Convention Center
Mile High Ballroom 3B

Two-Dimensional Materials for Energy & Fuel

Y. Lin, *Organizer*
V. Barone, G. Yu, *Organizers, Presiding*

8:00 ENFL **506.** Can graphene appear greener to galvanization industry? **V. Gadhamshetty**, **V.K. Upadhyayula**

8:20 ENFL **507.** Synthesis, chemical functionalization and electronic devices of 2D atomic and molecular crystals. **X. Wang**

8:50 ENFL **508.** How we look at graphene and graphene oxide: A material, a chemical, a tool. **Y. Shao**

9:20 Intermission.

9:30 ENFL **509.** Bulk graphene materials for energy applications. **Y. Chen**

10:00 ENFL **510.** Synthesis of 2D materials for energy applications. **S. Eichfeld**, J.A. Robinson

10:30 ENFL **511.** Synthesis and modification of holey graphene for energy storage. **Y. Lin**, J. Kim, J.W. Connell

11:00 ENFL **512.** NSF support of advanced materials for sustainable energy. **G.L. Rorrer**

11:30 Concluding Remarks.

Section E

Colorado Convention Center
Mile High Ballroom 4C

C1 Chemistry

Syngas Chemistry

Cosponsored by MPPG‡

N. Kumar, J. J. Spivey, *Organizers, Presiding*

8:00 ENFL **513.** Reactor design and catalysts testing for hydrogen production by methanol steam reforming for fuel cells applications. **F. Vidal Vazquez**

8:20 ENFL **514.** O-functionalized CNT mediated CO hydrodeoxygenation and chain growth. **K. Mondal**, S. Talapatra, M. Terrones, S. Pokhrel, C. Frizzel, B. Sumpter, V. Meunier, A. Elias

8:40 ENFL **515.** Metal organic mediated synthesis of highly stable and active FTO catalysts. V.P. Santos, **T. Wezendonk**, J. Delgado Jaén, A. Dugulan, A. Chojecki, S. Sina, A. Koeken, M. Ruitenbeek, T. Davidian, G. Meima, F. Kapteijn, M. Makkee, J. Gascon

9:00 ENFL **516.** Citrate-nitrate auto-combustion synthesis of Co-Ce mixed bulk oxides with different cobalt content for the oxidation of CO. **Z. Lin**, **J. Liu**, **Z. Zhao**, **K. Cheng**, **C. Xu**

9:20 Intermission.

9:30 ENFL **517.** Investigation of low temperature water-gas shift over MOF-assisted catalysts. O. Kavakli, **A.K. Avci**

9:50 ENFL **518.** Influence of coexisting metal oxide on the activity of copper catalyst for water-gas-shift reaction. **H. Yahiro**, K. Sagata

10:10 ENFL **519.** Homogeneous water-gas shift and production of methanol and ethanol from CO and H_2O without added H_2. **M.V. Mundschau**

10:30 ENFL **520.** Effect of Cu dopant in zeolite on catalytic properties and deactivation in carbonylation of dimethyl ether. **S. Huang**, X. Ma, H. Zhan, W. Huang

ENVR

Division of Environmental Chemistry

Souhail Al-Abed, *Program Chair*

OTHER SYMPOSIA OF INTEREST:

Applied Nanotechnology for Food & Agriculture *(see AGFD, Tue, Wed)*
Fundamental Research in Colloids, Surfaces & Nanomaterials *(see COLL, Sun)*
Analytical Chemistry of Natural Resources: Environmental Analysis *(see ANYL, Wed)*
Ask Dr. Safety: EH&S Support of Nanotechnology R&D *(see CHAS, Tue)*
Basic Research in Colloids, Surfactants & Nanomaterials *(see COLL, Sun, Wed, Thu)*

SOCIAL EVENTS:

Reception, 6:00 PM: Tue

BUSINESS MEETINGS:

ENVR Programs Planning Meeting, 2:00 PM: Sun
ENVR Long Range Planning Committee Meeting, 3:00 PM: Sun
ENVR Division Executive Committee Meeting, 7:00 PM: Sun

SUNDAY MORNING

Section A

Colorado Convention Center
Room 703

Green Chemistry and the Environment

Cosponsored by CEI and MPPG

S. O. Obare, *Organizer*
A. M. Balu, R. Luque, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 ENVR **1.** Aqueous chemistry in organic synthesis. **C. Len**

9:10 ENVR **2.** Deoxygenation and hydroisomerization of algae oils to hydrocarbon fuels. **J.S. Kruger**, E.D. Christensen, R.L. McCormick, P.T. Pienkos

9:30 ENVR **3.** Adipic acid production from lignin. **D.R. Vardon**, M. Franden, C. Johnson, E. Karp, M. Guarnieri, J. Linger, M. Salm, T.J. Strathmann, G. Beckham, G.A. Ferguson

9:50 ENVR **4.** Mechanism of lignin pyrolysis – from model compound to actual lignin. **V. Custodis**, P. Hemberger, J.A. Van Bokhoven

10:10 Intermission.

10:25 ENVR **5.** Use of green chemistry of chalcones synthesis. **E. Alarcón**, N. Romero, H. Aguilar, J.L. Terán, **A. Gómez Rivera**, L.F. Roa, **C. Lobato**, A. Escobar

10:45 ENVR **6.** Photochemical transformation of aliphatic-aromatic polyesters and its impacts to degradability. **M.A. Maurer-Jones**, M. Zumstein, M. Sander, K.P. Mc Neill

11:05 ENVR **7.** Transesterification of waste vegetable oil under simultaneous microwave and ultrasound Irradiations. **V. Gude**, **E. Martinez-Guerra**

11:25 ENVR **8.** Modified heterogeneous nickel catalysts for the production of chemicals and fuels from biodervied light olefins. **M. Menart**, J. Hensley, R.M. Richards

11:45 ENVR **9.** Overcoming production limitations of biosynthesis and tailoring rhamnolipid biosurfactant properties through chemical synthesis. **J.E. Pemberton**, R. Palos Pacheco, C. Coss, R. Polt

Section B

Colorado Convention Center
Room 705

Assessing Toxicity of Environmental Contaminants

Cosponsored by AGRO, CEI and MPPG‡

S. M. Uchimiya, B. Zhang, *Organizers*
X. Pan, J. Wang, *Organizers, Presiding*

8:00 Introductory Comments.

8:05 ENVR **10.** Measurement and evaluation of the rate of emission of semivolatile organic compounds from poly (vinyl chloride) sheets. M. Noguchi, **A. Yamasaki**

8:30 ENVR **11.** Environmental and human health risk assessment of amine emissions from post combustion power plants. **S. Manzoor**, A. Korre, S. Durucan, A. Simperler

8:55 ENVR **12.** Biological risk assessment of EDCs degradation by ozone. **L. Li**, K. Yeung

9:20 ENVR **13.** Assessing the uptake and effects of polycyclic aromatic hydrocarbons and their oxygenated derivatives on zebrafish using a metabolomics approach. **M.R. Elie**, R.L. Tanguay

9:45 ENVR **14.** Kinetic toxicity profile of haloacetonitriles, haloacetamides, and haloacetic acids. **Y. Yu**, D. Reckhow

10:10 Intermission.

10:25 ENVR **15.** Toxicity of silica nanomaterials: Effects of porosity and surface chemistry, and correlations with in vitro and in vivo results. **S.E. Lehman**, A. Wongrakpanich, A. Morris, A. Dodd, A.K. Salem, P.S. Thorne, V.H. Grassian, S.C. Larsen

10:50 ENVR **16.** Inhibition of thyroid hormone sulfotransferase activity by brominated flame retardants in a human choriocarcinoma cell line, BeWo. **C. Leonetti**, T. Neufeld, C. Butt, H.M. Stapleton

11:15 ENVR **17.** Identifying disinfection by-products (DBPs) capable of endocrine disruption through binding to the androgen receptor. **B.E. Holmes**, L. Smeester, R.C. Fry, H. Weinberg

11:40 ENVR **18.** Resistance measurements for Ar/O_2 and H_2O plasma modified SnO_2 nanomaterials for enhanced gas sensing. **E.P. Stuckert**, E.R. Fisher

Section C

Colorado Convention Center
Room 707

Chemical Processes at Environmental Interfaces

Chemistry and Imaging at Air/Liquid(Solid) Interfaces of Atmospheric Systems

Cosponsored by COLL

H. M. Ali, N. Kabengi, *Organizers*
H. A. Al - Abadleh, R. Z. Hinrichs, *Organizers, Presiding*

8:00 Introductory Remarks.

8:10 ENVR **19.** Role(s) of adsorbed water in the surface chemistry of oxide nanoparticles with atmospherically relevant molecules. **V.H. Grassian**

8:40 ENVR **20.** Effects of particle size, relative humidity, and sulfur dioxide on iron solubility in atmospheric particulate matter. **B.T. Cartledge**, A.R. Marcotte, A.D. Anbar, P. Herckes, B. Majestic

9:00 ENVR **21.** Complexation and dark degradation of catechol by iron(III): Bulk vs. surface chemistry. **H.A. Al - Abadleh**

9:20 ENVR **22.** Chemical imaging of atmospheric particles. **A. Laskin**

9:50 Intermission.

10:10 ENVR **23.** Ozone initiated heterogeneous oxidation of atmospheric organics. **Y. Liu**, C. Leng

10:40 ENVR **24.** Reactive uptake of biogenic volatile organic compounds on mineral aerosol substrates and their subsequent heterogeneous ozonolysis. **R.Z. Hinrichs**

11:00 ENVR **25.** Cascade oxidation of atmospheric aerosol dicarboxylic acids by gas-phase OH-radicals. S. Enami, M.R. Hoffmann, **A.J. Colussi**

11:30 ENVR **26.** Atmospheric oxidation of benzene: Effect of temperature, pH, ionic strength, and oxygen content at the air-water interface. **A.A. Heath**, L.C. Cormier, C.A. Leger, K.T. Valsaraj

11:50 ENVR **27.** Elucidating the mechanisms of HONO formation from nitrate photochemistry on environmental surfaces. **J.D. Raff**

Section D

Colorado Convention Center
Room 709

Environmental Reactivity of Organic Micropollutants and Their Transformation Products in Receiving Waters

Cosponsored by AGRO and MPPG‡

W. Arnold, Y. Chin, K. H. Wammer, *Organizers, Presiding*

8:30 Introductory Remarks.

8:30 ENVR **28.** Environmental photochemistry of altrenogest. **K.H. Wammer**, K.C. Anderson, P.R. Erickson, S. Kliegman, K. McNeill, D. Martinovic-Weigelt, D.M. Cwiertny, E.P. Kolodziej

8:50 ENVR **29.** Characterizing lampricide photoproduct formation under laboratory based and field based conditions. **M. McConville**, C.K. Remucal

9:10 ENVR **30.** Comparative triplet photochemistry of natural and treated effluent organic matter: Wavelength dependence of quantum yields for singlet oxygen and oxidizing triplets. **C.M. Sharpless**, J. Laszakovitz

9:30 ENVR **31.** Environmental photochemistry of bacitracin. R. Lundeen, C. Chu, M. Sander, **K. McNeill**

9:50 Intermission.

10:05 ENVR **32.** Matrix effects in the photodegradation of 2,4,6-trinitrotoluene. **K.A. Thorn**

10:25 ENVR **33.** Does debromination dominate BDE-47 photodegradation in natural environments? **M.L. Wei-Haas**, Y. Chin

10:45 ENVR **34.** Insights into photochemical transformation pathways of triclosan and 2'-HO-BDE-28. **Y. Zhang**, J. Chen, Q. Xie

11:05 ENVR **35.** Distinct photolytic mechanisms and products for different dissociation and metal complexation species of ciprofloxacin. X. Wei, **J. Chen**

Section E

Colorado Convention Center
Room 711

Biogenically Enhanced Recovery and Bioremediation in Fossil Fuel Reservoirs

Cosponsored by MPPG‡

D. L. Drogos, M. Urynowicz, *Organizers, Presiding*

8:00 Introductory Remarks.

8:10 ENVR **36.** Enhancing production of coalbed biogenic natural gas: History, status, and perspectives. **S. Jin**, R.M. Flores

8:30 ENVR **37.** Biogenic methane potential of Bowen Basin, Queensland coal preparation plant rejects. **S.K. Lane**, H. Zheng, V. Rudolph, S. Golding, P.C. Gilcrease

8:50 ENVR **38.** Impacts of natural gas developments on methanogenesis in deep aquifers in natural gas field. **T. Katayama**, H. Yoshioka, S. Sakata, Y. Muramoto, J. Usami

9:10 Intermission.

9:30 ENVR **39.** Decarbonization of shallow unconventional biogenic gas: Bridging the gap between fossil fuels and renewable energy. **M. Urynowicz**

9:50 ENVR **40.** Subsurface bio-electrochemical conversion of carbon dioxide into methane by using indigenous microorganisms. **H. Maeda**, M. Ikarashi, H. Kobayashi, N. Fukushima, K. Sato

10:10 ENVR **41.** Impact of CO_2 injection into depleted oil field on the methanogenic activity and pathway. H. Maeda, **T. Wakayama**, M. Ikarashi, D. Mayumi, S. Sakata, H. Tamaki, Y. Kamagata

10:30 ENVR **42.** Stimulating effect of protein-rich matter on the biogenic recycling of CO_2 to CH4. **J. Vilcaez**

10:50 Panel Discussion.

SUNDAY AFTERNOON

Section A

Colorado Convention Center
Room 703

Green Chemistry and the Environment
Cosponsored by CEI and MPPG

R. Luque, *Organizer*
A. M. Balu, S. O. Obare, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 ENVR **43.** Green photoelectrochemical solar cell based on water redox. H. Zhang, H. Xu, H. Wang, **J. Xuan**

2:05 ENVR **44.** Pd- reduced-graphene oxides with oxygen annealing for advanced direct formic acid fuel cells. D. Li, D. Leung, H. Xu, H. Wang, **J. Xuan**

2:25 ENVR **45.** Simultaneous energy generation and organics removal from real pharmaceutical wastewater by packed bed-microbial fuel cell. **Z.Z. Ismail**, A.A. Habeeb

2:45 ENVR **46.** Withdrawn.

3:05 Intermission.

3:20 ENVR **47.** Binary hierarchical systems for green chemistry processes. **R.R. Ozer**, H.A. Al-Zubaidi, S.O. Obare

3:40 ENVR **48.** Upcycling of packing-peanuts into carbon electrodes for electrochemical energy storage. **V. Etacheri**, C. Hong, V. Pol

4:00 ENVR **49.** Facile microwave-induced rapid synthesis of triazepinone: An adduct of metformin and methylglyoxal. **B. Dayal**, R. Gohil, B. Garsondiya, S. Nirujogi, M.A. Lea

4:20 ENVR **50.** Tyrosinase-catalyzed immobilization of catalase onto regenerated silk fibroins. P. Wang, G. Tang, L. Cui, **Q. Wang**, X. Fan

4:40 ENVR **51.** Multipurpose application of Sacha inchi *Plukentia volubilis* L plant: Panacea from the Andean region. **B. Kumar**, L. Cumbal, A. Debut

Section B

Colorado Convention Center
Room 705

Assessing Toxicity of Environmental Contaminants
Cosponsored by AGRO, CEI and MPPG‡

S. M. Uchimiya, B. Zhang, *Organizers*
X. Pan, J. Wang, *Organizers, Presiding*

1:30 ENVR **52.** Utilizing high-throughput bioassays associated with US EPA ToxCast Program to assess biological activity of environmental contaminants: A case study of chemical mixtures. **B. Blackwell**, A. Schroeder, G. Ankley, M. Lee, K. Jensen, K. Houck, R. Judson, D. Villeneuve

1:55 ENVR **53.** Uptake and reproductive toxicity of the metal oxide nanoparticle ZnO in Caenorhabditis elegans. **L.A. Bush**

2:20 ENVR **54.** Sublethal impacts of engineered and biogenic nanomaterials on social behavior of environmental bacteria. **A. Mohanty**, B. Cao

2:45 ENVR **55.** New measuring method of nicotine in tobacco smoke to estimate personal exposure of secondhand smoke. **M. Noguchi**, A. Yamasaki

3:10 ENVR **56.** Impacts of nanomaterials on bacterial growth, biofilm Formation, and microbial community function. **Y. Liu**, P. Ymele-Leki, M. Ramamoorthy

3:35 Intermission.

3:50 ENVR **57.** Toxicity of binary and ternary mixtures of nickel, copper, zinc and cadmium to *Daphnia magna*. **E. Traudt**, J.F. Ranville, S. Smith, K. Ebeling, J. Meyer

4:15 ENVR **58.** Simulated sunlight induces oxygen loss and decreases nanosheet size for graphene oxide in aqueous suspensions demonstrating zebrafish toxicity. **J.N. Wheeler**, M. Kim, W. Heideman, R.E. Peterson, J.A. Pedersen, R.J. Hamers

4:40 ENVR **59.** Effect of *Daphnia magna* age on the variability of cadmium toxicity. **S. Smith**

5:05 ENVR **60.** Metabolic pathways of polychlorinated biphenyls (PCBs) mediated by the active center of cytochrome P450s: A computational study with PCB-52 and PCB-77. **Z. Fu**, Y. Wang, Z. Wang, J. Chen

5:30 Concluding Remarks.

Section C

Colorado Convention Center
Room 707

Chemical Processes at Environmental Interfaces

Chemistry and Imaging at Air/Liquid(Solid) Interfaces of Atmospheric Systems
Cosponsored by COLL

H. A. Al - Abadleh, R. Z. Hinrichs, N. Kabengi, *Organizers*
H. M. Ali, *Organizer, Presiding*

1:30 ENVR **61.** Photolysis of secondary organic aerosol material as a source of small oxygenated volatile organic compounds. **K. Malecha**, S.A. Nizkorodov

1:50 ENVR **62.** Sunlight-driven synthesis and self-assembly of a model amphiphile at the air-water interface. **R. Rapf**, E. Griffith, V. Vaida

2:10 ENVR **63.** Effects of solutes on pollutant photolysis kinetics at ice surfaces. **T.F. Kahan**, P. Malley, J. Grossman

2:40 ENVR **64.** Attenuated total reflection spectroscopy of frozen aqueous salt solutions and vapor-deposited ice. **R.R. Michelsen**, H. Marrocco, K. Searles, R. Walker

3:00 Intermission.

3:20 ENVR **65.** Effects of air pollution and climate change on allergenic protein containing aerosols in the anthropocene. **C.J. Kampf**, F. Liu, K. Reinmuth-Selzle, M. Shiraiwa, U. Pöschl

3:40 ENVR **66.** In situ probing of environmental liquid surfaces and interfaces by time-of-flight secondary ion mass spectrometry. **X. Yu**

4:00 Discussion.

4:05 ENVR **67.** Adsorption and self-assembly of alkylammonium surfactants at silica/water interfaces studied by interface-specific vibrational spectroscopy: Investigating pH and ionic strength conditions relevant to hydraulic fracturing. **P. Hayes**, L.L. Torres

4:35 ENVR **68.** Characterization of quantum dot suspensions with SEC-ICP-MS. **P. Larese-Casanova**, P. Paydary

Section D

Colorado Convention Center
Room 709

Environmental Reactivity of Organic Micropollutants and Their Transformation Products in Receiving Waters
Cosponsored by AGRO and MPPG‡

W. Arnold, Y. Chin, K. H. Wammer, *Organizers, Presiding*

1:30 ENVR **69.** Insights into the (bio)transformation processes of benzotriazoles from compound-specific isotope analysis and transformation product identification. B. Rani, S. Spahr, S. Emma, J. Hollender, **T.B. Hofstetter**

1:50 ENVR **70.** Establishing predictive relationships between specific bacterial 16S rRNA sequences and micropollutant biotransformation rates. **D.E. Helbling**, D. Johnson, T. Lee, A. Scheidegger, K. Fenner

2:10 ENVR **71.** Experimental and computational evidence for reduction mechanisms of N-oxides by soluble Fe^{II} species. **Y. Chen**, H. Zhang

2:30 ENVR **72.** Fate of urban micropollutants and their transformation products in black carbon amended stormwater bioinfiltration systems. **B.A. Ulrich**, E. Im, D. Werner, C.P. Higgins

2:50 Intermission.

3:05 ENVR **73.** Withdrawn.

3:25 ENVR **74.** Ozone degradation of cylindrospermopsin (cyanotoxin): Degradation mechanisms and toxicity assessments. **S. Yan**, A. Jia, **S. Merel**, S.A. Snyder, W. Song

3:45 ENVR **75.** Doxycycline transformation during water disinfection with chlorine. **N. Kennedy**, O. Keen

4:05 ENVR **76.** Electroperoxone treatment of the anti-inflammatory drug ibuprofen:operation parameters and degradation mechanism. **X. Li**, Y. Wang, G. Yu

Section E

Colorado Convention Center
Room 711

Biogenically Enhanced Recovery and Bioremediation in Fossil Fuel Reservoirs
Cosponsored by MPPG‡

D. L. Drogos, M. Urynowicz, *Organizers, Presiding*

1:30 ENVR **77.** Relationship between coal biodegradation, microbial methane generation, and redox conditions in coalbeds indicated by coupled water, gas, and microbial analyses. **D. Ritter**, E. Barnhart, H. Schweitzer, D. Vinson, J.C. McIntosh, M. Fields

1:50 ENVR **78.** Molybdate, cobalt, and copper affect microorganisms associated with deep on subsurface coal by enhancing methane production and shifting the methanogenic community structure. **B. Unal**, M. Sanderson, V. Ryan Perry, K. Chin, K. Nusslein

2:10 ENVR **79.** Enhanced production of biogenic coalbed methane from coals following chemical oxidation. **Z. Huang**, M.A. Urynowicz

2:30 ENVR **80.** Use of a kinetic model to identify rate-limitations for biological methane production from coal. **S.L. Papendick**, S. Golding, V. Rudolph, P.C. Gilcrease

2:50 Intermission.

3:10 ENVR **81.** Characterization of microbial communities of methanogenically productive and unproductive coals. **L. Gallagher**, A.W. Glossner, L.L. Landkamer, L.A. Figueroa, K.W. Mandernack

3:30 ENVR **82.** Biodegradation pathways and organic intermediates in the conversion of coal geoplymers to methane. **W.H. Orem**, D.M. Akob, E. Barnhart, A. Clark, A. Cunningham, D. Dunlap, M. Fields, J.C. McIntosh, L. Ruppert, M. Varonka

3:50 ENVR **83.** Molecular characterization of microbes and metagenome of an Indian coal bed for biotransformation of coal into methane and other valued products. **D.N. Singh**, A. Kumar, M.P. Sarbhai, A. Gupta, A.K. Tripathi

4:10 ENVR **84.** Evolution of acetate metabolism in methanogenic *Archaea*. **E. Barnhart**, M. McClure, K. Johnson, S. Cleveland, K. Hunt, M. Fields

4:30 Panel Discussion.

4:50 Concluding Remarks.

MONDAY MORNING

Section A

Colorado Convention Center
Room 703

Green Chemistry and the Environment
Cosponsored by CEI

A. M. Balu, *Organizer*
R. Luque, S. O. Obare, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 ENVR **85.** Sonochemical water treatment of dyeing waste water on carpet workshop. **S. Sedaghat**

8:55 ENVR **86.** Morphology-dependent of alpha-MnO_2 for catalytic decomposition of ozone. **J. Jia**, P. Zhang

9:15 ENVR **87.** Effect of initial pH on iron-oxidizing bacteria assisted pyrite oxidation system for mine tailings treatment. **W. Ju**, E. Jho, K. Nam

9:35 ENVR **88.** Biotic and abiotic treatment methods for alkaline leachates from steel slags. **S. Kim**, K. Nam, E.G. Jho

9:55 ENVR **89.** Environmental application of PEI based hydrogels in different morphology and sizes: Bulk, microgel, and cryogel. **N. Sahiner**, S. Demirci, M. Sahiner, H.A. Al-Lohedan, **N. Aktas**

10:15 Intermission.

10:30 ENVR **90.** Effect of two-phase pretreatment of rice straw on polyhydroxyalkanoates (PHAs) synthesis by *Cupriavidus necator*. **J. Ahn**, E.G. Jho, K. Nam

10:50 ENVR **91.** Insights on the solubility of CO_2 in 1-Ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide from the microscopic point of view. **L.T. Costa**, T. Lourenço, D. Van Der Spoel

11:10 ENVR **92.** Novel vapor-phase hydrolysis approach for preparing of nanosilica: Recycling of silicon tetrachloride. **F. Yan**, **J. Jiang**, M. Zhao

11:30 ENVR **93.** Nitrous oxide emission from de-ammonification process. **P.L. Noophan**

11:50 ENVR **94.** [Bmim]Cl ionic liquid as a novel solvent and reaction medium for the preparation of keratin biodegradable thermoplastic. **J. Yuan**, Y. Yu, P. Wang, X. Fan, Q. Wang

12:10 ENVR **95.** Metal occurrence in and potential recovery from municipal biosolids. **K.S. Smith**, P.L. Hageman, G.S. Plumlee, J.G. Crock, T.J. Yager, R.B. Brobst, S.C. Gebhard

Section B

Colorado Convention Center
Room 705

Environmental Chemistry and Health Impacts of Fine and Ultrafine Particulate Matter
Cosponsored by MPPG

S. M. Lomnicki, *Organizer, Presiding*

8:00 ENVR **96.** Exposure to combustion-derived particulate matter: an unrecognized risk factor in severity of respiratory viral infection in infants. **S. Cormier**, G. Lee, J. Saravia, D. You, B. Shrestha, S. Jaligama, V. Hebert, T.R. Dugas

8:30 ENVR **97.** Withdrawn.

8:50 ENVR **98.** Temporal-spatial variations, sources, and transport of $PM_{2.5}$ and associated trace metals in the Yangtze River Delta (YRD), China. L. Ming, J. Li, G. Zhang, **X. Li**

9:10 ENVR **99.** Spatial variation of rainwater chemistry in Ile-Ife, Osun State, Nigeria. **A.A. Okoya**

9:30 ENVR **100.** Chemical speciated components of atmospheric organic aerosol in the St. Louis Region, U.S. **Y. Zhang**, B. Williams, R. Martinez, D. Mitroo, M. Walker, C. Oxford, X. Zuo, D. Hagan, J. Turner, L. Du, D. Millet, M. Baasandorj, L. Hu, R. Weber, L. King

9:50 Intermission.

10:05 ENVR **101.** Oxidant production from source-oriented particulate matter: hydrogen peroxide and hydroxyl radical. **N.K. Richards-Henderson**, J.G. Charrier, K.J. Bein, A.S. Wexler, C. Anastasio

10:25 ENVR **102.** Formation of biologically persistent free radicals (BPFR) via reaction of nano metal oxide with a selected component of broncho-alveolar lavage fluid (BALF). **A.N. Dela Cruz**, S.M. Lomnicki

10:45 ENVR **103.** Effect of black carbon nanoparticles on epithelial cell proliferation. **N. Beebe**, A.M. Johansen

11:05 ENVR **104.** Main contributors to the diesel exhaust and wood smoke particles toxicity. Do we know them? **A. Kubátová**, R. Cochran, K. Ondrušová, J. Rousová, A.I. Totlandsdal, J. Øvrevik, P.E. Schwarze, M. Låg

11:25 ENVR **105.** Determination of atmospheric organosulfates using HILIC chromatography with MS detection. **E.A. Stone**, A. Hettiyadura, S. Kundu, Z. Baker, E. Geddes, K. Richards, T. Humphry

11:45 ENVR **106.** Particulate matter containing environmentally persistent free radicals induce aryl hydrocarbon receptor-dependent cytokine production in human bronchial epithelial cells. V. Hebert, S. Cormier, R. Reed, W. Backes, **T.R. Dugas**

‡ *Cooperative Cosponsorship*

Section C

Colorado Convention Center
Room 707

Chemical Processes at Environmental Interfaces

Chemistry at Aqueous/Mineral(Solid) Interfaces

Cosponsored by COLL

H. A. Al - Abadleh, H. M. Ali, R. Z. Hinrichs, *Organizers*
N. Kabengi, *Organizer, Presiding*

8:00 Introductory Remarks.

8:10 ENVR **107.** Structure, dynamics, and reactivity of the interface between aqueous solutions and mineral surfaces. **D. Wesolowski**, A.G. Stack, H. Wang

8:40 ENVR **108.** Integrated approach to study surface reactions using spectroscopy and calorimetry. **M. Chrysochoou**, N. Kabengi

9:10 ENVR **109.** Speciation dynamics of metal at biochar-soil interface: Effects of biochar and soil properties. **R. Huang**, Y. Tang

9:30 ENVR **110.** Zinc interaction with struvite during and after mineralization from phosphorus-rich sources. **A. Rouff**, K. Juarez

9:50 Intermission.

10:10 ENVR **111.** Adsorption of Cr(VI), Cd(II), and Pb(II) on nanomaghemite and maghemite-coated silica. **C. Koretsky**, M. Komarek, D. Alessi, K. Stephen, A. Troy

10:40 ENVR **112.** DFT calculations in support of XANES and NMR studies of Cd and Pb on gibbsite and kaolinite. **J.D. Kubicki**, H. Watts, E. Poweleit, K.T. Mueller, N. Govind, P. ODay, M. Small

11:10 ENVR **113.** Development of DFT methods to aid in NMR data interpretation for Cd(II) adsorbed to clay minerals. **H.D. Watts**, E.T. Poweleit, K.T. Mueller, J.D. Kubicki

11:30 ENVR **114.** Exploring nano shape effects on reactivity in Keggin-type aluminum hydroxide clusters through DFT studies. **K.W. Corum**, S.E. Mason

11:50 ENVR **115.** Surface chemistry enhanced microbial electrodes: Biofilm modeling and characterization. **J.A. Cornejo**, K. Artyushkova, C. Santoro, S. Babanova, L.K. Ista, A.J. Schuler, P.B. Atanassov

Section D

Colorado Convention Center
Room 709

Hydraulic Fracturing Impacts on Water, Soil and Air Quality

Groundwater Impacts

Cosponsored by MPPG‡

R. Jackson, R. D. Vidic, *Organizers*
J. Blotevogel, T. Borch, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENVR **116.** Approaches for groundwater monitoring for shale gas impacts: Concepts and field examples. B. Parker, J. Cherry, **A. Cahill**

8:35 ENVR **117.** Controls on methane occurrences in aquifers in the footprint of Texas shale plays. **J. Nicot**, P. Mickler, T.E. Larson, M. Castro, Z. Hildenbrand, R. Darvari, K. Uhlman, R.C. Smyth, L. Bouvier, B.R. Scanlon

9:00 ENVR **118.** Simulating mobility and degradation of chemical contaminants from unconventional gas development. **C. Kanno**, D. Edlin, T. Borrillo-Hutter, J.E. McCray

9:25 ENVR **119.** Fate of hydraulic fracturing chemicals in agricultural topsoil. **M. McLaughlin**, T. Borch, J. Blotevogel

9:50 Intermission.

10:05 ENVR **120.** Trace levels of diesel range organic compounds in shallow groundwater wells in northeastern Pennsylvania elevated near Marcellus shale gas wells. **B. Drollette**, K. Schreglmann, N. Warner, T.H. Darrah, M.P. O'Connor, O. Karatum, R. Nelson, M. Elsner, C.M. Reddy, A. Vengosh, R. Jackson, D.L. Plata

10:30 ENVR **121.** Toxicity and fate of the chemicals of matrix acidization, an unconventional oil stimulation technique. **K. Abdullah**, **J. Taylor**, I. Suffet

10:55 ENVR **122.** Fate and transport of four organic compounds frequently used in hydraulic fracturing fluids in laboratory columns containing aquifer sediments. **J.D. Rogers**, S.G. Osborn, J.N. Ryan

11:20 ENVR **123.** WII4HF: A conceptual model for computing water impact index for hydraulic fracturing. **R. Kandiah**, K. Nedunuri, X. Wei, N. Zhang, M.G. Smith

Section E

Colorado Convention Center
Room 711

Modern Analytical Approaches for the Characterization of Natural Organic Matter in the Environment

Use of Mass Spectrometry and Other Methods to Characterize NOM in Diverse Environments

Cosponsored by ANYL and MPPG

G. Aiken, K. Cawley, *Organizers*
J. A. Korak, F. L. Rosario, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENVR **124.** From molecular analyses to remote sensing: Characterization of dissolved organic matter in the Gulf of Maine. **G. Aiken**, X. Cao, J. Mao, K. Schmidt-Rohr, R. Spencer, S. Belanger, W. Balch, T. Huntington

8:35 ENVR **125.** Ultrahigh resolution mass spectrometry study of sea spray aerosol water soluble and water insoluble organic matter composition. **A.S. Wozniak**, A.S. Willoughby, S.D. McElhenie, P.K. Quinn, D.J. Coffman, P. Hatcher

9:00 ENVR **126.** Using Fourier transform ion cyclotron resonance mass spectrometry to identify potential disinfection byproduct precursors in leaf litter leachate. **G. McKee**, C.C. Rhoades, T. Borch

9:25 ENVR **127.** Meta-metabolomics as a systems-level tool for examining shifts in organic matter composition driven by environmental change. **C.M. Boot**

9:50 ENVR **128.** Halogenated moieties incorporated into humic acid as a result of oxidation of tetrahalobisphenol A and their characterization using a TMAH-pyrolysis-GC/MS. R. Kodama, T. Miyamoto, Q. Zhu, M. Igarashi, **M. Fukushima**

10:15 Intermission.

10:30 ENVR **129.** Antarctic ice-locked reservoirs of organic matter: Probing the bulk and molecular level chemical nature of organic matter by fluorescence spectroscopy and mass spectrometry. **J. D'Andrilli**, C.M. Foreman, H.J. Smith

10:55 ENVR **130.** Transformations in autochthonous DOM: An Antarctic supraglacial case study. **H.J. Smith**, M.L. Wei-Haas, M. SanClements, J. D'Andrilli, C.M. Foreman, Y. Chin, D. McKnight

11:20 ENVR **131.** Patterns in DOC absorbance with photodegradation and microbial processing in tundra watersheds in the Kolyma River Basin. **M. Behnke**, J. Schade, K. Whittinghill, N. Zimov

11:45 ENVR **132.** DOC variability and characteristics in alpine watersheds. **K. Dee**, J.F. Ranville, K. Walton-Day, K.S. Smith

MONDAY AFTERNOON

Section A

Colorado Convention Center
Room 703

Dispersion of Nanoparticles and its Implication for Interfacial, Biological and Environmental Processes

Interface and Transport

N. B. Saleh, B. Xing, *Organizers*
B. Pan, P. J. Vikesland, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 ENVR **133.** Interaction between graphene oxide and minerals in aqueous phase. J. Zhao, Z. Wang, **B. Xing**

2:10 ENVR **134.** Natural organic matter's influence on pollutant toxicity: An interface point of view. R.D. Williams, C.L. Schneider, L.M. Ojwang', **R.L. Cook**

2:45 ENVR **135.** Effect of extracellular polymeric substances on the fate and transformation of engineered nanomaterials. **A.S. Adeleye**, A.A. Keller

3:05 ENVR **136.** Measuring iron particle formation in seawater through advances in spICP-MS. B.T. Cartledge, E.K. Cutler, K.E. Whitworth, **B. Majestic**

3:25 Intermission.

3:45 ENVR **137.** Heteroaggregation of carboxylated multiwalled carbon nanotubes (COOH-MWCNTs) and kaolinite in aquatic systems and their cotransport behavior in porous media. **T. Wang**, **P. Coogan**, Q. Li

4:05 ENVR **138.** Promoted dispersion of cerium oxide nanoparticles from Fe^{2+}-induced redox reactions at the nanoparticle surface. **Y. Jun**, J.R. Ray, X. Liu, C.W. Neil, Q. Li

4:25 ENVR **139.** Elucidating critical roles of light and electron acceptors during aqueous colloidal C_{60} (nC_{60}) formation. **J. Wu**, A. Montoya, W. Li, J. Fortner

4:45 ENVR **140.** Controlled evaluation of copper-based nanomaterial dissolution kinetics. **R.D. Kent**, P.J. Vikesland

Section B

Colorado Convention Center
Room 705

Chemistry in the Marine Boundary Layer

Cosponsored by MPPG

J. Donaldson, *Organizer*
B. DAnna, *Organizer, Presiding*

1:30 ENVR **141.** Ocean-atmosphere interaction and marine multiphase chemistry. **H. Herrmann**, M. van Pinxteren, D. van Pinxteren, K. Müller, W. Fomba, P. Bräuer

1:55 ENVR **142.** Impact of biological activity in the sea surface microlayer on sea spray aerosol and cold cloud formation. J.Y. Aller, P. Alpert, W.P. Kilthau, D. Bothe, T.W. Wilson, B. Murray, **D.A. Knopf**

2:15 ENVR **143.** Sea spray organic matter and virus-induced plankton dynamic. **M. Facchini**, C.D. O'Dowd, R. Danovaro

2:35 ENVR **144.** Surface-atmosphere exchange of ammonia in the summertime Canadian Arctic marine boundary layer. **G. Wentworth**, J. Murphy, J. Tremblay, J. Gagnon, J. Côté, I. Courchesne

2:55 Intermission.

3:05 ENVR **145.** Bringing the ocean into the laboratory for detailed studies on sea spray aerosols. **K.A. Prather**

3:30 ENVR **146.** Impact of air-sea exchanges on the Mediterranean marine boundary layer composition. **N. Marchand**, J. Pey, H.L. Dewitt, B. Temime-Roussel, S. Hellebust, A. Même, B. Rmili, B. Charrière, R. Sempéré, S. Mas, D. Parin, J. Cerro, N. Perez, C. Rose, A. Schwier, M. Elser, S. Szidat, A.S. Prévôt, K. Sellegri, B. D'Anna

3:50 ENVR **147.** Size-resolved sea spray aerosol particles studied by vibrational sum frequency generation. **F. Geiger**

4:10 Intermission.

4:20 ENVR **148.** Sunlight-driven photochemical halogenation of dissolved organic matter in seawater: A natural abiotic source of organobromine and organoiodine. **J.J. Pignatello**, J. Méndez-Díaz, K. Shimabuku, J. Ma, Z.O. Enumah, W. Mitch, M.C. Dodd

4:45 ENVR **149.** Simulation of the photochemical heterogeneous activation of halogens (Cl and Br) from salt pans and salt aerosol in chamber experiments. **C. Zetzsch**

5:05 ENVR **150.** On the reaction of CH_3O_2 radicals with OH radicals and its impact on the MBL. **C. Fittschen**

5:25 ENVR **151.** Impact of organosulfur compounds at the marine/urban interface in a decreasing SO_2 world. **V. Perraud**, S. Meinardi, D.R. Blake, J. Horne, M. Dawson, A. Martinez, D. Dabdub, J. Kalinowski, R.B. Gerber, B.J. Finlayson Pitts

Section C

Colorado Convention Center
Room 707

Solutions to Metals Contamination of Water

Cosponsored by MPPG‡

S. Ahuja, J. W. Finley, J. N. Seiber, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 ENVR **152.** Notable solutions to water contamination. **S. Ahuja**

2:00 ENVR **153.** Arsenic removal technology for drinking water for developing countries. **S. Chaudhari**, T. Banerji

2:25 ENVR **154.** Quantification of arsenic and uranium in unregulated water sources on the Navajo and Hopi reservations. **J. Credo**, E.R. Peaches, T. Rock, S.B. Garcia, J.C. Ingram

2:50 ENVR **155.** Feasibility study of iron oxide nanoparticles prepared by different synthetic methods for arsenic removal. **N.I. Gonzalez Pech**, C. Avendano, G. Escalera, A. Bohloul, V.L. Colvin

3:15 Intermission.

3:30 ENVR **156.** Influence of acid-base properties of zinc oxide nanomaterials on their arsenic uptake capacity. **E. Rukundo**, A. Apblett

3:55 ENVR **157.** Extraction, recovery, and identification of Inorganic contaminants from water. **R.E. Del Sesto**, A. Newsham, M. Jones, B.H. Barton, A.T. Koppisch, D. Fox

4:20 ENVR **158.** Optimizing the treatment performance of graphene oxide-based hydrogels. **T.A. Duster**, L.F. Greenlee

4:45 ENVR **159.** Removal of heavy metals with steel furnace slag. B. Mercado-Borrayo, R. Contreras, A. Sánchez, X. Font, R. Schouwenaars, **R. Ramírez-Zamora**

Section D

Colorado Convention Center
Room 709

Hydraulic Fracturing Impacts on Water, Soil and Air Quality

Surface Water Impacts/Fluid Chemistry

Cosponsored by MPPG‡

J. Blotevogel, T. Borch, *Organizers*
R. Jackson, R. D. Vidic, *Organizers, Presiding*

1:30 ENVR **160.** Water quality challenges associated with energy resource extraction from Marcellus Shale. **R.D. Vidic**

2:00 ENVR **161.** Appropriation of fresh water for shale gas development in Pennsylvania's Marcellus Shale. **J. Saiers**, E. Barth-Naftilan

2:25 ENVR **162.** Transformation kinetics and pathways of hydraulic fracturing biocides under downhole conditions: Focus on glutaraldehyde. **G. Kahrilas**, J. Blotevogel, T. Borch

2:50 ENVR **163.** Exploring the potential for rare earth elements as geochemical fingerprints of salinity sources. **A. Karamalidis**, C.W. Noack, D.A. Dzombak

3:15 Intermission.

3:25 ENVR **164.** Analysis of hydraulic fracturing flowback and produced waters using accurate mass: IIdentification of ethoxylated surfactants. **E. Thurman**, I. Ferrer, J. Blotevogel, T. Borch

3:55 ENVR **165.** Endocrine disrupting activity of hydraulic fracturing chemicals and health outcomes following prenatal exposure in mice. **C. Kassotis**, C. Lin, D.E. Tillitt, S.C. Nagel

4:20 ENVR **166.** Contaminant mobilization via reactions between Marcellus shale and synthetic fracturing fluids. **W.D. Burgos**, T. Tasket

4:45 ENVR **167.** Ultrahigh resolution mass spectrometry of hydraulic fracturing produced waters. **L. Jenna**, M. Gonsior, P. Schmitt-Kopplin, J. Batista

5:10 ENVR **168.** Molecular-level characterization of water-soluble organic species from eagle ford shale oil by ultrahigh resolution ft-icr mass spectrometry. **A.M. McKenna**, D.C. Podgorski, H. Chen, L.C. Krajewski, Y. Corilo

Section E

Colorado Convention Center
Room 711

Modern Analytical Approaches for the Characterization of Natural Organic Matter in the Environment

Extraction Techniques to Isolate NOM and Characterization of Pyrogenic Organic Matter (Biomass Burning)

Cosponsored by ANYL and MPPG

J. A. Korak, F. L. Rosario, *Organizers*
G. Aiken, K. Cawley, *Organizers, Presiding*

1:30 ENVR **169.** Solid phase extraction of organic matter, past to present: A review of isolation mechanisms from XAD to today's sorbents. **E.M. Thurman**, I. Ferrer

2:00 ENVR **170.** Characterization of soil organic matter (SOM) using online supercritical fluid extraction (SCFE) techniques coupled with liquid chromatography-ultrahigh resolution mass spectrometry (LC-UHR MS). **K.M. Roscioli**, Y. Shen, R. Zhao, T. Fillmore, N. Tolic, M. Tfaily, B. Anderson, N.J. Hess, L. Paša-Tolić, E.W. Robinson

2:25 ENVR **171.** New solvent methods for molecular characterization of SOM by high resolution spectrometry. **M.M. Tfaily**, R. Chu, N. Tolic, K.M. Roscioli, L. Paša-Tolić, E.W. Robinson, N.J. Hess

2:50 ENVR **172.** Effects of chemical treatments on soil organic matter composition identified by DRIFT, NMR and py-MBMS characterization. **F.J. Calderón**, **A.J. Margenot**, K.A. Magrini, R.J. Evans

3:15 Intermission.

3:30 ENVR **173.** Structural interrogation of dissolved organic matter and pyrogenic black carbon and molecular characterization by ultrahigh resolution FT-ICR mass spectrometry. **A.M. McKenna**, D.C. Podgorski, Y. Corilo, W.T. Cooper, D.F. Smith, N.K. Kaiser

3:55 ENVR **174.** Speciation of organics in aged atmospheric particles from a biomass burning event: Relationship to light absorption and comparison to humic acids. **R.A. Di Lorenzo**, K.J. Jobst, X. Ortiz, C.J. Young

4:20 ENVR **175.** Comparative analysis of wood stove smoke. **V.M. Porden**

4:45 ENVR **176.** Characterization and concentration of water soluble organic matter (WSOM) and inorganic constituents from wildfire impacted stream bank material. **K. Cawley**, A.K. Hohner, P. Omur-Ozbek, R. Summers, F.L. Rosario

MONDAY EVENING

Section A

Colorado Convention Center
Halls C/D

Sci-Mix

S. R. Al-Abed, *Organizer*

8:00 - 10:00

ENVR **177.** Profile of metal bioaccumulation in selected invertebrates from the eastern and western shores of the Susquehanna River near Hummels Wharf Pennsylvania. **A. Pritzlaff**, C.P. Hallen, C. Venn

ENVR **178.** Organic matter and nitrogen removal within field-scale constructed wetlands: Reduction performance and microbial identification studies. **T. Yeh**

203, 210, 336, 351, 360, 362-363, 366, 370-371, 374, 377, 379, 381, 383, 386, 388-389, 394, 396, 400-401, 403, 407, 414-415, 417, 419, 422, 430-431, 438, 443, 446-447, 450-451, 454, 460. See subsequent listings.

TUESDAY MORNING

Section A

Colorado Convention Center
Mile High Ballroom 4D

Dispersion of Nanoparticles and its Implication for Interfacial, Biological and Environmental Processes

Sorption and Dispersion

B. Pan, N. B. Saleh, P. J. Vikesland, *Organizers*
B. Xing, *Organizer, Presiding*
R. L. Cook, *Presiding*

8:00 ENVR **179.** Toward a mechanistic understanding of the effect of natural organic matter coatings on nanoparticle aggregation. **G.V. Lowry**, S. Louie, E.R. Spielman-Sun, R.D. Tilton

8:35 ENVR **180.** Coadsorption, desorption hysteresis, and sorption thermodynamics of sulfamethoxazole and carbamazepine on graphene oxide and graphite. **B. Pan**, C. Wang, H. Li, B. Xing

9:10 ENVR **181.** Arsenic adsorption in highly dispersed conductive TiO_2-CNT nanosystems: Enhanced sorption behavior due to mass transport, electrosorption, and adsorbent dispersion. **H. Liu**, K. Zuo, C.D. Vecitis

9:30 ENVR **182.** Role of air bubbles overlooked in the adsorption of perfluorooctane sulfonate on carbon nanotubes. **S. Deng**, P. Meng, B. Xing

9:50 Intermission.

10:10 ENVR **183.** Influence of humic acid on the dispersion and transport of $nTiO_2$ particles in water-saturated porous media. **Y. Wu**, T. Cheng

10:30 ENVR **184.** Surface engineering magnetic nanoparticles for aqueous applications: Design and characterization of tailored organic bilayer. **W. Li**, C.H. Hinton, S. Lee, J. Wu, Y. Jiang, J.D. Fortner

10:50 ENVR **185.** Disruption of quorum sensing by adsorption of acyl-homoserine lactone to engineered nanomaterials. **K.B. Gregory**, J.M. Vanbriesen, E. McGivney

11:10 ENVR **186.** Synthesis and characterization of anion exchange resin coated SWCNTs for dissolved organic content removal. **J.C. Poler**, B. Johnson, Y.J. Baik, R. Furst

Section B

Colorado Convention Center
Room 705

Advances in Analytical Chemistry for Discovering Emerging Contaminants in the Natural Environment

Cosponsored by AGRO, ANYL and MPPG

D. Alvarez, *Organizer*
T. L. Jones-Lepp, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 ENVR **187.** New environmental monitoring framework for contaminants of emerging concern (CECs). **K.A. Maruya**, N.G. Dodder, A.C. Mehinto

8:55 ENVR **188.** Microplastics emerging contaminants: a new source of toxic compounds. **L.M. Rios Mendoza**, E. Soto

9:15 ENVR **189.** Naphthenic acid analysis using differential mobility spectrometry coupled with accurate mass time of flight mass spectrometry. **P. Winkler**, L. Campbell, T. Sakuma, A. Schreiber, K. Peru, j. Headley

9:35 ENVR **190.** Quantification and risk assessment of emerging organic contaminants in Ikpa River basin, Niger Delta, Nigeria. N.O. Offiong, **E. Inam**, J. Essien, S. Kang, G. Udofia, B. Antia, S. Kang, P. Yang

9:55 Intermission.

10:15 ENVR **191.** Using a novel photo-micro-reactor to remove benzoylecgonine in wastewater treatment: Uncovering phototransformation products and the reaction pathways with advanced mass spectrometry tools. **S.D. Richardson**, K.H. Cochran, M. Vaccaro, D. Russo, D. Spasiano, R. Marotta, R. Andreozzi, N.M. Reis, G. Li Puma

10:35 ENVR **192.** Novel methods for sampling perfluorinated acids in the atmosphere. J.J. MacInnis, T.C. Vandenboer, **C. Young**

10:55 ENVR **193.** Adsorption and disposition of pharmaceuticals by bluegill exposed at constant concentrations in a flow-through aquatic exposure system. J. Zhao, **E.T. Furlong**, D.W. Kolpin, E.A. Schwab, D.J. Feifarek, K.L. Bird, H. Schoenfuss, G. Ying

11:15 ENVR **194.** Presence of UV filters (sunscreens) in marine surface waters of bays within the Virgin Islands National Park. **D. Alvarez**, T. Bargar

11:35 ENVR **195.** Using 5-hydroxyindoleacetic acid as an anthropogenic population biomarker in wastewater treatment plant influent. **D.A. Burgard**, H. Fryhle, M.C. Pellman

Section C

Colorado Convention Center
Room 707

Solutions to Metals Contamination of Water

Cosponsored by MPPG‡

S. Ahuja, J. W. Finley, J. N. Seiber, *Organizers, Presiding*

8:30 ENVR **196.** Immobilization of mercury by stabilized iron sulfide nanoparticles: Reaction mechanisms and effects of stabilizer. **D. Zhao**, Y. Gong, Y. Liu, Z. Xiong

8:55 ENVR **197.** Solar UV photooxidation as pretreatment for stripping voltammetric trace metal analysis in river water. **G. Flechsig**, G. Woldemichael

9:20 ENVR **198.** Lignin-coated magnetic nanoparticles for mercury adsorption. **L. Peña Duque**, N. Robitaille Brown

9:45 ENVR **199.** Mercury uptake by oysters in the New York Harbor indicates early success of novel approach to water restoration. **E. Park**

10:10 Intermission.

10:25 ENVR **200.** Binding of inorganic mercury in surface water to DOM and alum flocs: How much removal can we get? **F.A. Diaz**, L.E. Katz, D.F. Lawler

10:50 ENVR **201.** Utilization of fruit juice with high vitamin C content for the remediation of wastewater contaminated with chromium (VI). Y.S. Mendoza, **J.R. Pinzón**

11:15 ENVR **202.** Efficient and robust removal of chromium using engineered metal-reducing biofilms. **Y. Ding**, B. Cao

11:40 ENVR **203.** Adsorption of Cs, Sr, and Co by mesoporous materials. **K. Guo**, F.X. Han, Z. Arslan, H. Yu

Section D

Colorado Convention Center
Room 709

Hydraulic Fracturing Impacts on Water, Soil and Air Quality

Air & Water Quality

Cosponsored by MPPG‡

R. Jackson, R. D. Vidic, *Organizers*
J. Blotevogel, T. Borch, *Organizers, Presiding*

8:00 ENVR **204.** Characterizing air quality impacts of oil and gas development in the Bakken formation region. **J.L. Collett**, A. Evanoski-Cole, A. Prenni, D. Day, A. Sullivan, Y. Li, B.C. Sive, Y. Zhou, J. Hand, K. Gebhart, M. Schurman, B. Schichtel

8:30 ENVR **205.** Observations of acyl peroxyl nitrates (PANs) during the Front Range Air Pollution and Photochemistry Éxperiment (FRAPPÉ) field campaign. **J. Zaragoza**, E.V. Fischer, E.E. McDuffie, W.P. Dubé, S.S. Brown, D.K. Farmer, F.M. Flocke

8:55 ENVR **206.** Locating, quantifying, and attributing methane emissions from fossil-fuel extraction. **E. Kort**, M. Smith, A. Gvakharia, C. Sweeney, A. Karion, J. Peischl, T.B. Ryerson, C. Frankenberg, M. Dubey

9:20 Intermission.

9:35 ENVR **207.** Influence of salinity, concentration, and redox on the biodegradability of organic additives in hydraulic fracturing fluids. **P. Mouser**

10:05 ENVR **208.** Disinfection by-products formed during the treatment of produced waters at wastewater treatment plants. **M.L. Hladik**, M. Focazio

10:30 ENVR **209.** Produced water exposure from hydraulic fracturing alters bacterial response to biocides. A. Vikram, D. Lipus, **K. Bibby**

10:55 ENVR **210.** Anaerobic biodegradation of polypropylene glycols within hydraulic fracturing fluid. **K.M. Heyob**, J. Blotevogel, T. Borch, P.J. Mouser

11:20 ENVR **211.** Feasibility of reusing barite recovered from the produced for drilling mud formulation. **N. Cely**

Section E

Colorado Convention Center
Room 711

Modern Analytical Approaches for the Characterization of Natural Organic Matter in the Environment

NMR and Photochemical Analysis of NOM

Cosponsored by ANYL and MPPG

J. A. Korak, F. L. Rosario, *Organizers*
G. Aiken, K. Cawley, *Organizers, Presiding*

8:00 ENVR **212.** Combined mass spectrometry - NMR spectroscopy approach for characterizing organic phosphorus in treatment of wetlands. **W.T. Cooper**, L. Skiba, C. Stulz, S. Newman

8:30 ENVR **213.** New forms of dissolved organic nitrogen Identified by multibond 2D NMR spectroscopy. X. Cao, M.R. Mulholland, P.W. Bernhardt, J. Helms, **J. Mao**, K. Schmidt-Rohr, Z. Zhou

8:55 ENVR **214.** Composition and structure of natural organic matter isolated by reverse osmosis and ultrafiltration. **Y. Ran**, W. Huang, X. Cao, J. Mao

9:20 Intermission.

9:35 ENVR **215.** Further insights on the chemical structure of humic substances (HS) and chromophoric dissolved organic matter (CDOM) in relation to their optical/chemical properties. **R. Del Vecchio**, T. Schendorf, N.V. Blough

10:00 ENVR **216.** pH effects on DOM photodegradation using semi-continuous fluorescence excitation emission matrices. **S. Timko**, M. Gonsior, W.J. Cooper

10:25 ENVR **217.** Temperature dependence of the photochemical formation of hydroxyl radical from dissolved organic matter. **G. McKay**, F.L. Rosario

10:50 ENVR **218.** Comparing triplet reaction mechanisms for DOM characterization. **A. Maizel**, W. Kamp, C.K. Remucal

11:15 ENVR **219.** Dynamic light scattering and zeta potential investigation of fulvic and humic acid reversible self-assembly in low electrolytic conductivity solutions. **M.J. Wells**, M.R. Esfahani, H.A. Stretz

11:40 ENVR **220.** Assessment of novel natural organic matter characterization tools: Application to the drinking water industry. **Y. Park**, A. Stoddart, M. Brophy, W. Krkosek, G.A. Gagnon

TUESDAY AFTERNOON

Section A

Colorado Convention Center
Room 703

Dispersion of Nanoparticles and its Implication for Interfacial, Biological and Environmental Processes

Benefit and Risk

B. Pan, P. J. Vikesland, B. Xing, *Organizers*
N. B. Saleh, *Organizer, Presiding*
Z. Zhang, *Presiding*

1:30 ENVR **221.** Interactions between plants and rare earth oxide nanoparticles. **Z. Zhang**, Y. Ma, P. Zhang, X. He, Y. Zhao

‡ *Cooperative Cosponsorship*

2:05 ENVR **222.** Bioaccumulation of ionic silver and silver nanoparticles within freshwater crayfish using inductively coupled plasma optical emission spectroscopy. **S.W. Brittle**, D.P. Foose, M.T. Ruis, M.T. Amato, S.A. Paluri, N.H. Lam, B. Buttigieg, Z.E. Gagnon, I.E. Pavel Sizemore

2:25 ENVR **223.** Bioavailability of fullerene in the presence of environmentally relevant matrices: Effects of humic acid and fetal bovine serum (FBS) on the lipid accumulation and cellular uptake. **Y. Ha**, H. Liljestrand, L.E. Katz, J. Maynard

2:45 ENVR **224.** Interaction strength of supported lipid bilayers with the underlying substrate influences the disruptive effect of engineered nanoparticles. N. Yousefi, A. Wargenau, **N. Tufenkji**

3:05 Intermission.

3:25 ENVR **225.** Application of carbon nanotube yarn as a filter media to treat nitroaromatic-contaminated water. **S.R. Kanel**, B. Doane, H. Misak, S. Mall, S.W. Brittle, I.E. Pavel Sizemore, T. Ebrahimian, D. Kempisty, M.N. Goltz

3:45 ENVR **226.** Engineered carbon nanoparticle tracers: Groundwater transport and implications for the migration of environmental nanoparticles. **C.N. King**, W.E. Sanford, Y.V. Li

4:05 ENVR **227.** Probing photosensitization by functionalized carbon nanotubes in aquatic environments. **C. Chen**, R.G. Zepp

4:25 ENVR **228.** Modification of zero-valent iron nanoparticles and its application for the decoloration of malachite green. **X. Wang**, J. He, L. Le

4:45 Concluding Remarks.

Section B

Colorado Convention Center
Room 705

Advances in Analytical Chemistry for Discovering Emerging Contaminants in the Natural Environment

Cosponsored by AGRO, ANYL and MPPG

T. L. Jones-Lepp, *Organizer*
D. Alvarez, *Organizer, Presiding*

1:30 ENVR **229.** Spatial and temporal variability of excitation emission matrix (EEM) fluorescence spectra in a wastewater effluent impacted river. **M.J. Wells**, G.A. Mullins, K.Y. Bell, A.K. Da Silva, E.M. Navarrete

1:50 ENVR **230.** Application of field portable PLOT-cryoadsorption headspace sampling apparatus for detection of diesel fuel in soil. **S. Bukovsky-Reyes**, T. Bruno, M. Harries

2:10 ENVR **231.** Analysis of complex environmental samples by 2D-GC combined with high-resolution mass spectrometry. **A. Dane**, M. Ubukata, R.B. Cody

2:30 ENVR **232.** Detection, quantification, and partitioning property estimation of bioaccumulative pollutants in aquatic environments using GCxGC-ENCI-TOFMS and GCxGC-ECD. **J.S. Arey**, S. Samanipour, P. Dimitriou-Christidis, D. Nabi, J. Gros

2:50 Intermission.

3:10 ENVR **233.** Determination of perchlorate in polar ice cores down to sub-ng L^{-1} level using ion chromatography-tandem mass spectrometry. **K.M. Peterson**, J. Cole-Dai, D. Brandis, T. Cox, S. Splett

3:30 ENVR **234.** Periodic table of elements for the water heavy metal monitoring on paper. **M. Li**, R. Cao, A. Nilghaz, L. Guan, W. Shen

3:50 ENVR **235.** Hydroxyl radical generation on graphite and modified graphite surfaces for AOP's: An EPR investigation. **M.A. Morsy**, A.M. Kawde, M.A. Daous, T.A. Saleh

4:10 ENVR **236.** Identifying trace environmental contaminant in CO_2 capture solvents from coal-fired power plants using ICP-MS and high resolution time-of-flight mass spectrometry (TOF-MS). **J.G. Thompson**, Q. Huang, K. Liu

4:30 Concluding Remarks.

Section C

Colorado Convention Center
Room 707

Solutions to Metals Contamination of Water

Cosponsored by MPPG‡

S. Ahuja, J. W. Finley, J. N. Seiber, *Organizers, Presiding*

1:30 ENVR **237.** Efficient and versatile carbon-based nanocomposite for the adsorption of heavy metal ions from aqueous environments. A.B. Dichiara, M.R. Webber, **R.E. Rogers**

1:55 ENVR **238.** Effects of the presence of oxyanions during birnessite synthesis on birnessite particle sizes and application for removal of lead. **Q. Wang**, X. Liao, M. Zhu

2:20 ENVR **239.** Engineered superparamagnetic iron oxide nanoparticles for uranyl separation in water. **W. Li**, S. Lee, C.H. Hinton, J. Wu, J.D. Fortner

2:45 ENVR **240.** Cr(VI) removal using magnetite-non oxidative graphene composite as a new sorbent: A comparative study with magnetite-graphene oxide and magnetite-reduced graphene oxide. **M. Zheng**, Y. Yoon, W. Park, W. Yang, J. Kang

3:10 Intermission.

3:25 ENVR **241.** Double-stranded DNA encased single-walled carbon nanotubes for optical sensing of cupric ions. **B. Ergul**, W. Zhao

3:50 ENVR **242.** Speciation behavior of transition and rare earth metal binding by monorhamnolipids. **R. Eismin**, R.M. Maier, J.E. Pemberton

4:15 ENVR **243.** Water purification through graphene oxide-insoluble salt composite membranes. **D. Wang**, W. Zhao

4:40 Concluding Remarks.

Section D

Colorado Convention Center
Room 709

Hydraulic Fracturing Impacts on Water, Soil and Air Quality

Treatment and Regulations

Cosponsored by MPPG‡

J. Blotevogel, T. Borch, *Organizers*
R. Jackson, R. D. Vidic, *Organizers, Presiding*

1:30 ENVR **244.** Origin of radioactivity in Marcellus Shale flowback water and potential concerns with radioactivity in wastes generated by unconventional gas industry. **T. Zhang**, R.D. Vidic

1:55 ENVR **245.** Advanced treatment for water-recycling: Characterization and pretreatment of the particulate foulants for microfiltration in flowback and produced water from Marcellus shale gas play. **B. Xiong**, M. Kumar, A.L. Zydney

2:20 ENVR **246.** Composition and associated hazards of well stimulation fluids used in California (USA). **W. Stringfellow**, T. McKone, W. Sandelin, R. Maddalena, M. Heberger, C. Varadharajan, P. Jordan, J. Domen, H. Cooley, M. Reagan, R. Tinnacher, M. Camarillo, J. Houseworth, J. Birkholzer

2:50 ENVR **247.** Identifying gaps in hydraulic fracturing wastewater management practices across four North American basins. **D.S. Alessi**, C.A. Notte, D. Thompson, S. Kletke, J. Brisbois, D.M. Allen, J. Gehman, G.G. Goss

3:15 ENVR **248.** Characterization and analysis of liquid waste from Marcellus Shale gas development. J. Shih, J. Saiers, S.C. Anisfeld, J. Chu, L. Mueclenbachs, S. Olmstead, **A. Krupnick**

3:40 Intermission.

3:55 ENVR **249.** Perspectives on hydraulic fracturing in Atlantic Canada: Overview of recent regulatory activities and social license to operate with an environmental context. G.A. Gagnon, **W. Krkosek**, B. Trueman, L. Anderson

4:20 ENVR **250.** Examining memorandums of understanding as a policy solution for hydraulic fracturing in Colorado. **S. Zilliox**, A. Shaffer, J.S. Rolston

4:45 ENVR **251.** Managing the risks of shale gas development using innovative legal and regulatory approaches. **S. Olmstead**, N. Richardson

5:10 Concluding Remarks.

WEDNESDAY MORNING

Section A

Colorado Convention Center
Room 703

Water Sustainability in Oil and Gas Exploration: Treatment Issues

Cosponsored by CEI and MPPG‡

T. Y. Cath, K. Linden, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENVR **252.** Chemicals used for matrix acidization, an unconventional oil stimulation technique. **K. Abdullah**, M. Stenstrom, I. Suffet

8:30 ENVR **253.** Water supply and unconventional energy development in the Denver-Julesburg basin: A case study in the South Platte watershed. **E. Walker**, A. Anderson, C. Barry, T.S. Hogue

8:55 ENVR **254.** Feasibility of thermal technologies for reuse of oil and gas exploration and production wastewaters. **V. Gadhamshetty**, V. Gude

9:20 ENVR **255.** Mechanically strong aerogel fabrics for oil capture and recovery. **O. Karatum**, S.A. Steiner III, D.L. Plata

9:45 ENVR **256.** Application of AMD for produced water reuse: Equilibrium and kinetics of solid precipitation and solid waste management. **C. He**, R.D. Vidic

10:10 Intermission.

10:10 ENVR **257.** Comparing electrocoagulation, dissolved air flotation, and traditional coagulation/flocculation as pretreatment for hydraulic fracturing wastewater. K. Sitterley, **J. Rosenblum**, K. Linden

10:35 ENVR **258.** Removal mechanisms of boron during aluminum electrocoagulation of hydraulic fracturing flowback water. **S. Chellam**, M. Sari

11:00 ENVR **259.** Coupling magnetic Pickering emulsions to membrane filtration for non-fouling oil/water separations. **D. Jassby**

11:25 ENVR **260.** Engineered osmosis technology for desalination of oil and gas exploration wastewaters: Progressive assessment of membrane performance and process sustainability. **B.D. Coday**, T.Y. Cath

Section B

Colorado Convention Center
Room 705

Surface Physicochemical Processes in Engineered and Natural Systems

Cosponsored by AGRO and MPPG‡

H. J. Zhang, *Organizer*
J. M. Cerrato, H. Liu, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 ENVR **261.** Multifunctional nanostructured composite materials for highly active reductive catalysis water treatment applications. J. Liu, X. Chen, Y. Wang, P. Wang, C.J. Werth, **T.J. Strathmann**

9:15 ENVR **262.** Photocatalytic reductive treatment of hexavalent chromium using barium doped TiO_2. M. Chen, W. Wang, Y. Yin, **H. Liu**

9:35 ENVR **263.** Transformation of hexavalent chromium via redox pathways in drinking water: Implications on Cr(VI) control and treatment. **H. Liu**, M. Chebeir, H. Sohn

9:55 ENVR **264.** Hexavalent chromium removal by electrocoagulation in drinking water system. **C. Pan**, D. Giammar, M. Marni, J.G. Catalano

10:15 ENVR **265.** Effects of water hardness and humic substances on Cr(VI) removal from aqueous systems using pyrite as the reducing agent. **C. Kantar**, M.S. Bulbul

10:35 Intermission.

10:50 ENVR **266.** Impact of hematite nanoparticle ($n\alpha$-Fe_2O_3) morphology and size on photocatalytic potential as exampled by reduction of chromate. **A.W. Lounsbury**, J. Yamani, N. Billmyer, J.B. Zimmerman

11:10 ENVR **267.** Functionalization of boron-doped diamond electrodes for the minimization of perchlorate formation during electrochemical advanced oxidation processes. **B.P. Chaplin**, W. Jawando, P. Gayen

11:30 ENVR **268.** One-pot electrospinningfFabrication of Pd-carbon nanofiber catalysts for contaminant hydrogenation. **T. Ye**, D. Shuai

11:50 ENVR **269.** Visible-light-responsive graphitic carbon nitride for photocatalytic degradation of persistent waterborne contaminants. **Q. Zheng**, D. Shuai, N. Bensalah

Section C

Colorado Convention Center
Room 707

Microalgae: A Renewable Energy Source and a Sustainable Solution for the Environment

Cosponsored by AGRO

D. Shuai, *Organizer*
B. P. Chaplin, W. Zhang, *Organizers, Presiding*

8:30 Introductory Remarks.

8:40 ENVR **270.** Green algae cultivation and engineering of its fatty acid synthase. **M.D. Burkart**

9:20 ENVR **271.** Using a pH-stat to understand how the N source affects the concentration of inorganic carbon in microalgae culture. **B. Nguyen**, B.E. Rittmann

9:40 ENVR **272.** Using carbon dioxide to maintain the abundance of the oleaginous microalgae *Scenedesmus dimorphus* in mixed-culture growth reactors. **M.J. Giannetto**, A. Retotar, H. Rismani Yazdi, J. Peccia

10:00 Intermission.

10:20 ENVR **273.** Energy efficient urban wastewater treatment using *Galdieria sulphuraria*. **T. Selvaratnam**, N. Nagamany, L. Peter

10:40 ENVR **274.** Novel shortcut nitrogen removal process by algal-bacterial consortia in a sequencing batch photobioreactor (SBPR). **M. Wang**, H. Yang, **S. Ergas**, P. van der Steen

11:00 ENVR **275.** Role of filamentous cyanobacteria in granular biofilms containing microalgae and bacteria. **K. Stauch-White**, C. Kuo-Dahab, K. Milferstedt, C. Park, C. Butler

11:20 ENVR **276.** Light and COD effects on the performance of photosynthetic microbial desalination cells. **B. Kokabian**, **V. Gude**

11:40 ENVR **277.** Passive membrane photobioreactor for the isolated cultivation of algal resource utilizing selectivity (ICARUS) using wastewater as a feed stock. **I. Drexler**, M. Pickett, M. Heintz, D. Yeh

Section D

Colorado Convention Center
Room 709

Trace Materials in Air, Soil, and Water

Cosponsored by MPPG‡

A. Rihana, *Organizer*
M. A. Benvenuto, K. R. Evans, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 ENVR **278.** Flame retardants in Chicago's atmosphere and sediment of the Chicago Sanitary and Ship Canal. **A. Peverly**, M. Venier, Y. Ma, Z. Rodenburg, K.C. Hornbuckle, R.A. Hites

8:55 ENVR **279.** Are pink salt, blue salt, and other "healthy" salts worth their price? Their analysis by energy dispersive X-ray fluorescence spectrometry. **S. Maurice**, C. Roberts, C. Kashat, M.A. Benvenuto, E. Roberts-Kirchhoff

9:15 ENVR **280.** New insights into mercury speciation in freshwaters using mercury-thiourea complex ion chromatography with ICP-MS detection. **T.H. Huang**, O.A. Todd, R.J. Hudson

9:35 ENVR **281.** Single extraction methodology for amino sugars as biomarkers in environmental matrices. **T.C. Vandenboer**, R. Hems, R. Di Lorenzo, S. Ziegler, C. Young

9:55 Intermission.

10:10 ENVR **282.** Molecular sensing at graphene grain boundaries. **P. Kral**

10:30 ENVR **283.** Iron analysis in aging water pipes using cloud point extraction method. **Z. Li**, A. Rihana, K.C. Lanigan

10:50 ENVR **284.** Analyzing the correlation of volatile organic compounds with ozone formation in the Houston-Galveston-Brazoria area Using CAMx. M. Shahriar, A. Kadiyala, **R.R. Kommalapati**, Z. Huque

11:10 ENVR **285.** Fate of oxyhalide disinfection by-products in hypochlorite solution storage tanks. **A. Breytus**, S. Prabakar, A.P. Kruzic

11:30 Concluding Remarks.

Section E

Colorado Convention Center
Room 711

Environmental Implications of Nano: Release from Consumer Products and Advances in Nanometrology

C. P. Higgins, J. F. Ranville, *Organizers*
R. B. Reed, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 ENVR **286.** Tracking nanomaterials through the laundry wash cycle: Release, dissolution, and complexation. **D. Mitrano**, B. Nowack

8:25 ENVR **287.** Prospecting silicon dioxide in foods: Occurrence, characterization, and toxicity. Y. Yang, J. Faust, J. Schoepf, K. Hristovski, R.L. Tanguay, D.G. Capco, P. Herckes, **P.K. Westerhoff**

8:45 ENVR **288.** Characterization of nanosilica release from a weathered nanosilica/polyurethane coating. **L. Sung**, S. Huang, Y. Cheng, D. Stanley, S. Rabb, P. Krommenhoek, L. Yu, T. Nguyen

9:05 ENVR **289.** Evaluation of nanoparticle release from polymer nanocomposites loaded with fluorescent quantum dots. **K. Pillai**, P. Gray, C. Tien, R. Bleher, L. Sung, T.V. Duncan

9:25 ENVR **290.** Influence of loading on the degradation and release of carbon nanotubes from polymer nanocomposites. **H. Fairbrother**, R. Lankone, D.G. Goodwin, E.J. Bouwer, J.F. Ranville, J. Wang

9:45 ENVR **291.** Evaluation of silver nanoparticle– impregnated fabrics across their life cycle. **R.B. Reed**, J.F. Ranville, R.L. Tanguay, J.E. Hutchison, P.K. Westerhoff, T. Zaikova

10:05 Intermission.

10:20 ENVR **292.** Engineered nanoparticles in the environment: From theory to practice. A.P. Gondikas, **F. Von Der Kammer**, R.B. Reed, R. Kaegi, T. Hofmann

10:40 ENVR **293.** Single particle ICP-MS (SP-ICP-MS) for the detection of metal-based nanoparticles in environmental matrices. **C. Stephan**

11:00 ENVR **294.** Development of novel methodology to quantify silver release from polymer nanocomposites. **A. Barber**, R. Lankone, J. Wang, H. Fairbrother, P.K. Westerhoff, J.F. Ranville

11:20 ENVR **295.** Improvements in the detection and characterization of silica nanomaterials using spICP-MS. **M.D. Montano**, B. Majestic, J.F. Ranville

11:40 ENVR **296.** Measuring nanocarbon fluxes by tracing stable isotope labelled nanomaterials. **T.D. Berry**, T.R. Filley

Elucidation of Mechanisms & Kinetics on Surfaces

Sponsored by COLL, Cosponsored by CATL and ENVR

WEDNESDAY AFTERNOON

Section A

Colorado Convention Center
Room 703

Water Sustainability in Oil and Gas Exploration: Treatment Issues

Cosponsored by CEI and MPPG‡

T. Y. Cath, K. Linden, *Organizers, Presiding*

1:30 ENVR **297.** Removal of radium from shale gas wastewater using cation exchange resin. **Y. Bi**, H. Zhang, K.F. Hayes, B. Ellis

1:55 ENVR **298.** Fate of radium in wastewater produced during unconventional gas extraction during carbonate precipitation reactions. **Y. Li**, R.D. Vidic

2:20 ENVR **299.** Fate of NORM in flowback water and waste management strategies during water reuse for hydraulic fracturing in Marcellus Shale. **T. Zhang**, R.D. Vidic

2:45 ENVR **300.** Biological treatment of flowback water from a hydraulically fractured well. **J. Rosenblum**, K. Sitterley, I. Morrissey, K. Linden

3:10 Intermission.

3:30 ENVR **301.** Anammox biocathode for sustainable microbial desalination of brackish waters. **B. Kokabian**, **V. Gude**

3:55 ENVR **302.** Microbial mats as a biological treatment approach for produced water from hydraulic fracturing. B. Akyon, E. Stachler, N. Wei, **K. Bibby**

4:20 ENVR **303.** Microbial capacitive desalination for organic and salt removal and energy production from unconventional natural gas produced water. C. Forrestal, A. Haeger, L. Dankovich, **Z. Ren**

4:45 ENVR **304.** Biological active filtration treatment of O&G flowback and produced waters. **T.Y. Cath**, D.E. Freedman, S.M. Riley

5:10 Concluding Remarks.

Section B

Colorado Convention Center
Room 705

Surface Physicochemical Processes in Engineered and Natural Systems

Cosponsored by AGRO and MPPG‡

H. J. Zhang, *Organizer*
J. M. Cerrato, H. Liu, *Organizers, Presiding*

1:30 ENVR **305.** Interactions and reactions of organic compounds at interfaces between water and pyrogenic carbonaceous materials. **J.J. Pignatello**

2:10 ENVR **306.** Oxidative reactivity of MnO_2 in mixtures with Fe^{III} oxides and/or natural organic matter (NOM). **H. Zhang**, S. Taujale

2:30 ENVR **307.** Oxidative degradation of trinitrotoluene by mixed metal oxide nanoparticles in water. **G.S. Harbison**, Y. Kye, M.A. Langell, M. Kumbier

2:50 ENVR **308.** Adsorption and photocatalysis of ciprofloxacin using alumina-titania particles synthesized via sol-gel process. **C. Dozier**, L.E. Katz, H. Liljestrand

3:10 ENVR **309.** Mechanistic comparison of isomeric oxorhenium(V) complexes coordinated with a oxazoline-phenolate ligand for highly active perchlorate reduction in water. **J. Liu**, D. Wu, S.Y. Kimura, J.R. Shapley, M.M. Abu-Omar, C.J. Werth, T.J. Strathmann

3:30 Intermission.

3:45 ENVR **310.** Post-pyrolysis air oxidation of biochars: A simple and effective method for enhancing adsorption of ionizable organic compounds. **F. Xiao**, J.J. Pignatello

4:05 ENVR **311.** Photoenhanced chlorination of hydroxylated fullerene (fullerol) in water. **J. Wu**, L. Alemany, D.N. Benoit, W. Li, J. Fortner

4:25 ENVR **312.** Insight into anti-scaling mechanisms of phosphonates and organic polymers for the control of barium sulfate scales. **C. He**, R.D. Vidic

4:45 ENVR **313.** Mesoporous silica supported bimetallic Pd/Fe nanocompositea for enhanced reductive dechlorination of tetrachloroethylene. **R. Doong**, C. Lee

Section C

Colorado Convention Center
Room 707

Microalgae: A Renewable Energy Source and a Sustainable Solution for the Environment

Cosponsored by AGRO

B. P. Chaplin, *Organizer*
D. Shuai, W. Zhang, *Organizers, Presiding*

1:30 Introductory Remarks.

1:40 ENVR **314.** Applications of polymer-coated magnetic nanoparticles for algal biomass harvesting. **W. Zhang**, S. Ge, M. Agbakpe

2:00 ENVR **315.** Fluorescein induced spectral conversion for the growth of *Chlorella vulgaris*. Y. Orduz, **J.R. Pinzón**

2:20 ENVR **316.** Direct visualization of nutrient consumption within microbial communities using NanoSIMS. **C.R. Anderton**, J.K. Cole, J.J. Moran, J.M. Mobberley, M. Hess, S.R. Lindemann, L. Paša-Tolić

2:40 ENVR **317.** Photogeneration of reactive oxygen species (ROS) by extracellular organic matter (EOM) in *Chlamydomonas reinhardtii* photobioreactor cultures. **R. Tenorio**, J. Guest, T.J. Strathmann

3:00 Intermission.

3:20 ENVR **318.** Predicting microalgae hydrothermal liquefaction biocrude oil yield and properties from microalgae biochemical composition. **S. Leow**, J.R. Witter, D.R. Vardon, B.K. Sharma, J.S. Guest, T.J. Strathmann

3:40 ENVR **319.** Coupling fluid dynamics with kinetic modeling to quantify the effects of photosynthetic bioreactor design and operation on yield performance. **R. Manavi**, S. Yamamoto, J.W. Levis, J. Ducoste, F. De Los Reyes, R. Ranjithan

4:00 ENVR **320.** Life cycle-optimization framework for photosynthetic biorefineries. **R. Manavi**, A. Karam, C. McMillan, J.W. Levis, F. De Los Reyes, J. Ducoste, R. Ranjithan

4:20 ENVR **321.** Environmental and economic performance analysis of three techniques for breaking microalgae cell wall in the biodiesel production process. M. Collotta, R. Lee, A. Ramos, **P. Champagne**, P.G. Jessop, W. Mabee

Section D

Colorado Convention Center
Room 709

Trace Materials in Air, Soil, and Water

Cosponsored by MPPG‡

K. R. Evans, *Organizer*
M. A. Benvenuto, A. Rihana, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 ENVR **322.** Elemental characterization of $PM_{2.5}$ and PM_{10} emitted from light duty vehicles in the Washburn Tunnel of Houston, Texas: Release of rhodium, palladium, and platinum. **S. Chellam**, A. Bozlaker, N. Spada, M. Fraser

1:55 ENVR **323.** Synthesis of a series of highly multi-dentate podand ligands as possible water remediation agents. **C. Kashat**, M.A. Benvenuto

2:15 ENVR **324.** Metal concentrations and soluble iron speciation in fine particulate matter from light rail activity in the Denver-Metropolitan area. **B.T. Cartledge**, B. Majestic

2:35 ENVR **325.** Nontoxic, air stable quantum dots for low level metal detection in water. **H. Meylemans**, L. Cambrea

2:55 Intermission.

3:10 ENVR **326.** Stable isotopes of lead and strontium as tracers of sources of airborne particulate matter in Kyrgyzstan. **N. Dewan**, B.J. Majestic, M.E. Ketterer, J.P. Miller-Schulze, M.M. Shafer, J.J. Schauer, P.A. Solomon, M. Artamonova, B.B. Chen, S.A. Imashev, G.R. Carmichael

3:30 ENVR **327.** Monitoring metal contamination from artisanal and small-scale gold mining (ASGM) communities in Ecuador Part I: Mercury emissions to air. **A.M. Kiefer**, C.S. Seney

3:50 ENVR **328.** Monitoring metal contamination from artisanal and small-scale gold mining (ASGM) communities in Ecuador Part II: Analysis of water, soil, and tailings. **C.S. Seney**, A.M. Kiefer, J.D. Mimbs

4:10 ENVR **329.** New diffusive gradients in a thin film technique for measuring nitrate using ion exchange resin. **J. Huang**, W. Bennett, P. Teasdale, D. Welsh

4:30 ENVR **330.** Modeling TCE concentration in groundwater using MATLAB. A. Rihana, **Y. Pang**, Y. Gao

4:50 Concluding Remarks.

Elucidation of Mechanisms & Kinetics on Surfaces

Sponsored by COLL, Cosponsored by CATL and ENVR

WEDNESDAY EVENING

Section A

Colorado Convention Center
Hall C

Advances in Analytical Chemistry for Discovering Emerging Contaminants in the Natural Environment

Cosponsored by MPPG

D. Alvarez, T. L. Jones-Lepp, *Organizers*

6:00 - 8:00

ENVR **331.** Quantitation and identification of PPCP in environmental samples using accurate mass MS/MS technology. **C. Borton**, R. Kern, A. Schreiber

ENVR **332.** Contaminants of emerging concern in effluent dominated coastal waterways in southern California.. **K.A. Maruya**, N.G. Dodder, T. Anumol, S. Shane, W. Lao, A. Sengupta, J. Drewes

Section A

Colorado Convention Center
Hall C

Assessing Toxicity of Environmental Contaminants

Cosponsored by MPPG‡

S. M. Uchimiya, J. Wang, *Organizers*
X. Pan, B. Zhang, *Organizers*

6:00 - 8:00

ENVR **333.** Influences of environmental conditions on the aquatic toxicity of silver nanoparticles to *Daphnia magna*.. **R.M. Sofield**, A. Nieman, M. Abernathy, A. Gibson

ENVR **334.** Hydrogen peroxide production in the presence of soot and biological electron donors. D. Hinz, **J. Barnes**, A.M. Johansen

Section A

Colorado Convention Center
Hall C

Bioavailability and Biogeochemical Interactions Affecting Remediation of Hazardous Substances in the Environment

Cosponsored by MPPG‡

M. F. Benedetti, *Organizer*
H. Henry, J. F. Ranville, *Organizers*

6:00 - 8:00

ENVR **335.** Remediation of soil polluted area in Ondo State, Nigeria. **A.E. Folorunso**

ENVR **336.** Phytoremediation on heavy metal contaminants in sewage river sediment. **X. Mao**, F.X. Han, K. Guo

ENVR **337.** Relative impact of temperature, groundwater chemistry, and groundwater hydrology on inorganic nitrogen processing and nitrogen cycle functional genes in sediments of a groundwater flow-through lake. **D.L. Stoliker**, D.A. Repert, R.L. Smith, B. Song, C.H. Conaway, D.R. LeBlanc, T.D. McCobb, S. Hyun, D. Koh, H. Moon, K. Ha, D.B. Kent

‡ *Cooperative Cosponsorship*

Section A

Colorado Convention Center
Hall C

Biogenically Enhanced Recovery and Bioremediation in Fossil Fuel Reservoirs

Cosponsored by MPPG‡

D. L. Drogos, M. Urynowicz, *Organizers, Presiding*

6:00 - 8:00

ENVR **338.** Impacts of microbial community diversity on the occurrence and quantity of crude oil biodegradation and microbial methanogenesis. **J. Shelton**, D.M. Akob, J.C. McIntosh, J.E. McCray

Section A

Colorado Convention Center
Hall C

Chemical Processes at Environmental Interfaces

H. A. Al - Abadleh, H. M. Ali, R. Z. Hinrichs, N. Kabengi, *Organizers, Presiding*

6:00 - 8:00

ENVR **339.** Adsorptive removal of taste and odor compounds onto granular mesoporous carbon (GMC). **S. Kim**, Y. Kim, H. Choi

ENVR **340.** Au nanostar-enabled multifunctional reverse osmosis membranes for reduced mineral scaling, organic-, and bio-fouling. **J. Ray**, S. Tadepalli, S.Z. Nergiz, K. Liu, L. You, Y. Tang, S. Singamaneni, Y. Jun

Section A

Colorado Convention Center
Hall C

Chemistry in the Marine Boundary Layer

Cosponsored by MPPG

B. DAnna, J. Donaldson, *Organizers*

6:00 - 8:00

ENVR **341.** Ocean organics vs. inorganics: The contributions to suppressed $ClNO_2$ yield from the ocean surface following N_2O_5 uptake. **O.S. Ryder**, N. Campbell, T.H. Bertram

ENVR **342.** On the role of dimethyl sulfide and marine biogenic volatile organic compounds in sea spray aerosol growth post production. **N.R. Campbell**, M.J. Kim, M. Zoerb, T.H. Bertram

Section A

Colorado Convention Center
Hall C

Environmental Chemistry and Health Impacts of Fine and Ultrafine Particulate Matter

Cosponsored by MPPG

S. M. Lomnicki, *Organizer*

6:00 - 8:00

ENVR **343.** Using the chemical mass balance for the changes of source apportionment at the heating time of three period in Tianjin, China. W. Hong, **X. Bi**, Y. Feng, J. Wu, K. Chen

ENVR **344.** Comparative study of $PM_{2.5}$ vertical characteristics between heavy pollution weather and clean weather in Tianjin, China. **W. Hong**, **S. Han**, **Y. Zhang**, J. Wang, Y. Feng

Section A

Colorado Convention Center
Hall C

Environmental Chemistry: Pedagogical Models and Practices

Cosponsored by CHED, MPPG‡ and YCC

K. C. Lanigan, E. Roberts-Kirchhoff, *Organizers*

6:00 - 8:00

ENVR **345.** Paper spectrometers: The intersection of environmental chemistry and engineering. **A. Kahl**

Section A

Colorado Convention Center
Hall C

Environmental Implications of Nano: Release from Consumer Products and Advances in Nanometrology

C. P. Higgins, J. F. Ranville, R. B. Reed, *Organizers, Presiding*

6:00 - 8:00

ENVR **346.** Role of CO_2 in the equimolar C_2H_2-CO_2 reaction to synthesize carbon nanotubes: Environmental and mechanistic implications. **W. Shi**, Y. Peng, D.L. Plata

ENVR **347.** Detection of single walled carbon nanotubes using microsecond single particle ICP-MS. **J. Wang**, R. Lankone, H. Fairbrother, C.P. Higgins, J.F. Ranville

ENVR **348.** Aggregation and stabilization of multiwalled carbon nanotubes in aquatic system: Influence of carboxymethyl cellulose, starch, and humic acid. **W. Liu**, X. Zhao, D. Zhao

ENVR **349.** Theoretical and experimental studying of sedimentation of TiO_2 nanoparticles in aqueous solutions. **J. Lu**, D. Liu, H. Liu, X. Yang, F. Cui

ENVR **350.** Dissolved organic matter adsorption to titanium dioxide nanoparticles: Effect of molecular weight fractions and the interaction mechanisms. **X. Yang**, T. Jiang, F. Cui

ENVR **351.** Comparative study of Fe(II)-GAC for bromate or perchlorate removal. **H. Xu**

ENVR **352.** Challenges in the differentiation of nanoparticles when analyzing complex sample matrices using spICP-MS. **E. Gray**, J.F. Ranville, A. Bednar, C.P. Higgins

ENVR **353.** Titanium dioxide nanoparticles induces mitochondrial dysregulation and loss of liver functions. V. Natarajan, C. Wilson, S.L. Hayward, **S. Kidambi**

ENVR **354.** Isotopically-labeled core-shell-shell Ag_{107}@Au@Ag_{109}) nanoparticles to ion and particle bioavailability. **R.C. Merrifield**, J. Lead

ENVR **355.** Asymmetric flow field flow fractionation online with Single particle – inductively coupled plasma mass spectrometry: Detection and quantification of silver nanoparticles in aqueous samples. **K. Huynh**, E. Siska, E. Heithmar

Section A

Colorado Convention Center
Hall C

Environmental Reactivity of Organic Micropollutants and Their Transformation Products in Receiving Waters

Cosponsored by AGRO and MPPG‡

W. Arnold, Y. Chin, K. H. Wammer, *Organizers*

6:00 - 8:00

ENVR **356.** Polychromatic method to determine the wavelength dependence of singlet oxygen quantum yields for natural and effluent organic matter. **J.R. Laszakovits**

Section A

Colorado Convention Center
Hall C

General Posters

S. R. Al-Abed, *Organizer*

6:00 - 8:00

ENVR **357.** Electrolytic disinfection of water contaminated with *E. coli* by treatment with an alternating current using stainless steel and copper electrodes: Role of hydroxyl radicals and hydrogen peroxide formation. **N. Barashkov**, **T. Sakhno**, **I. Irgibayeva**

ENVR **358.** Hydrooligomerization of acetylene from electrocracking gas over Ni/CNFs catalyst. **A.S. Ismail**

ENVR **359.** Removal of micropollutants from surface water and groundwater by portable water filtering system designed for rural communities in underdeveloped countries. **S. Jeong**, K. Koo, **Y. Jeong**

ENVR **360.** Functional forms of the unburned carbon present in coal fly ashes: Role of surface oxygen species in the formation of organic fluorine forms on the carbon surface. **N. Tsubouchi**, Y. Ohtsuka

ENVR **361.** Development of a sheathless particle classifier with an electrometer to measure the particles from automobile. H. Yamada, **H. Okuda**

ENVR **362.** Behavior of mercury in coal combustion residue contaminated sediments. **T.R. Gofstein**, A. Heyes

ENVR **363.** Compared fluorescence characterization of salt marsh pore water using PARAFAC analysis. **J. Bowen**, W.J. De Bruyn, C.D. Clark

ENVR **364.** Analysis of diazepam, diphenhydramine, carbamazepine and metabolites drugs in fish from grocery markets by gas chromatography – mass spectrometry (GC-MS) using SIM mode. M. Arafat, C. Stowe, **D. Johnson**, M.J. Meziani, **M. Mottaleb**

ENVR **365.** Withdrawn.

ENVR **366.** Trace metals in trout species collected from high altitude Colorado lakes. **M. Spedale**

ENVR **367.** Study on the adsorption of ammonia Nntrogen on zeolite modified by ultrasonic and sodium. **W. Qun**, Y. Zhichao, G. Mingkun, C. Bin, X. He, C. Shuang

ENVR **368.** GCMS identification and quantification of the lipids produced via esterification to FAMEs in *Neochloris minuta* (UTEX 776) algae induced by nitrogen deprivation. **D.G. Giarikos**, R. Razeghifard, M. Margupuram, C. Chiafair

ENVR **369.** Enhanced reductive degradation of *p*-chloronitrobenzene in a coupled bioelectrode-UASB system. **L. Zhu**, X. Xu, K. Gao, J. Jin

ENVR **370.** Race for the gold metal: A novel approach for reclaiming specialty metals from industrial waste and processing streams. **M.P. O'Connor**, D.L. Plata

ENVR **371.** Spectroscopic and microscopic investigation of soil mineral and natural organic matter-treated silver nanoparticles. **S.R. Kanel**, B.A. Manning, S.W. Brittle, I.E. Pavel Sizemore, D. Felker, D. Kempisty, M.N. Goltz

ENVR **372.** Assessment of clay minerals selectivity for adsorption of humic acid fraction. **M.E. ElSayed**, M.M. Khalaf, J.A. Rice

ENVR **373.** Quantitative analysis of single-particle mass spectra acquired in Northfield, MN. **A. Janes**, D.S. Gross

ENVR **374.** Airborne metal concentrations during and after pollution restrictions in Shenzhen. **N. Dewan**, B. Majestic, Y. Wang, Z. Yuan-Xun

ENVR **375.** Photoluminescence quenching of graphene oxide by enzymatic reaction for optical sensing of pesticides. **T. Kang**, S. Jeon, H. Kim, J. Kim

ENVR **376.** Combining Fenton's oxidation and biodegradation to degrade decabromodiphenyl ether in soil. C. Lin, C. Yang, **Y. Chang**

ENVR **377.** Assessment and spatial variation analysis of water quality in Grand Bay national estuarine research reserve. **J. McComb**, C.C. Thomas, Z. Arslan, F.X. Han

ENVR **378.** Groundwork for the development of a model for determining atmospheric mercury in the arid West using leaves. D.W. Lehmpuhl, **L.M. Bartolo**, K.A. Wager

ENVR **379.** Photochemical inactivation of *E. faecalis* in the presence of organic matter. **S. Mostafa**, M. Rubinato, F.L. Rosario, K. Linden

ENVR **380.** Disinfection by-products as endocrine active substances. **B.E. Holmes**, L. Smeester, R.C. Fry, H. Weinberg

ENVR **381.** Dissolved organic carbon (DOC) release following drought: influence of DOC source and drought severity on drinking water treatment. **J. Ritson**, N. Graham, M. Templeton, J. Clark, C. Freeman

ENVR **382.** Synthesis and characterization of nanocomposites of Au@Ag@rGO and their use in degradation of organic dyes. E. Mejía-Ospino, R. Cabanzo, **S.E. Castellanos**

ENVR **383.** Enhanced air-cathode microbial fuel cell (MFC) performance with oxygen supply from an externally connected algal bioreactor (ABR). **R. Kakarla**, B. Min

ENVR **384.** Microbial electrosynthesis of high-value products from volatile fatty acids present in anaerobic digestion effluent. S. Kondaveeti, **B. Min**

ENVR **385.** Reduced polyoxometalates initiate HO formation from aqueous ozone. **B. Solomon**, J. Ferry

ENVR **386.** Quantitative analysis of atmospheric aerosol with atomic force microscopy. **W. Kong**, L. Hawkins

ENVR **387.** Halide ions as tracers for human wastewater inputs to an agricultural watershed. **A. Thayer**, C. Spiese

ENVR **388.** Reductive remediation of trichloroethylene (TCE) solution by granulated nano zero-valent iron (nZVI). Y. Shih, C. Su, C. Chen, C. Chen, **C. Dong**

ENVR **389.** Photolysis and UV/H_2O_2 advanced oxidation processes of bisphenol-s in water. **M. Mbewe**, R. Beil, J. Jin, P.A. Ruiz-Haas

ENVR **390.** Exploring the relevant parameter space in shale rock geochemistry: Organic transformations at temperature and pressure. **A. Sumner**, B. Drollette, D.L. Plata

ENVR **391.** Silver nanoparticle adsorption to corundum surfaces as a function of solution pH and time. **J. Purvis**, K. O'Neil, S.W. Brittle, I.E. Pavel Sizemore, S.R. Higgins

ENVR **392.** Toxic effects of multiwall carbon nanotubes to *Pseudomonas aeruginosa* and its predator *Tetrahymena thermophila*. **M. Mortimer**, E. Orias, E. Petersen, B.A. Buchholz, P. Holden

ENVR **393.** Photolysis and toxicity of the organic UV filter chemical octylmethoxycinnamate and its photoproducts. **C.A. Berg**, L. MacManus-Spencer, M.G. Paulick

ENVR **394.** Heterogeneous photochemistry of nitrate chemisorbed on TiO_2 as a function of relative humidity. **D.M. Lesko**, H.D. Swomley, J.G. Navea

ENVR **395.** Improvement of antisintering of Ca-based sorbents by thermally treated vermiculite. **J. Meng**, H. Li, B. Meng, J. Li, L. Shan, Y. Yu, Y. Min, D. Xu

ENVR **396.** Experiment on CO_2 capturing capacity of attapulgite modified CaO-based sorbent in calcination/carbonation cycle. **L. Shan**, H. Li, J. Meng, B. Meng, J. Li, Y. Yu, Y. Min, D. Xu

ENVR **397.** Metal oxide modified limestone for CO_2 adsorption. **J. Li**, H. Li, B. Meng, Y. Yu, Y. Min, D. Xu

ENVR **398.** Enhancement of CO_2 sequestration of limestone with carbon additives. **B. Meng**, H. Li, W. Yang, J. Li, Y. Yu, Y. Min, D. Xu

ENVR **399.** Virucidal activity of a multilevel antimicrobial air filter. W. Han, Q. Chang, Y. Lai, **Y. Li**, Y. Yang, C. Wu, K.L. Yeung, C. Chao, Z. Yang

ENVR **400.** Design, synthesis, and characterization of isoprene hydroperoxides. **E. Lozano**, V. Kumar, A. Abdelhamid, A. Hasson, S. Maitra

ENVR **401.** Exploring the environmental controls on the degradation of oil by marine fungi. **C.M. Poutasse**, R. Simister, H.K. White

ENVR **402.** Exposure to engineered nanomaterials in various consumer products. **B. Lee**, G. Yu, M. Kim, H. Kim

ENVR **403.** Reactivity of an epoxy coating with free and combined chlorine in drinking water service lines. **E.F. Peltier**, Z.A. Breault, R.F. Lane, S.J. Randtke, R.E. Carter, C.D. Adams

ENVR **404.** Oxidation of surface-adsorbed anthracene on a quartz fiber substrate. **J. Bilek**, R. Cochran, H. Jeong, E.I. Kozliak, A. Kubatova

ENVR **405.** Effect of relative humidity on HCl formation from the reaction of H2SO4, HNO3 and with NaCl. **K. Newhouse**, B. Fong, H.M. Ali

ENVR **406.** Resistance of synthetic organic aerosol chromophores to photobleaching under oxidative conditions. **A. Lemire**, L. Hawkins

ENVR **407.** Degradation of diclofenac in water with TAML activators and hydrogen peroxide. **M.R. Mills**, A.V. Cheng, A.D. Ryabov, T.J. Collins

ENVR **408.** Limonene reactivity on mineral surfaces and the impact of relative humidity and adsorbed nitric acid. **A. Staniec**, R.Z. Hinrichs

ENVR **409.** Quantifying the solar energy absorbed by nitrophenols adsorbed on atmospheric aerosol substrates. **J. Trivedi**, R.Z. Hinrichs

ENVR **410.** Investigating the reversibility of self-assembled humic acid structures. **G. Chilom**, M.M. Khalaf, J.A. Rice

ENVR **411.** Withdrawn.

ENVR **412.** Use of chlorate, nitrate, and perchlorate to promote crude oil mineralization in salt marsh sediments. **M. Brundrett**, J. Horita, T.A. Anderson, D. Reible, J. Pardue, A. Jackson

ENVR **413.** Influence of stabilizer size and chelation strength on iron nanoparticle oxidation. **N. Rentz**, L.F. Greenlee

ENVR **414.** Online monitoring of ambient fungal spore concentrations in the harbour region of Cork, Ireland. **D.J. O'Connor**, D.A. Healy, J.R. Sodeau

ENVR **415.** Quantum mechanical calculations of nitric acid chemisorbed on several crystalline structures of TiO_2 anatase. **M.J. Lueckheide**, J.G. Navea

ENVR **416.** Simultaneous removal of SO_2 and NOx from combustion flue gas in a discharge plasma reactor. **L. Qi**, Y. Zhang

ENVR **417.** Array-based detection of carcinogens and carcinogen metabolites in urine. **L. Gareau**, N. Serio, L. Prignano, M. Levine

ENVR **418.** Arsenic release mechanism in the shallow and deep aquifer in Chiayi County, Taiwan. **C. Lee**, Y. Lin, S. Wang

ENVR **419.** Effect of photochemical weathering on the composition and spectroscopic properties of crude oil. **O.C. Stewart**, C.M. Sharpless, C.M. Reddy, B. Swarthout, C. Aeppli

ENVR **420.** Use of LIBS to detect CO_2 leaks from geological storage based on mineral carbonate interactions in groundwater. **J. Jain**, H. Edenborn, C. Goueguel, C. Carson, D. McIntyre

ENVR **421.** Examining the desorption of oil from persistent surface residual oil balls (SRBs). **S.L. Lyons**, H.K. White

ENVR **422.** Comparative evaluation of the dissolution of fly ash from different source regions under atmospherically relevant conditions. J.R. Borgatta, **A. Paskavitz**, J.G. Navea

ENVR **423.** Colorimetric evaluation of the cation exchange of aluminum with iron in humic acids. **J.R. Borgatta**, J.G. Navea

ENVR **424.** Electrochemical dechlorination of TCE in the presence of natural organic matter, metal ions and nitrates in a simulated karst aquifer. **N. Fallahpour**, X. Mao, L. Rajic, A. Alshawabkeh, S. Yuan

ENVR **425.** Electrochemical degradation of chlorobenzene in groundwater using Pd- catalytic electro-Fenton's reaction. **R. Nazari**, A. Ciblak

ENVR **426.** New spectroscopic method for characterizing the nutritional quality of fruit resources available to wildlife in a Western New York habitat. **S.B. Smith**, M. Bida, S. Schroeder, G. Wink, T.E. Pagano

ENVR **427.** Extraction and separation of contaminants in water systems. **M. Jones**, B. Caldwell, A. Newsham, B.H. Barton, R.E. Del Sesto, A.T. Koppisch, S. Iyer

ENVR **428.** Measuring the emission efficiency and nicotine delivery of electronic cigarette. **G. Wink**, R.J. Robinson, A.G. DeFrancesco, S.B. Smith, T.E. Pagano

ENVR **429.** Microbe-metal interactions along a produced water impacted stream system. **J. Klinges**, D.M. Akob

ENVR **430.** Airborne antibiotic resistant genes upwind and downwind of poultry concentrated animal feeding operation. **H.M. Sanchez**, J.A. Jay

ENVR **431.** Withdrawn.

ENVR **432.** Direct synthesis of V_2O_5-WO_3-TiO_2 nanoparticles with enhanced low-temperature activity for NH_3-SCR. **K. Cheng**, **Z. Zhao**, **J. Liu**

ENVR **433.** Enantioselective disposition of 2,2',3,5',6-hexachlorobiphenyl (PCB 95) and its metabolites in mouse dams dosed during pregnancy. **I. Korwel**, C. Barnhart, K. Truong, P. Lein, H.J. Lehmler

ENVR **434.** Withdrawn.

ENVR **435.** Use of flue gas desulfurization (FGD) gypsum as a heavy metal stabilizer in contaminated soils. **N.H. Koralegedara**, S.R. Al-Abed, D.D. Dionysiou

ENVR **436.** Trace metal emissions from the combustion of fecal char briquettes and a comparison to other solid fuels. **M.J. Price**, W.M. Champion, B.J. Ward, B.T. Cartledge, B. Majestic, L.D. Montoya

ENVR **437.** Hexadecyl trimethyl ammonium bromide dispersed nano zero-valent iron for discoloration of methyl orange. **X. Wang**, P. Wang, L. Le

ENVR **438.** Wireless glucose sensor utilizing magnetic nanoparticles embedded hydrogel. **J. Park**, C. Zhang, P.V. Braun, R.A. Siegel, **B. Ziaie**

ENVR **439.** Fecal and urinary elimination kinetics of cephalosporin and lincosamide antibiotics in dairy cows following intramammary infusion: Application of SPE clean-up and UPLC-MS/MS quantification approach. **P. Ray**, K.F. Knowlton, C. Shang, K. Xia

ENVR **440.** New insights into the function of potassium carbonate species and the superiority of base metals to noble metals in the polytitanate nanobelt supported LNT catalysts. **Y. Zhang**, M. Meng

ENVR **441.** Effects of filtration on the detection, quantification, and characterization of engineered nanoparticles in water samples using single particle inductively coupled plasma mass spectrometry. **E. Siska**, K. Huynh, E.M. Heithmar

ENVR **442.** Analysis of water and soil of La Encantada fall in Anasco, Puerto Rico. **K. Matias**

ENVR **443.** Effects of speciation on mercury co-selection for antibiotic resistance genes in fresh and brackish water microcosms. **C.M. Echeverria Palencia**, S. Hafeznezami, C. Marambio Jones, A. Zimmer-Faust, V. Thulsiraj, S. Mahendra, J.A. Jay

ENVR **444.** Withdrawn.

ENVR **445.** Developing tailored bioreactive silica-gels for pollutant removal and biodegradation. **J.K. Sakkos**, A. Ish Am Radian, B.R. Mutlu, L.P. Wackett, A. Aksan

Section A

Colorado Convention Center
Hall C

Green Chemistry and the Environment

A. M. Balu, R. Luque, S. O. Obare, *Organizers*

6:00 - 8:00

ENVR **446.** Multi-electron transfer process for the degradation of toxic organophosphorus contaminants. **S. Santos**, S.O. Obare

ENVR **447.** Superoxide radical as a green reagent and an ultimate solution of environmental problems. **U. Stoin**, Y. Sasson

ENVR **448.** Development of low density solvent DLLME-GC/MS method for quantitation of tetrabromobisphenol-A from dust. **J.E. Owens**, C. Barrett, D.A. Orban, S.E. Seebeck, L. Lowe

ENVR **449.** Glow in the dark: Luminescent metal organic frameworks (MOFs) grown from cotton fibers. **R.R. Ozer**, J.P. Hinestroza

Section A

Colorado Convention Center
Hall C

Modern Analytical Approaches for the Characterization of Natural Organic Matter in the Environment

Cosponsored by ANYL and MPPG

G. Aiken, K. Cawley, J. A. Korak, F. L. Rosario, *Organizers*

6:00 - 8:00

ENVR **450.** Evaluating the treatability and reactivity of wildfire-impacted DOM using leachates from burned sediments. **A.K. Hohner**, K. Cawley, P. Omur-Ozbek, R. Summers, F.L. Rosario-Ortiz

ENVR **451.** Photochemical processing of wastewater impacted streams. **C. Glover**, F.L. Rosario

ENVR **452.** Development of a novel microscope spectrofluorometer for individual bioparticle characterization. **B.E. Swanson**, J.A. Huffman, D.R. Huffman

ENVR **453.** Evaluation of total petroleum hydrocarbon analysis specificity. **D.A. Gratson**

Section A

Colorado Convention Center
Hall C

Solutions to Metals Contamination of Water

Cosponsored by MPPG‡

S. Ahuja, J. W. Finley, J. N. Seiber, *Organizers*

6:00 - 8:00

ENVR **454.** Novel method for measuring arsenic in water using nanostructured surface. N. Mosquera, **W. Marimon Bolivar**, L. Yate, E. Coy, E. Gonzalez

ENVR **455.** Biosurfactants as a tool for metal removal from waste effluents. **D. Hogan**, J.E. Pemberton, R.M. Maier

ENVR **456.** Chitosan-grafted carbon for the sequestration of heavy metals in aqueous solution. **A.A. Okoya**

Section A

Colorado Convention Center
Hall C

Water Recycling in Domestic Use, Energy Extraction, and Agricultural Use

Cosponsored by AGRO and MPPG‡

I. C. Escobar, J. Hestekin, *Organizers*

6:00 - 8:00

ENVR **457.** Pilot-scale study on the removal of nutritional elements in agricultural runoff by iron-modified biochar. **T. Chi**, J. Zuo, F. Liu

ENVR **458.** Kinetics of hydroxyl radical reactions with chloramines in support of recycling wastewater. K. Couch, **S.P. Mezyk**, K.P. Ishida

ENVR **459.** Sulfate radical remediation of pharmaceuticals in DOM containing wastewaters. **T. Reutershan**, S.P. Mezyk

Section A

Colorado Convention Center
Hall C

Water Sustainability in Oil and Gas Exploration: Treatment Issues

Cosponsored by CEI and MPPG‡

T. Y. Cath, K. Linden, *Organizers*

6:00 - 8:00

ENVR **460.** Evaluation of forward osmosis membranes in long-term oil and gas wastewater treatment stud. **L. Bell**, T.Y. Cath, B.D. Coday

THURSDAY MORNING

Section A

Colorado Convention Center
Room 703

Bioavailability and Biogeochemical Interactions Affecting Remediation of Hazardous Substances in the Environment

Cosponsored by MPPG‡

M. F. Benedetti, *Organizer*
H. Henry, J. F. Ranville, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENVR **461.** Toxicity implications of sulfate radical based oxidative treatment for groundwater remediation. W. Li, D.L. Sedlak, D. Schlenk, **H. Liu**

8:25 ENVR **462.** Methods for simulating the restoration and recovery of acid mine drainage-impacted stream sediment. **J. Williamson**, J.F. Ranville, M.R. Pastorinho, J. Meyer, W.H. Clements

8:45 ENVR **463.** Diffusive gradient in thin film (DGT) passive samplers for monitoring metals in contaminated sediments: Contribution of metal sulfide nanoparticles. **A. Pham**, D. Manley, C. Johnson, H. Hsu-Kim

9:05 ENVR **464.** Biogeochemical processes controlling trace elements in the Grand Bay National Estuarine Reserve in the northern Gulf of Mexico. J. McComb, **F.X. Han**, C. Rogers, C.C. Thomas, Z. Arslan, A. Ardeshir, P. Tchounwou

9:25 ENVR **465.** Stable oxygen isotope enrichment during biotic and abiotic reduction of selenate. **A. Schellenger**, L. Xia, D. Jaisi, P. Larese-Casanova

9:45 ENVR **466.** In situ immobilization of uranium in Hanford sediments with the amendment of phosphate. **Z. Pan**, D. Giammar, V. Mehta, L. Troyer, J.G. Catalano, Z. Wang

10:05 Intermission.

10:20 ENVR **467.** D. Magna metal toxicity in a mining impacted stream: Comparing results in simulated and field-collected waters. **K. Ebeling**

10:40 ENVR **468.** Comparing the partition and sorption behavior to agricultural soils of Bisphenol A (BPA) and BPA alternatives: BPS and BPAF. **Y. Choi**, L.S. Lee

11:00 ENVR **469.** Perfluoroalkyl acids inhibit TCE dechlorination by repressing *Dehalococcoides* growth. **T.S. Weathers**, K. Harding, L. Alvarez-Cohen, C.P. Higgins, J.O. Sharp

11:20 ENVR **470.** Enantioselective biotransformation of chiral PCBs in aquatic to riparian food webs. **C.M. Lee**, V.D. Dang, D. Delach, K. Mitra

11:40 ENVR **471.** Compound specific isotope analysis of aromatics and chlorinated aromatics at a fine vertical resolution across the groundwater – surface water sediment interface. **E. Passeport**, R. Landis, K. Chu, G. Lacrampe-Couloume, E. Lutz, E.E. Mack, B. Sherwood Lollar, K. West

Section B

Colorado Convention Center
Room 705

Surface Physicochemical Processes in Engineered and Natural Systems

Cosponsored by AGRO and MPPG‡

H. J. Zhang, *Organizer*
J. M. Cerrato, H. Liu, *Organizers, Presiding*

8:30 ENVR **472.** Fe(II)-catalyzed recrystallization of hematite and goethite revisited. **M. Scherer**, A.J. Frierdich, R.M. Handler, M. Helgeson, K. Rosso, C. Johnson

9:10 ENVR **473.** Interfacial processes affecting the mobility of metals from abandoned uranium mine wastes. **S. Avasarala**, J. Blake, K. Artyushkova, M. Ali, A. Brearly, C. Shuey, P. Robinson, E. Escheverria, F. Escheverria, C. Hirani, J.M. Cerrato

9:30 ENVR **474.** Identification of Mackinawite surface products formed upon reaction with carbon tetrachloride. **Y. Lan**, E.C. Butler

9:50 ENVR **475.** Acoustically enhanced sediment remediation: Characterization of cavitation and pore flow in porous media. **Z. Wei**, J.J. Lenhart, L. Weavers

10:10 ENVR **476.** Characterizing the reactivity of naturally occurring reducing materials with agarose-bound powder disk electrodes. **M.J. Bradley**, R. Meuuwsen, P.G. Tratnyek

10:30 Intermission.

‡ *Cooperative Cosponsorship*

10:45 ENVR **477.** Mechanisms of fluoride removal: Adsorption and co-precipitation with aluminum hydroxide in the presence and absence of NOM. L.E. Katz, D.F. Lawler, K. Alfredo, **M. Stehouwer**, C. Ernst

11:05 ENVR **478.** Heterogeneous nature of permanganate oxidation reactions. **X. Xia**, A.T. Stone

11:25 ENVR **479.** Efficacy of $CaCO_3$ and $CaSO_4$ scaling resistance of polyethylene glycol hydrophilically-modified reverse osmosis membranes in the presence of humic acid. **J. Ray**, W. Wong, Y. Jun

11:45 ENVR **480.** Radioluminescent/photocatalytic composite materials for pursuing fixed-bed heterogeneous advanced oxidation using X-rays. **F. Li**, E.L. Cates

12:05 Concluding Remarks.

Section C

Colorado Convention Center
Room 707

Environmental Chemistry: Pedagogical Models and Practices

Cosponsored by CHED, MPPG‡ and YCC

K. C. Lanigan, E. Roberts-Kirchhoff, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENVR **481.** Environmentally-themed chemistry activities and experiments focused on water quality for a range of instructional levels. **K.C. Lanigan**, E. Roberts-Kirchhoff

8:25 ENVR **482.** Engaging undergraduates: Investigating local environmental issues at the intersection of science and society. **S.L. Scribner**, J. Hammang-Buhl

8:45 ENVR **483.** Using environmental chemistry to teach analytical chemistry. **K.H. Weaver**, D.J. Eves

9:05 ENVR **484.** Integrating environmental and sustainability challenges into a capstone chemistry course. **K. Miller**, B. Murugaverl

9:25 ENVR **485.** Chemistry lab water quality analysis in an integrated thematic learning community. **W.J. Donovan**, E.R. Wheland, A. Bilia, G.A. Smith, T.A. Wagler

9:45 Intermission.

10:00 ENVR **486.** Using climate change context to engage students in general chemistry. **D.B. King**, J.E. Lewis, K. Anderson, D.E. Latch, S. Sutheimer, G.H. Webster, C.H. Middlecamp, R.S. Moog

10:20 ENVR **487.** Using models of growth in the Amazon to bring an environmental chemistry topic into the general chemistry class. **M.A. Benvenuto**, D. Archey

10:40 ENVR **488.** Teaching environmental toxicology by cooperative learning methods: Capstone travel course on the environment of Thailand. **L.J. Berliner**

11:00 ENVR **489.** Benefits of working in an envrionmental water-testing laboratory: How applying what you learn prepares you for the real world. **D.J. Eves**, J.T. Redd, K.H. Weaver, N.S. Werner, M. Valentine, S. Potter, D. Callison

11:20 ENVR **490.** Southern Utah University internship: A working model of peer mentorship. **J.T. Redd**, K.H. Weaver

11:40 Concluding Remarks.

Section D

Colorado Convention Center
Room 709

Water Recycling in Domestic Use, Energy Extraction, and Agricultural Use

Cosponsored by AGRO and MPPG‡

I. C. Escobar, J. Hestekin, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENVR **491.** Recycling wastewater: Quantitative removal of antibiotic activity in waters using advanced oxidation processes. **S.P. Mezyk**, S.C. Otto

8:30 ENVR **492.** A few options for energy and water autarky in water-power systems. **V. Gude**

8:55 ENVR **493.** Water reuse: Right technology for you. **V. Frenkel**

9:20 Intermission.

9:35 ENVR **494.** Reactivity of chlorine atoms with antibiotics under wastewater treatment conditions. **C.A. Rice**, S.P. Mezyk

10:00 ENVR **495.** Feasibility of integrated bioelectrochemical/membrane technologies for wastewater reuse in power plants. **V. Gadhamshetty**, **N. Shrestha**

10:25 ENVR **496.** Smart event detection system for online water quality monitoring and wastewater source control. **T. Li**, S. Zhang, H. Zhao

10:50 ENVR **497.** Adsorption mechanism of phosphorus removal in agricultural runoff by iron-modified biochar. **T. Chi**, J. Zuo, F. Liu

11:15 ENVR **498.** Phosphorus speciation in anaerobic digestion of biosolids for efficient phosphorous recovery. **C.F. Gutierrez**, K. Kinney, L.E. Katz

FLUO

Division of Fluorine Chemistry

V. Petrov, *Program Chair*

SUNDAY MORNING

Section A

Embassy Suites Denver–Downtown Convention Center
Silverton Ballroom 1

ACS Award for Creative Work in Fluorine Chemistry: Symposium in Honor of Véronique Gouverneur

Cosponsored by WCC

D. A. Dixon, *Organizer, Presiding*

8:25 Introductory Remarks.

8:30 FLUO **1.** Green metrics for the assessment of selective direct fluorination processes. **G. Sandford**

9:00 FLUO **2.** Preparation and structure of 1,2,3,4,5,6,-hexafluorocyclohexane stereoisomers. **D. O'Hagan**

9:30 FLUO **3.** Probe solute association via the water proton NMR signal. Y. Feng, M. Taraban, **Y.B. Yu**

10:00 Intermission.

10:20 FLUO **4.** Recent progress in the synthesis of aryl triflones. **N. Shibata**

10:50 FLUO **5.** Use of 1,3-dipolar cycloadditions for the preparation of SF_5-substituted heterocycles. **W.R. Dolbier**, S.E. Lopez, A. Mitani

11:20 FLUO **6.** Influence of fluorination on alcohol hydrogen bonding and lipophilicity properties. **B.J. Linclau**

SUNDAY AFTERNOON

Section A

Embassy Suites Denver–Downtown Convention Center
Silverton Ballroom 1

ACS Award for Creative Work in Fluorine Chemistry: Symposium in Honor of Véronique Gouverneur

Cosponsored by WCC

D. A. Dixon, *Organizer*
D. O'Hagan, G. Sandford, *Presiding*

1:30 Introductory Remarks.

1:50 FLUO **7.** AgF-mediated fluorinative cross-coupling of two olefins. **B. Gao**, Y. Zhao, **J. Hu**

2:20 FLUO **8.** Our recent studies in fluoroalkylation chemistry. **S.G. Prakash**

2:50 FLUO **9.** New frontier in fluorine chemistry. **K. Mikami**

3:20 FLUO **10.** Reagents and catalysts for fluorination and perfluoroalkylation reactions. **A. Togni**

3:50 FLUO **11.** Computational studies of fluorine containing molecules: Lewis acidities and radical reaction mechanisms. **D.A. Dixon**

4:20 FLUO **12. Award Address** (ACS Award for Creative Work in Fluorine Chemistry sponsored by the Juhua Group Technology Center (China)). Expanding the range of 18F-tags for PET applications. **V. Gouverneur**

MONDAY EVENING

Section A

Colorado Convention Center
Halls C/D

Sci-Mix

V. Petrov, *Organizer*

8:00 - 10:00

FLUO **13.** Solvation/desolvation and crystal structures of monovalent metal salts of the superweak anion $B_{12}F_{12}^{2-}$. **E.V. Bukovsky**, D. Peryshkov, T.C. Folsom, S.H. Strauss

FLUO **14.** Spectral characterization of steroids following fluorination by selectfluor. **H. Hakk**, S. Svendsen

FLUO **15.** Expansion of polyaromatic π systems via fluoroannulation reactions. **K. Rippy**, I.V. Kuvychko, T. Clikeman, E.V. Bukovsky, O. Boltalina, S.H. Strauss, Y. Chen

FLUO **16.** Acid cation salts of the superweak anion $B_{12}F_{12}^{2-}$. **W.M. Jones**, E.V. Bukovsky, M. Malischewski, D.V. Peryshkov, K. Seppelt, S.H. Strauss

FLUO **17.** Withdrawn.

FLUO **18.** Self-assembly of novel fluorosurfactants with polyoxometalates (POMs) as polar component in acetonitrile/water solution. **B. Zhang**

FLUO **19.** Biological applications of trifluoromethylfullerene. **K.P. Castro**, A. Mitchell, J.M. Sloan, S.A. Rolfe, A.J. Fleming, A. Ferguson, J. Blackburn, S.H. Strauss, O.V. Boltalina

FLUO **20.** Molecular design of fluorine-containing fullerene electron acceptor materials for organic photovoltaics. **N. DeWeerd**, L. San, S.H. Strauss, O.V. Boltalina

FLUO **21.** Synthesis, structural features, and dielectric properties of coordination polymers based on poly(azolate) ligands. **A. Cimino**, A. Maspero, S. Galli, C. Giacobbe, G. Palmisano, C. Yang, S. Tekarli, M. Omary

TUESDAY MORNING

Section A

Embassy Suites Denver–Downtown Convention Center
Cripple Creek Ballroom 2

ACS Award for Creative Research and Applications of Iodine Chemistry: Symposium in Honor of Karl O. Christe

Cosponsored by INOR

D. A. Dixon, *Organizer, Presiding*

8:25 Introductory Remarks.

8:30 FLUO **22.** Our excursions into iodine chemistry. **S.G. Prakash**

9:10 FLUO **23.** Iodocarbon molecules and materials. **N.S. Goroff**

9:50 Intermission.

10:10 FLUO **24.** Organohypervalent iodine chemistry. **V.V. Zhdankin**

10:50 FLUO **25.** Iodine driven self-assembly processes. **G.P. Resnati**, P. Metrangolo, G. Terraneo, G. Cavallo

11:30 FLUO **26.** Recent progress in the chemistry of iodine fluorides, oxofluorides, and oxides. **R. Haiges**, K.O. Christe

TUESDAY AFTERNOON

Section A

Embassy Suites Denver–Downtown Convention Center
Cripple Creek Ballroom 2

ACS Award for Creative Research and Applications of Iodine Chemistry: Symposium in Honor of Karl O. Christe

Cosponsored by INOR

D. A. Dixon, *Organizer*
R. M. Haiges, *Presiding*

1:30 FLUO **27.** Iodine serving fluorine. **A. Togni**

2:10 FLUO **28.** Formation, characterization, and uses of 3D metallacages via coordination directed self-assembly. **P.J. Stang**

2:50 Intermission.

3:10 FLUO **29.** Role of iodine in the chemical oxygen iodine laser. **W. McDermott**

3:50 FLUO **30.** Computational studies of iodo compounds. **D.A. Dixon**

GEOC

Division of Geochemistry

S. Kerisit, *Program Chair*

OTHER SYMPOSIA OF INTEREST:

Analytical Chemistry of Natural Resources: Environmental Analysis (see ANYL, Wed)

Analytical Chemistry of Natural Resources: Instrumentation and Methods *(see ANYL, Wed)*

BUSINESS MEETINGS:

GEOC Executive Meeting, 6:30 PM: Sun

GEOC Business Meeting, 5:30 PM: Tue

SUNDAY MORNING

Section A

Colorado Convention Center
Room 710

Understanding the Geochemical Interactions of Organic Compounds in the Subsurface

Cosponsored by MPPG‡

J. Blotevogel, V. Glezakou, A. Karamalidis, *Organizers, Presiding*

8:00 GEOC **1.** Structure-dependent interactions between feldspars and organic compounds: Implications for geologic carbon sequestration. **Y. Jun**, Y. Yang, Y. Min

8:30 GEOC **2.** Determination of binding geometry, local water structure and topological at FeOOH surfaces. **E.J. Bylaska**, Y. Chen, J. Weare

9:00 GEOC **3.** Effects of organic ligands on $scCO_2$ saturated brine-biotite interactions: Implications for organic-rich geologic CO_2 sequestration. **L. Zhang**, Y. Jun

9:20 GEOC **4.** Effects of carboxylic acid ligands on plagioclase dissolution under conditions relevant to geologic sequestration. **Y. Min**, Y. Jun, J.D. Kubicki

9:40 Intermission.

10:00 GEOC **5.** NMR and computational molecular dynamics investigation of mineral-NOM interactions at atmospheric and elevated pressures. **R.J. Kirkpatrick**, G.M. Bowers, A.O. Yazaydin, B. Ferguson, D.W. Hoyt, S. Burton, T. Varga, V. Reddy

10:30 GEOC **6.** Molecular-scale Interactions of Ca^{2+}, NOM, H_2O, and smectites in Ca-NOM-H_2O and Ca-Smectite-NOM-H_2O systems: Roles of pH history, NOM activity, H_2O activity, and ionic strength. **G.M. Bowers**, B. Ferguson, H.E. Argersinger, T. Johnson, V. Reddy, R.J. Kirkpatrick, B. Arey

11:00 GEOC **7.** Chemical controls of the micro-structure of NOM-smectite composite materials. **B. Ferguson**, H. Argersinger, R.J. Kirkpatrick, B. Arey, G.M. Bowers

11:20 GEOC **8.** Water - supercritical CO_2 partitioning of selected organic compounds: Comparison of in-situ batch reactor experiments and model predictions. **A. Burant**, C.J. Thompson, G.V. Lowry, A. Karamalidis

11:50 GEOC **9.** Measurement of organic partitioning coefficients in water-supercritical CO_2 systems by simultaneous in situ UV and near-infrared spectroscopies. **C.J. Thompson**, D. Bryce, H. Shao, K. Cantrell, J.S. Loring, B.P. McGrail

Section B

Colorado Convention Center
Room 712

Coupled Cycling of Biogeochemical Critical Elements and Contaminants

Metals/Contaminants: Field-scale

J. R. Bargar, B. Gu, M. Keiluweit, H. Lin, *Organizers, Presiding*

8:05 Introductory Remarks.

8:10 GEOC **10.** Carbon and contaminants in the critical zone. **J.D. Chorover**

8:40 GEOC **11.** Influence of natural organic matter on uranium mobility in the upper Colorado River Basin. **J.R. Bargar**, N. Janot, D.Q. Pham, M.E. Jones, S.E. Bone, J. Lezama-Pacheco, S.E. Fendorf, K. Williams, P.E. Long

9:00 GEOC **12.** Uranium immobilization in acidic wetlands by natural organic matter and plant roots. **D. Li**, D. Kaplan, J. seaman, P. Jaffe, K. Scheckel, C.U. Segre

9:20 GEOC **13.** Assessment of tellurium in semi-arid mine tailings at Delamar, Nevada: Implications for human and ecosystem health. **N.A. Knight**, S.M. Hayes

9:40 GEOC **14.** Tc migration, reduction, and redox rate scaling in Fe(II)-containing sediments from a natural redox transition zone at Hanford site. **C. Liu**, Y. Liu, R. Kukkadapu, j. McKinley, J. Zachara

10:10 Intermission.

10:30 GEOC **15.** Fate of U and As in biostimulated mine tailings sediments. **T. Borch**, L.D. Troyer, K. Campbell, J. Stone, J. Lezama-Pacheco, J.R. Bargar

11:00 GEOC **16.** Characterization of effluent and stormwater metal sources and influence on bioavailability in developed streams. **H. Luan**, T.M. Vadas

11:20 GEOC **17.** Speciation and mobility of U, As, and co-occurring constituents at abandoned mine waste sites in the Southwest, USA. **J. Blake**, S. Avasarala, K. Artyushkova, M. Ali, A. Brearly, C. Shuey, P. Robinson, S. Bill, F. Escheverria, E. Escheverria, C. Hirani, J.M. Cerrato

11:40 GEOC **18.** Silica availability in the volcanic Klamath Basin and its effect on bioavailability of phosphorus in Upper Klamath Lake, Oregon. **N.S. Simon**, K. Conko, T. Robertson, A. Vinci, K. Fischer

SUNDAY AFTERNOON

Section A

Colorado Convention Center
Room 710

Understanding the Geochemical Interactions of Organic Compounds in the Subsurface

Cosponsored by MPPG‡

J. Blotevogel, V. Glezakou, A. Karamalidis, *Organizers, Presiding*

1:15 GEOC **19.** Understanding soil organic matter: Mineral interactions with large-scale molecular dynamics simulation of biopolymer-mineral interfaces. **A. Andersen**, N. Washton, P. Reardon, S. Chacon, M. Kleber

1:45 GEOC **20.** Adsorption of light hydrocarbons and carbon dioxide confined in nanoporous synthetic sandstone rocks and shale. **G. Rother**, L. Vlcek

2:15 GEOC **21.** CH_4 and CO_2 interactions with model clay minerals. **M. Lee**, B.P. McGrail, H. Schaef, V. Glezakou

2:35 GEOC **22.** Use of LC-QTOF mass spectrometry in characterization of produced water for organic compounds: Application to geologic carbon storage and unconventional gas exploration. **V. Mishra**, A. Karamalidis, **J. Jain**, S. Hedges, A. Hakala

2:55 GEOC **23.** Autoclave experiments to investigate possible interactions between black shales and stimulation fluid during unconventional gas production. **A. Vieth-Hillebrand**, F.D. Wilke, J. Erzinger, B. Horsfield

3:25 Intermission.

3:45 GEOC **24.** Partitioning and reactivity of trace organics in unconventional oil and gas plays. **G.V. Lowry**, A. Burant, N. Edwards, A. Karamalidis

4:15 GEOC **25.** How stable are hydraulic fracturing fluid chemicals deep below the Earth's surface? **T. Borch**, G. Kahrilas, E.M. Thurman, I. Ferrer, J. Blotevogel

4:45 GEOC **26.** Minerals can be catalysts for organic reactions in hydrothermal environments. **H.E. Hartnett**, J. Shipp, Z. Yang, L. Williams, I.R. Gould, E. Shock

5:15 GEOC **27.** Chromatographic fractionation and structural diversity of petroporphyrins isolated from natural petroleum seeps by FT-ICR MS. **A.M. McKenna**, J.C. Putman, S.M. Rowland, D.L. Valentine, M.Y. Kellermann, C. Aeppli, C.M. Reddy, R.P. Rodgers

5:35 GEOC **28.** Computer simulation of the ascent, liquid-gas repartitioning, and dissolution of oil hydrocarbons in the deep water column during the *Deepwater Horizon* disaster. **J.S. Arey**, J. Gros, S. Socolofsky, C.M. Reddy

Section B

Colorado Convention Center
Room 712

Coupled Cycling of Biogeochemical Critical Elements and Contaminants

Metals/Contaminants: Molecular-scale

J. R. Bargar, B. Gu, M. Keiluweit, H. Lin, *Organizers, Presiding*

1:15 GEOC **29.** Viral influence on subsurface biogeochemical cycling and contaminant mobility. **D. Pan**, Z. Tan, J. Nolan, K. Williams, M.J. Robbins, N. Kananizadeh, Y. Li, K.A. Weber

1:45 GEOC **30.** Behavior of antimony(V) under Fe(III)- and sulfate-reducing conditions. C.R. Johnson, D. Antonopoulos, M. Boyanov, T. Flynn, K.M. Kemner, J. Koval, **E.J. O'Loughlin**

2:05 GEOC **31.** Complex roles of cysteine in methylmercury production by *G. sulfurreducens* PCA. **H. Lin**, X. LU, L. Liang, B. Gu

2:25 GEOC **32.** Differentiating kinetic and thermodynamic controls of microbial uranium reduction in the presence of iron oxides. **K.M. Belli**, T.J. DiChristina, P. Van Cappellen, M. Taillefert

2:45 GEOC **33.** From plant materials to biochars: Speciation and transformation of sulfur and potassium during biofuel production. **S. Cheah**, N. Laroco, J. Olstad

3:05 Intermission.

3:25 GEOC **34.** Coupled cycling of biogeochemically important elements (iron, sulphur, carbon) and toxic metal(oid)s (As, Pb, Cu, Zn, Cd, Ni, U, Th) in pelagic redoxclines of acidic pit lakes. **J. Sánchez-España**

3:55 GEOC **35.** Rates and mechanisms of uranyl oxyhydroxide mineral dissolution. **E. Reinoso-Maset**, W. Um, J.D. Chorover, C. Steefel, P. O'Day

4:15 GEOC **36.** Elucidating the role of monomeric U(IV) in uranium ore deposit genesis. **A. Bhattacharyya**, K. Campbell, S. Weyer, T. Borch

4:35 GEOC **37.** Rapid mobilization of noncrystalline U(IV) coupled with FeS oxidation. **Y. Bi**, M. Stylo, R. Bernier-Latmani, K.F. Hayes

4:55 GEOC **38.** Structural study of Sb(V) adsorption on hematite(1-102) surface. **C. Qiu**, F. Majs, P.J. Eng, J. Stubbs, T. Trainor

5:15 GEOC **39.** Modelling Eu(iii) speciation in a Eu(iii)/PAHA/αAl_2O^3 ternary system. **M.F. Benedetti**, J. Noémie, P. Reiller

MONDAY MORNING

Section A

Colorado Convention Center
Room 710

Geochemistry and Reactive Transport in Nano-Pore Geomaterials

Cosponsored by MPPG‡

L. J. Criscenti, Y. Wang, H. Yoon, *Organizers, Presiding*

8:15 Introductory Remarks.

8:20 GEOC **40.** Non-Darcian flow, imaging, and coupled constitutive behavior of heterogeneous shale. **T. Dewers**, J. Heath, H. Yoon

8:50 GEOC **41.** Chemical and mechanical alterations of Portland Cement by aqueous CO_2 and SO_4^{2-} under geologic CO_2 sequestration relevant conditions. **Q. Li**, Y. Lim, Y. Jun

9:10 GEOC **42.** Role of advanced reactive surface area characterization in improving predictions of mineral reaction rates in subsurface porous media. **L.E. Beckingham**, S. Zhang, E. Mitnick, D. Cole, L. Yang, L. Anovitz, J. Sheets, A. Swift, T. Kneafsey, G. Landrot, S. Mito, Z. Xue, C. Steefel, D. DePaolo, J. Ajo-Franklin, M. Voltolini

9:30 GEOC **43.** Adsorption-enhanced mass transport in carbon nanotube. **S. Riewchotisakul**, I. Akkutlu, K. Bui

9:50 GEOC **44.** Characterization of shale pore topology and chemistry using combined TEM and FIB-SEM. **H. Yoon**, T. Dewers

10:10 Intermission.

10:30 GEOC **45.** Neutron investigation of hydrocarbon and water in low-permeability geomaterials. **M. Ding**, M. Hartl, R.P. Hjelm, Y. Wang, L. Daemen, Y. Wang, C. Jove-Colon

11:00 GEOC **46.** CO_2 hydrate dissolution in pore space of marine sediments. **D. Kyung**, T. Kwon, W. Lee

11:20 GEOC **47.** Nanopore wall effect on surface tension of methane. **K. Bui**, I. Akkutlu

11:40 GEOC **48.** Understanding radionuclide interactions with layered materials: The effect of nanopore confinement. **Y. Wang**

Section B

Colorado Convention Center
Room 712

Coupled Cycling of Biogeochemical Critical Elements and Contaminants

Fundamental Redox/Elemental Cycling

J. R. Bargar, B. Gu, M. Keiluweit, H. Lin, *Organizers, Presiding*

8:00 GEOC **49.** Properties and reactivity of Fe-organic matter associations. **D.L. Sparks**

8:30 GEOC **50.** Temperature effects on carbon sequestration by iron oxide coated mineral surfaces. **E. Daugherty**, T. Borch

8:50 GEOC **51.** Source of Mn(III)-L in the surface waters of the Saguenay Fjord, Quebec, Canada. V.**E. Oldham**, M. Jones, A. Mucci, B.M. Tebo, G.W. Luther

9:10 GEOC **52.** Episodic anoxia drives geochemical formation of reactive oxygen species in coastal environments. S.A. Murphy, S. Meng, B.R. Solomon, T.J. Shaw, **J.L. Ferry**

9:30 GEOC **53.** Timescales of soil redox oscillations and the role of iron in the critical zone. **A. Thompson**, B. Ginn, C. Meile, J. Wilmoth, D. Bacellos

10:00 Intermission.

10:20 GEOC **54.** Biogeochemical cycling of Fe and S: Where are the electrons going and who is moving them? **K.M. Kemner**, E.J. O'Loughlin, M. Boyanov, D. Antonopoulos, B. Mishra, T. Flynn, D. Latta, M. Scherer, M. Kwon, T.J. Dichristina, K. Skinner

10:50 GEOC **55.** Denitrification, reductive diffusion, and rate scaling in natural redox transition zone sediments. **Y. Liu**, S. Yan, C. Liu, L. Shi, J. Shang, H. Shan, J. Zachara, J. Fredrickson, D. Kennedy, C. Resch, C.J. Thompson, S. Fansler

11:10 GEOC **56.** Evidence for the coupling of nitrogen and iron redox transformations in marine sediments. **N. Kiriazis**, J. Beckler, M. Taillefert

11:30 GEOC **57.** Removal and behavior of metal contaminants during passive co-treatment of synthetic acid mine drainage and synthetic municipal wastewater. **P. Smyntek**, J. Bandstra, R.C. Wagner, W. Stronsnider, C. Marcillo

11:50 GEOC **58.** Copper removal by bio-adsorption: A biotechnology approach. **D.F. Rodrigues**

MONDAY AFTERNOON

Section A

Colorado Convention Center
Mile High Ballroom 3C

2015 Geochemistry Division Medal Symposium

D. B. Kent, *Organizer*
S. E. Fendorf, M. Hochella, *Presiding*

1:15 Introductory Remarks.

1:30 GEOC **59.** Incidental nanomaterials in the environment, and why it is critical that we pay attention. **M. Hochella**, J. Dale, R. French, C. Johnson, B. Kim, Y. Yang

2:10 GEOC **60.** Combined impact of (bio) chemical and physical processes in defining metal dynamics within soils. **S. Fendorf**, D. Hausladen, S. Ying

2:50 GEOC **61.** Energetics of CO_2 confinement: Amorphous carbonates, layered double hydroxides, and metal organic frameworks. **A. Navrotsky**

3:30 Intermission.

3:50 GEOC **62.** Geochemical reaction kinetics using nanometer-sized metal-hydroxide and -oxide ions. **W.H. Casey**

4:30 GEOC **63.** Kinetics and mechanisms of geochemical processes: It's about interfaces and scale. **D.L. Sparks**

MONDAY EVENING

Section A

Colorado Convention Center
Halls C/D

Sci-Mix

S. N. Kerisit, *Organizer*

8:00 - 10:00

GEOC **64.** Distribution and quantity of iodine with relationship to aquifer formations in northwestern Oklahoma brine waters. J.R. Wickham, **C. Hoffman**, **A. Anderson**, R. Fenton, D. Edlin

GEOC **65.** Distribution of uranium and uranyl minerals near and within hyalite opal. **T.L. Spano**, T.A. Olds, A.M. Burd, J. Kovacs, P.C. Burns

GEOC **66.** Seasonal changes in temperature and vadose zone gases due to microbial activity at a crude oil-contaminated site. **E. Warren**, J. Trost, N. Sihota, B. Bekins

GEOC **67.** Using geochemical analysis to identify local vs. exotic sources of glacial clasts, Friis Hills, Antarctica. **J. Wrage**, C. Jacobs, A. Lewis, B. Saini-Eidukat

GEOC **68.** Toward quantification of Mo and Re speciation in natural anoxic waters: Reverse phase ion pair chromatographic separation of oxythiomolybdate and oxythioperrhenate mixtures. **E. Stong**, **N. Young**, L. Groskreutz, A. Chappaz, T.P. Vorlicek

GEOC **69.** Abiotic addition of sulfide to dissolved organic matter. **B.A. Poulin**, J.N. Ryan, A. Stubbins, G. Aiken

‡ *Cooperative Cosponsorship*

GEOC **70.** Reactive surfaces of altered clay minerals and their effect on the retention of metal(loid)s by clays. **C.A. Legrand**, M. Schindler, M. Hochella

GEOC **71.** Disequilibrium of mineral phases in confined pore spaces in silica-rich coatings. **J. Caplette**, M. Schindler, M. Hochella

GEOC **72.** Numerical simulation of groundwater flow and solute transport: A case study for Manati-Vega Baja limestone karst aquifer, Puerto Rico. **B. Maihemuti**

GEOC **73.** Speciation of arsenic in water at Bakyrchik gold mine, Kazakhstan. **A. Seitkan**, S. Redfern

GEOC **74.** Environmental factors affect production of methylmercury by *Geobacter bemidjensis*. **X. Lu**, H. Lin, B. Gu

GEOC **75.** Thermodynamic studies of uranyl minerals: Enthalpies of formation of metatorbernite, metazeunerite, metaankoleite, metastudtite, and metaschoepite. **E. Dzik**, P.C. Burns

GEOC **76.** Copper sorption and lability from iron oxide and organic matter coprecipitates. **F. Koenigsmark**, T.M. Vadas

GEOC **77.** Redistribution of solid phase arsenic in aquaculture pond sediments. **S. Hafeznezami**, T. Lin, J.A. Jay

GEOC **78.** Effect of exposure time on Cu(II) adsorption and retention to iron oxyhydroxide nanoparticles. **A.V. Torossian**, J.A. Jacobs, C.S. Kim

GEOC **79.** Dark production of superoxide and hydrogen peroxide during oxidation of reduced dissolved organic matter in natural waters. **R. Marsico**, T. Rand, K. Roe, D.L. Macalady, B. Voelker

TUESDAY MORNING

Section A

Colorado Convention Center
Room 710

Iron Oxides: Formation, Structure, Reactivity and Applications

Formation and Transformation

Cosponsored by MPPG‡

T. Borch, W. D. Burgos, Y. Hu, M. Zhu, *Organizers, Presiding*

8:00 GEOC **80.** Initial mechanisms of iron oxyhydroxide precipitation: Results from molecular spectroscopy and MD simulations. **G. Waychunas**, M. Zhu, H. Zhang, C. Frandsen, J.D. Kubicki, B. Puls

8:30 GEOC **81.** Mineral formation by cluster self-assembly: Schwertmannite as a partially crystallized nanomineral. **F.M. Michel**, H.E. King

9:00 GEOC **82.** Size-dependent solubility, stability, and nucleation of ferrihydrite. **T. Hiemstra**

9:20 GEOC **83.** Interactions among aqueous ions, quartz, and Fe (hydr)oxide polymers during heterogeneous Fe hydroxide nucleation and growth. C. Dai, **Y. Hu**

9:40 GEOC **84.** Nucleation and growth of synthetic chrysotile nanotubes: Insights into the structure of proto-serpentine. **A. Fernandez-Martinez**, **R. Lafay**, G. Montes-Hernandez, A. Auzende, A. Poulain

10:00 Intermission.

10:15 GEOC **85.** Fe(III) (hydr)oxide nucleation, and growth: Influences of local saturation changes, structural matches, and hydrophilicity. **Y. Jun**, Y. Hu, J.R. Ray, C.W. Neil, B. Lee

10:45 GEOC **86.** Natural organic matter impacts on heterogeneous iron(III) (hydr)oxide nucleation, growth, and composition in the presence of arsenate. **C.W. Neil**, B. Lee, Y. Jun

11:05 GEOC **87.** Thermodynamics of mixing of spinel solid solutions with magnetite end-member Part I: Mixing of normal and inverse spinels. **S. Sahu**, K. Lilova, B. Huang, B.F. Woodfield, A. Navrotsky

11:25 GEOC **88.** Thermodynamics of mixing of spinel solid solutions with magnetite (Fe_3O_4) end-member Part II: Mixing of two inverse spinels. **K. Lilova**, S.K. Sahu, C. Pearce, K. Rosso, A. Navrotsky

11:45 GEOC **89.** Nucleation and growth of $(Fe,Cr)(OH)_3$ nanoparticles: Implications for aqueous Cr removal. **C. Dai**, Y. Hu

Section B

Colorado Convention Center
Room 712

Molecular-Scale Processes Controlling Reactivity at Mineral-Water Interfaces

Cosponsored by COLL

S. E. Mason, *Organizer*
A. Ilgen, S. Lee, *Organizers, Presiding*

8:05 Introductory Remarks.

8:10 GEOC **90.** Janus, striped and coarse-grained particles. **R. Hernandez**

8:40 GEOC **91.** Molecular simulation analysis of nanoparticle-biomolecule interactions: challenges and developments. **Q. Cui**

9:00 GEOC **92.** DFT-MD simulations of the quartz (101)-water interface as a function of pH, ionic strength, salt type and temperature: Implications for dissolution mechanisms. **J.D. Kubicki**, M. DelloStritto, J.O. Sofo, M. Fedkin, L. Vlcek, A.A. Chialvo, D. Wesolowski, O. Kroutil, M. Predota, F. Bellucci, P. Fenter, F. Geiger, S.A. Saslow, A. Bandura

9:30 GEOC **93.** Structure of water at the quartz(101) surface: Effect of ions and pH. **M. DelloStritto**, J.D. Kubicki, J.O. Sofo

9:50 Intermission.

10:10 GEOC **94.** Measure of absolute surface potential at the water–silica nanoparticle interface: Specific ion effects and pH dependence. **M.A. Brown**

10:30 GEOC **95.** Second harmonic generation studies of aqueous R-cut α-quartz and fused silica interfaces. **F. Geiger**

10:50 GEOC **96.** Monitoring the influence of ions on acid-base chemistry at the silica/water interface at low and high salt concentration using nonlinear optical methods. **J. Gibbs-Davis**, A. Darlington, M. Azam

11:10 GEOC **97.** Surface energies for Pt catalysts comprising C, CO, methanol, and glycerol adsorbates in liquid water calculated using density functional theory and molecular dynamics. **C. Bodenschatz**, R. Getman

11:40 GEOC **98.** Structure dynamics and reactivity of water-saturated supercritical CO_2 and anorthite interface from ab initio molecular dynamics. **V. Glezakou**, M. Lee, B.P. McGrail, R. Rousseau

TUESDAY AFTERNOON

Section A

Colorado Convention Center
Mile High Ballroom 3A

Symposium in Honor of Dr. Donald Sparks, 2015 Geochemistry Medal Recipient

Kinetics and Mechanisms of Aqueous Geochemical Processes

S. E. Fendorf, D. B. Kent, *Organizers*
G. W. Luther, K. Scheckel, *Presiding*

1:15 Introductory Remarks.

1:20 GEOC **99.** Kinetic competence in bacterial iron oxide reduction: A model system study with proteoliposomes. **J. Zachara**, Z. Wang, L. Shi, G. White, D. Richardson, J. Fredrickson

1:55 GEOC **100.** Oxygen flux modulates net rates of Fe reduction and Fe solid phase composition in redox dynamic soils. **J. Wilmoth**, A. Thompson

2:20 GEOC **101.** Reduction kinetics of polymeric (soluble) manganese (IV) oxide (MnO_2) by ferrous iron (Fe^{2+}). **M. Siebecker**, G.W. Luther

2:40 GEOC **102.** Crystallite size effects on the structure and physicochemical properties of ferrihydrite. **X. Feng**, X. Wang, W. Li, M. Zhu, F. Liu, D.L. Sparks

3:00 GEOC **103.** Molecular-level explanation for humification in peats and soils based on ultrahigh resolution mass spectrometry. **P. Hatcher**, H. Chen, B. Hartman, N. DiDonato, D. Waggoner

3:20 Intermission.

3:35 GEOC **104.** Characterizing high affinity binding sites within bacterial cell envelopes and on bacterial EPS molecules. **J. Fein**, Q. Yu

4:00 GEOC **105.** Role of NOM complexation in Fe(II) stabilization. **T. Borch**, E. Daugherty, P.S. Nico, B. Gilbert

4:25 GEOC **106.** Behavior of nitrite with goethite and surface Fe(II)-goethite complexes. **C.J. Matocha**, P. Dhakal

4:45 GEOC **107.** In-situ Cu(II)-fulvic acid systems studied using complementary spectroscopic techinques. **C. Phillips**, J. Hamilton, D. Hilger, D. Peak

5:05 GEOC **108.** Adjunctive, disjunctive, and "Interjunctive"? Influence of ligand structure on kinetic pathways of ligand exchange. **N.E. Boland**, A.T. Stone, T. Nelson, M. Harned, A. Wildman

Section B

Colorado Convention Center
Room 710

Molecular-Scale Processes Controlling Reactivity at Mineral-Water Interfaces

Cosponsored by COLL

S. Lee, *Organizer*
A. Ilgen, S. E. Mason, *Organizers, Presiding*

1:30 GEOC **109.** Molecular dynamics simulations of cation adsorption at mica-water interfaces. **I.C. Bourg**

2:00 GEOC **110.** Adsorption properties of cesium ions to micaceous clay minerals. **M. Okumura**, H. Nakamura, M. Machida, S.N. Kerisit

2:20 GEOC **111.** New insights into thermal effects of K, Na, Ca, Mg, and Cs-exchanged montmorillonite by in situ USAXS/SAXS study. **S. Lee**, T.B. Fischer, M.R. Stokes, R.J. Klingler, J. Ilavsky, D.K. McCarty, M.O. Wigand, R.E. Winans

2:40 GEOC **112.** Deciphering populations of Cd surface complexes on gibbsite and kaolinite with combined experimental and computational methods. **P.A. O'Day**, M. Small, N. Govind, H.D. Watts, J.D. Kubicki, K.T. Mueller

3:00 GEOC **113.** Reactivity of Sb(V) and Pb(II) on environmentally active (1-102) surface of hematite and alumina. **S. Ramadugu**, S.E. Mason

3:20 Intermission.

3:40 GEOC **114.** Co-sorption of Fe(II) with As(III) and As(V) at the solid-water interface of aluminum oxide. **Y. Zhu**, E.J. Elzinga

4:10 GEOC **115.** Characterization of Ba^{2+} adsorption on oxide minerals: Combined effects of solution and surface properties in complex systems. **J. Han**, S. Chun, L.E. Katz

4:30 GEOC **116.** Enhanced phosphate sorption on metal-doped birnessite. **Y. Tang**, R. Huang, B. Fields, M. Zhu, S. Zhao

4:50 GEOC **117.** Microfluidic device to determine the rate of mineral weathering. **D. Ciceri**, A. Allanore

Section C

Colorado Convention Center
Room 710

Iron Oxides: Formation, Structure, Reactivity and Applications

Formation and Transformation

Cosponsored by MPPG‡

T. Borch, W. D. Burgos, Y. Hu, M. Zhu, *Organizers, Presiding*

1:20 GEOC **118.** Iron oxides in reactive systems. A.M. Vindedahl, J.H. Strehlau, J.A. Soltis, B.M. Toner, W. Arnold, **R. Penn**

1:50 GEOC **119.** Effect of solution and solid-phase conditions on the Fe(II)-accelerated transformation of ferrihydrite to lepidocrocite and goethite. **T.D. Waite**, D. Boland, R. Collins, C. Miller

2:20 GEOC **120.** Abiotic phase transformation of schwertmannite pelagic particles in acidic pit lakes: Influence on metal mobility. **J. Sánchez-España**, I. Yusta

2:40 GEOC **121.** Mineralogical changes in goethite during goethite-Fe(II) atom exchange: A microscopic and 55Fe-tracer study. **P. Joshi**, C. Gorski

3:00 GEOC **122.** Revisiting the α-Fe_2O_3 (0001) phase diagram using a surface specific GGA + *Ud+p* approach. **X. Huang**, S. Ramadugu, S.E. Mason

3:20 Intermission.

3:35 GEOC **123.** Dissolution, aggregation, surface chemistry, and biological effects of iron oxide nanomaterials. **V.H. Grassian**

4:05 GEOC **124.** Structure and thermodynamics of ferrihydrite from first principles. **M. Sassi**, K. Rosso

4:25 GEOC **125.** Withdrawn.

4:45 GEOC **126.** On the join between goethite and hematite: X-ray diffraction and FT-IR studies of "hydrohematite". **P.J. Heaney**, K.M. Peterson, F.T. Ling, J.E. Post

5:05 GEOC **127.** Technetium incorporation into goethite: An atomic-scale investigation. **F.N. Smith**

WEDNESDAY MORNING

Section A

Colorado Convention Center
Mile High Ballroom 3A

Symposium in Honor of Dr. Donald Sparks, 2015 Geochemistry Medal Recipient

Kinetics and Mechanisms of Aqueous Geochemical Processes

S. E. Fendorf, D. B. Kent, *Organizers*
M. Hochella, A. L. Seyfferth, *Presiding*

8:00 Introductory Remarks.

8:05 GEOC **128.** Determining chemical and microbial Fe(II) oxidation kinetics in situ: Iron oxidizing bacteria compete with chemical Fe(II) oxidation. **G.W. Luther**, C. Chan, D. Emerson

8:40 GEOC **129.** Mechanisms and kinetics of contaminant transformation by Mn(IV) oxides. **M.A. Ginder-Vogel**

9:05 GEOC **130.** Transformation of triclinic to hexagonal birnessite by common biological buffers. **F. Ling**, P. Heaney, X. Gao, J. Post

9:45 GEOC **131.** Co-sorption of aqueous Fe(II) and Mn(II) in anoxic aluminum-oxide suspensions. **E. Elzinga**, Y. Zhu

10:05 Intermission.

10:20 GEOC **132.** Iron mineral formation in an iron- and sulfide-rich early ocean model habitat. **E. Koeksoy**

10:40 GEOC **133.** Time resolved in situ spectroscopic studies of aqueous geochemical reactions. **D. Peak**

11:05 GEOC **134.** Novel synchrotron-based hard x-ray approaches to understanding controls on metal ion fate in subsurface and terrestrial environments. **K.M. Kemner**, M. Boyanov, B. Mishra, E.J. O'Loughlin, S.L. O'Brien, D. Sholto-Douglas, B. Lai, M. Balasubramanian, R. Gordon, S. Kelly, V. Bailey

11:30 GEOC **135.** Tackling rapid reaction kinetics at the mineral-water interface using quick-scanning X-ray absorption spectroscopy. **W. Li**, M. Siebecker, D.L. Sparks

11:50 GEOC **136.** Development of a rate law for arsenite oxidation by manganese oxides to assess the impact of the recycling of arsenic on microbial respiration processes. **S. Owings**, M. Taillefert

Section B

Colorado Convention Center

Room 712

Molecular-Scale Processes Controlling Reactivity at Mineral-Water Interfaces

Cosponsored by COLL

A. Ilgen, *Organizer*

S. Lee, S. E. Mason, *Organizers, Presiding*

8:30 GEOC **137.** Pathways and kinetics of Fe(II)-catalyzed redox recrystallization of Fe(III)-oxides. **K. Rosso**, V. Alexandrov, P. Zarzycki, S.N. Kerisit, M. Sassi

9:00 GEOC **138.** Contribution of thiol structure on reduction kinetics of iron and manganese oxides. **E.M. Eitel**, M. Taillefert

9:20 GEOC **139.** Iron electron transfer and atom exchange in clay minerals. **D.E. Latta**, W. Premaratne, K. Rosso, M. Scherer, A. Neumann

9:50 GEOC **140.** Controls on the reactivity of clay structural Fe(II)/Fe(III) redox couple. **A.G. Ilgen**, D.R. Dunphy, J.N. Kruichak, R.K. Kukkadapu, J.M. Cerrato, J.M. Argo, R.E. Washington

10:10 Intermission.

10:30 GEOC **141.** Characterizing the dynamics of iron oxide aggregation and reactivity in aqueous systems. A.M. Vindedahl, J.H. Strehlau, W. Arnold, **R. Penn**

11:00 GEOC **142.** Resolving conflicting effects of surfaces, ligands, and concentration on the evolution of reactive oxygen species during iron oxidation. **S. Meng**, B.R. Solomon, J.L. Ferry

11:20 GEOC **143.** Effect of live *Acremonium strictum* KR21-2 fungus on the mobility of REEs during the biooxidation of Mn(II). **Q. Yu**, T. Ohnuki, K. Tanaka, N. Kozai, F. Sakamoto, Y. Tani

11:40 GEOC **144.** Prebiotic role of fluoride minerals in the montmorillonite catalyzed synthesis of RNA. **M.F. Aldersley**, P.C. Joshi

Section C

Colorado Convention Center

Room 710

Iron Oxides: Formation, Structure, Reactivity and Applications

Biotic and Abiotic Redox Reactions

Cosponsored by MPPG‡

T. Borch, W. D. Burgos, Y. Hu, M. Zhu, *Organizers, Presiding*

8:00 GEOC **145.** Speciation of particulate iron in marine geochemical gradients. **B.M. Toner**, P.J. Lam

8:30 GEOC **146.** Iron oxide – aqueous Fe(II) standard reduction potential measurements: A mediated electrochemical study. R.A. Edwards, A.C. Costa, **C.A. Gorski**

8:50 GEOC **147.** High spatial resolution analysis of biogeochemical iron cycling and iron mineral formation in freshwater sediments. **C.L. Lockwood**, T.K. Himpel, F. Schaedler, C. Schmidt, A. Kappler

9:10 GEOC **148.** Effect of natural and engineered electron transfer in living cells on the transformation of iron oxides. **K.K. Sand**, M. TerAvest, C.M. Ajo Franklin, J. De Yoreo

9:30 GEOC **149.** Harnessing community genomics to understand microbial iron and sulfur cycling in estuary sediments. **B.J. Baker**

10:00 Intermission.

10:15 GEOC **150.** Biogeobattery: Redox cycling of Fe(II) and Fe(III) in magnetite by Fe-metabolizing bacteria. J. Byrne, N. Klüglein, C. Pearce, E. Appel, **A. Kappler**

10:45 GEOC **151.** Reactivity of bioreduced iron-bearing phyllosilicates towards nitroaromatic compounds. **W.D. Burgos**, F. Luan, C. Gorski

11:05 GEOC **152.** Role of microbial communities in linking Fe (hydr)oxide transformation and nutrient cycling. **M.A. Ginder-Vogel**, E. Tomaszewski, J. Mejia

11:25 GEOC **153.** Characterization of redox potential and reactivity of sorbed Fe(II). **D. Fan**, A. Hinkle, R. Johnson, P.G. Tratnyek

11:45 GEOC **154.** Evidence for the existence of soluble Fe(III) complexes in sedimentary environments. **M. Taillefert**, J. Beckler

WEDNESDAY AFTERNOON

Section A

Colorado Convention Center

Mile High Ballroom 3A

Symposium in Honor of Dr. Donald Sparks, 2015 Geochemistry Medal Recipient

Structure and Bonding at the Mineral-water Interface

S. E. Fendorf, D. B. Kent, *Organizers*

B. C. Bostick, M. A. Ginder-Vogel, *Presiding*

1:30 Introductory Remarks.

1:35 GEOC **155.** Structural environments of ligands associated with amorphous ferric hydroxides, and their impact on goethite nucleation. **S.C. Myneni**, N. Crompton, J. Majzlan

2:10 GEOC **156.** Silicate sorption on Fe oxyhydroxides: Identification of reaction sites from molecular spectroscopy, and reactive force field modeling of sorption/desorption processes. **G. Waychunas**, M. Kanematsu, J. Boily, C.B. Keller, A. Wallace

2:35 GEOC **157.** Alkaline earth metal ion sorption processes: From adsorption to precipitation. **L.E. Katz**, J. Choi, J. Han, L.J. Criscenti

3:00 GEOC **158.** Ligand controlled chemical fate of CeO_2 nanoparticles in heterogeneous geochemical system. **Y. Arai**

3:20 Intermission.

3:35 GEOC **159.** Adsorption and reaction at mineral/water interfaces: Relevance to natural products and agricultural chemicals. **A.T. Stone**

4:00 GEOC **160.** Sulfate coordination environment in Schwersmannite. **X. Wang**, C. Gu, X. Feng, M. Zhu

4:20 GEOC **161.** Identification and quantification of sulfate surface complexes on ferrihydrite. **C. Gu**, X. Wang, Z. Wang, M. Zhu

4:40 GEOC **162.** Organo-mineral associations in agricultural soils: insights from multi-elemental STXM-NEXAFS analysis. **C. Chen**, J. Wang, J.J. Dynes, D.L. Sparks

5:00 GEOC **163.** Ternary complexation of dissolved organic matter in kaolinite-Fe(III)-organic acid systems: An EXAFS spectroscopic study. **J. Yang**, D.L. Sparks, N. Bolan, R. Cornelia, W. Pan

5:20 GEOC **164.** Macroscopic and microscopic investigation of adsorption and precipitation of Zn on γ-alumina as affected by As. **Y. Wang**, T. Fan, D. Zhou, W. Li, M. Zhu, D.L. Sparks

Section B

Colorado Convention Center

Room 710

Molecular-Scale Processes Controlling Reactivity at Mineral-Water Interfaces

Cosponsored by COLL

S. E. Mason, *Organizer*

A. Ilgen, S. Lee, *Organizers, Presiding*

1:30 GEOC **165.** Uncovering the local atomic structure of a hydrated amorphous magnesium carbonate: The computational chemistry and total scattering iterative methodology. **C. White**, N. Henson, L. Daemen, M. Hartl, K. Page

2:00 GEOC **166.** How does the ionic strength control the nucleation of manganese oxide nanoparticles at quartz-water interfaces? **H. Jung**, Y. Jun

2:20 GEOC **167.** In-situ observation of a single-layer gibbsite film at the muscovite (001)–water interface. **S. Lee**, M. Schmidt, T.T. Fister, N.C. Sturchio, K.L. Nagy, P. Fenter

2:40 GEOC **168.** Mineralogical constraint of reverse weathering reactions. **E.M. Saad**, Y. Tang

3:00 Intermission.

3:20 GEOC **169.** Role of citric acid in $CaCO_3$ crystallization. **D.J. Tobler**, J. Rodriguez Blanco, K. Dideriksen, N. Bovet, K.K. Sand, S.S. Stipp

3:40 GEOC **170.** Role of borate ions in $CaCO_3$ crystallization. **J. Rodriguez-Blanco**, K. Dideriksen, D. Tobler, K. Sand, B. Vallina, L.G. Benning, S.S. Stipp

4:00 GEOC **171.** Effect of varying cation:anion ratio on growth of sparingly-soluble minerals. **J. Bracco**, A.G. Stack, S.R. Higgins

4:20 GEOC **172.** Impact of carbonate substitution on the interfacial kinetics and bulk stability of hydroxyapatite. **L.N. Lammers**

4:40 Concluding Remarks.

Section C

Colorado Convention Center

Room 710

Iron Oxides: Formation, Structure, Reactivity and Applications

Environmental Applications

Cosponsored by MPPG‡

T. Borch, W. D. Burgos, Y. Hu, M. Zhu, *Organizers, Presiding*

1:15 GEOC **173.** Reactions of nanoscale zero-valent iron (nZVI) with heavy metals: Atomic resolution imaging and applications. **W. Zhang**, L. Ling

1:45 GEOC **174.** Contaminant removal from water through oxidation-reduction and adsorption on iron oxides generated during electrocoagulation. **D. Giammar**, C. Pan, L. Wang, J.G. Catalano

2:15 GEOC **175.** Interaction of Cr(III) and Cr(VI) with hematite studied by second harmonic generation. **F. Geiger**

2:35 GEOC **176.** Sequestration of arsenate in zero-valent iron nanoparticles: Visualization of intraparticle reactions at Angstrom resolution. **L. Ling**, W. Zhang

2:55 GEOC **177.** Redox reactions and contaminant degradation by Fe(II) and iron oxides in complex groundwater systems. J.H. Strehlau, **B.M. Toner**, W. Arnold, R. Penn

3:15 Intermission.

3:30 GEOC **178.** Solute transport with pH variations through soil. **S. Bryant**, V. Prigiobbe

4:00 GEOC **179.** Immobilization of arsenate in soil and groundwater using starch-stabilized magnetite nanoparticles. **D. Zhao**, Q. Liang

4:30 GEOC **180.** Withdrawn.

4:50 GEOC **181.** Reactivity of various kinds of magnetite to adsorb heavy metals from contaminated wastewater. **M. Usman**, Z. Ajmal

5:10 GEOC **182.** Density functional theory modeling of ferrihydrite nanoparticle charging and adsorption behavior. **J.D. Kubicki**, E. Cerkez, D.R. Strongin

THURSDAY MORNING

Section A

Colorado Convention Center

Mile High Ballroom 3A

Symposium in Honor of Dr. Donald Sparks, 2015 Geochemistry Medal Recipient

Biogeochemical Processes in Soils and Sediments

S. E. Fendorf, D. B. Kent, *Organizers*

A. Navrotsky, J. Stuckey, *Presiding*

8:00 Introductory Remarks.

8:05 GEOC **183.** Rhizosphere processes controlling metal speciation and bioavailability in soils. **D.H. McNear**

8:30 GEOC **184.** Fate, transport, and cycling of hexavalent chromium in the soil environment. **J. Fischel**, D.L. Sparks

8:50 GEOC **185.** Potential impacts of sea level rise on arsenic mobility and cycling. **J.J. LeMonte**, R. Tappero, D.L. Sparks

9:10 GEOC **186.** Tracking the temporal dynamics of intracellular lead speciation in a model green alga by resonant X-ray emission spectroscopy. T. Stewart, J. Szlachetko, L. Sigg, R. Behra, **M. Nachtegaal**

9:30 GEOC **187.** Impact of sea level rise on arsenic and chromium sorption in *Phragmites australis* root plaques. **M. Fischel**, D.L. Sparks

9:50 Intermission.

10:05 GEOC **188.** Fate of arsenic at the soil-plant interface: Impacts of soil-incorporation of plant-available silicon on arsenic desorption, iron oxide plaque, and plant uptake. **A.L. Seyfferth**, R. Gill, E. Penido

10:30 GEOC **189.** Root cell wall polysaccharides are involved in Cd hyperaccumulation in *Sedum alfredii*. **T. Li**, Q. Tao, X. yang, D.L. Sparks, Y. Liang

10:50 GEOC **190.** Scaling up molecular reactions to ecosystem processes: Organic matter degradation controlled phosphorus cycling in the Chesapeake Bay. **D. Jaisi**, S. Joshi, R. Kukkadapu, D.L. Sparks

11:10 GEOC **191.** Identification of biologically inert phosphorus pools in river waters: An application of phosphate oxygen isotope ratios of particulate P pools in East Creek, a Chesapeake Bay watershed. **K. Bear**, S.R. Joshi, D. Jaisi

11:30 GEOC **192.** Using phosphorus distribution in soils and sediments to understand arsenic biogeochemistry. **D.G. Strawn**

11:50 GEOC **193.** Using synchrotron-based techniques to elucidate the fate of militarily relevant metals in the environment. **J. Seiter**, B. Lafferty, R. Tappero, A. Bednar, A. Kennedy, S. Brasfield, M. Chappell

Section B

Colorado Convention Center

Room 712

Precipitation, Dissolution and Adsorption under Confinement

Mineral Dissolution and Precipitation

A. Fernandez-Martinez, A. G. Stack, *Organizers, Presiding*

8:45 Introductory Remarks.

8:50 GEOC **194.** Mineral precipitation in porous materials. **A.G. Stack**, A. Gordon, H. Wang, A. Fernandez-Martinez, L. Anovitz, K. Page

9:10 GEOC **195.** Precipitates of Al(III), Sc(III), and La(III) at the muscovite-water interface. **F. Geiger**

9:30 GEOC **196.** Nucleation and growth of barite ($BaSO_4$) observed in-situ in porous media using X-ray computed tomography. **J. Godinho**, A.G. Stack, M. Rivers

9:50 Intermission.

10:10 GEOC **197.** Effects of reactivity and flow rate on dissolution of carbonates from the nano to the centimeter scale. **L. Anovitz**, C.A. Novack, T.R. Prisk, J. Ilavsky, J. Hammons, D.F. Mildner, M.J. Wasbrough, D.L. Jacobson, D.S. Hussey

10:40 GEOC **198.** Evolution of silica walls of nanopores filled of water and ions. **D. Rébiscoul**, J. Cambedouzou, M. Brossel

11:00 GEOC **199.** In situ X-ray diffraction and infrared spectroscopic investigation of magnesite precipitation in interfacial water films. **Q.R. Miller**, J.P. Kaszuba, H.T. Schaef, M.E. Bowden, C.J. Thompson, J.S. Loring

11:30 GEOC **200.** Nanogeochemistry issues arising from borosilicate leaching experiments. **S. Gin**, P. Jollivet, F. Angéli, P. Frugier

THURSDAY AFTERNOON

Section A

Colorado Convention Center

Mile High Ballroom 3A

Symposium in Honor of Dr. Donald Sparks, 2015 Geochemistry Medal Recipient

Biogeochemical Processes in Soils and Sediments

S. E. Fendorf, D. B. Kent, *Organizers*

D. Giammar, D. H. McNear, *Presiding*

1:30 Introductory Remarks.

‡ *Cooperative Cosponsorship*

1:35 GEOC **201.** Environmental fate and transformation of engineered nanoparticles from consumer products. **K. Scheckel**, E. Lombi, E. Donner, R. Sekine, B. Miller, K. Vasilev

2:00 GEOC **202.** Uranium(VI) uptake on iron oxide surfaces: The transition from adsorption to precipitatio. **D. Giammar**, A. Singh, V. Mehta, L.D. Troyer, F. Maillot, J.G. Catalano

2:25 GEOC **203.** Chemistry of depleted uranium in military firing range soils. **B. Lafferty**, J. Seiter, A. Bednar, R. Tappero, F. Hill, M. Chappell

2:45 GEOC **204.** Kinetics-based approaches of predicting aqueous arsenic concentrations in soil and groundwater systems. **B.C. Bostick**, J. Sun, S. Chillrud, A. van Geen, B. Mailloux

3:10 GEOC **205.** Wetland hydrology dictates organic carbon reactivity controlling microbial arsenic release within the Mekong Delta. **J. Stuckey**, M. Schaefer, B. Kocar, S. Benner, S. Fendorf

3:30 GEOC **206.** Development and applications of stabilized nanoparticles for in situ immobilization of metals/metalloids in soil and groundwater. **D. Zhao**, X. Zhao, W. Xie, X. Wang, S. Tian

3:50 Intermission.

4:05 GEOC **207.** Fe(III) affects arsenic mobilization and secondary mineral precipitate phase, morphology, and coverage during arsenopyrite oxidation. **C.W. Neil**, Y. Jun

4:25 GEOC **208.** Copper sequestration by black carbon in contaminated soil using STXM-C K-edge and Cu L-edge XANES spectroscopy. **J. Yang**, J. Liu, J. Wang, D.L. Sparks

4:45 GEOC **209.** Role of chlorite interlayers in Zn sequestration in smelter-affected soils. **J. Hamilton**, D. Peak

5:25 GEOC **211.** Modeling the impact of variable pH and dissolved salt concentration on sorption and transport of nickel, zinc, and lead in a quartz-sand aquifer. **D.B. Kent**, M. Kohler, G. Ng

Section B

Colorado Convention Center
Room 712

Precipitation, Dissolution and Adsorption under Confinement

Chemistry of Aqueous Solutions

A. Fernandez-Martinez, A. G. Stack, *Organizers, Presiding*

1:30 GEOC **212.** Adsorption and precipitation of Zn and Ni in nanoporous silica. **J.M. Nelson**, J.R. Bargar, G.E. Brown, K. Maher

1:50 GEOC **213.** Hydration-induced morphological evolution at glass-liquid interfaces. **J. Ryan**, P. Rieke, S.N. Kerisit

2:10 GEOC **214.** Inhibition mechanism of DTPMP based on the analysis of barite nucleation and crystal growth using laser detection method and novel crystal growth model supported by cryo-TEM measurements. **Z. Dai**, F. Zhang, A.T. Kan, Z. zhang, Y. Liu, L. Wang, F. Yan, N. Bhandari, V. Bolanos, M.B. Tomson

2:30 GEOC **215.** Inelastic neutron scattering techniques for the study of water confined in swelling clay minerals. **M. Jimenez-Ruiz**

3:00 Intermission.

3:20 GEOC **216.** Aqueous geochemistry of water confined in clay and silica nanopores. **I.C. Bourg**

3:50 GEOC **217.** Structure, dynamics, and reactivity of geofluids in confined geometries. **D. Cole**, D.W. Hoyt, A. Kolesnikov, T. Liu, E. Mamontov, K.T. Mueller, S. Gautam, G. Rother, J. Sheets, A. Striolo, N. Washton, S. Welch

4:20 GEOC **218.** Confined pore spaces in mineral coatings of contaminated soils: Disequilibria between abiotic and biotic processes and their environment. **M. Schindler**, M. Hochella

4:40 Concluding Remarks.

HIST

Division of the History of Chemistry

S. C. Rasmussen, *Program Chair*

BUSINESS MEETINGS:
HIST Division Executive Committee Meeting, 5:00 PM: Sun

SUNDAY AFTERNOON

Section A

Sheraton Denver Downtown Hotel
Tower Court A

HIST Tutorial and General Papers

S. C. Rasmussen, *Organizer, Presiding*

1:00 HIST **1.** HIST Tutorial: Elemental sulfur – a natural (and unnatural) resource. **M.E. Schott**

1:40 HIST **2.** James Hyatt, chemist, scientist, and communicator: A man of his times. W.P. Palmer

2:10 HIST **3.** Inaccuracy of dates in accounts of the history of chemistry: A case of deliberate falsification? **J. Gal**

2:40 Intermission.

2:55 HIST **4.** Rules, formulas, names: The lexical legacy of the 1892 Geneva Nomenclature Congress. **E. Hepler-Smith**

3:25 HIST **5.** NMR characterization of resin blocks from 13th century *Java Sea Wreck*. **J.B. Lambert**, A. Levy

3:55 HIST **6.** Investigation into the first isolation of carbonic acid. **R.L. Hudson**

4:25 HIST **7.** Foundation and influence of the Sydney School of Coordination Chemistry. **A.T. Baker**

MONDAY MORNING

Section A

Sheraton Denver Downtown Hotel
Tower Court A

Chemical Technology in Antiquity

Cosponsored by MPPG‡

S. C. Rasmussen, *Organizer*
C. L. Heth, *Presiding*

8:25 Introductory Remarks.

8:30 HIST **8.** Pigments in antiquity: Colorful forerunners of every aspect of modern chemistry. **M. Orna**

9:15 HIST **9.** First artificial material: Ceramics from prehistory to the fall of Rome. **N. Zumbulyadis**

10:00 Intermission.

10:15 HIST **10.** From honey wine to cultivation of the grape: An early history of fermented beverages. S.C. Rasmussen

11:00 HIST **11.** Metals of antiquity and their alloys. **V.V. Mainz**

MONDAY AFTERNOON

Section A

Sheraton Denver Downtown Hotel
Tower Court A

Chemical Technology in Antiquity

Cosponsored by MPPG‡

S. C. Rasmussen, *Organizer, Presiding*

1:30 HIST **12.** The skin they were in: Leather and tanning in antiquity. **C.L. Heth**

2:00 HIST **13.** Modern chemistry of the ancient chemical processing of organic dyes and pigments. **Z.C. Koren**

2:45 HIST **14.** Scented oils and perfumes in antiquity. **N. Balasubramanian**

3:15 Intermission.

3:30 HIST **15.** Soap production and use in antiquity. **K.L. Konkol**, S.C. Rasmussen

4:00 HIST **16.** Modern materials in antiquity: An early history of the art and technology of glass. **S.C. Rasmussen**

MONDAY EVENING

Section A

Colorado Convention Center
Halls C/D

Sci-Mix

S. C. Rasmussen, *Organizer*

8:00 - 10:00
11-12, 14. See previous listings.

TUESDAY MORNING

Section A

Sheraton Denver Downtown Hotel
Tower Court A

Modern Chemical Warfare: History, Chemistry, Toxicology, Morality

J. Gal, *Organizer*
J. A. Asper, *Presiding*

8:00 Introductory Remarks.

8:05 HIST **17.** Modern chemical warfare: A historical overview. **J. Gal**

8:35 HIST **18.** German chemists and chemical weapons: Fritz Haber and his legacy. **S. Everts**

9:05 HIST **19.** Chemical warfare and French chemists. **P. Laszlo**

9:35 Intermission.

9:50 HIST **20.** American chemists and chemical warfare. **T.T. Tidwell**

10:20 "Haber: The Father of Chemical Warfare", a film by Daniel Ragussis.

11:00 Q&A with Daniel Ragussis.

George C. Pimentel Award in Chemical Education: Symposium in Honor of I. Dwaine Eubanks

Sputnik to Smartphones: A Half-Century of Chemistry Education

Sponsored by CHED, Cosponsored by HIST‡

TUESDAY AFTERNOON

Section A

Sheraton Denver Downtown Hotel
Tower Court A

Modern Chemical Warfare: History, Chemistry, Toxicology, Morality

J. Gal, *Organizer, Presiding*

1:00 HIST **21.** Chemical weapons: Clinical description and discussion of basic injuries. **D. Gilmore**

1:30 HIST **22.** Aiming chemical weapons at student engagement: Chemistry and war as a first year seminar. **J.A. Asper**

2:00 HIST **23.** Modern chemical warfare: A philatelic chronology. **D. Rabinovich**

2:30 HIST **24.** Chemical warfare: The American WWII aftermath. **D.C. Neckers**

3:00 Intermission.

3:15 HIST **25.** Nerve agents: From inception to current concepts. **S.W. Wiener**

3:45 HIST **26.** Ethics of chemical weapons research. **J.D. Kovac**

4:15 HIST **27.** OPCW: Working for a world free of chemical weapons. D. Feakes, **A. Kelle**

George C. Pimentel Award in Chemical Education: Symposium in Honor of I. Dwaine Eubanks

Sputnik to Smartphones: A Half-Century of Chemistry Education

Sponsored by CHED, Cosponsored by HIST‡

I&EC

Division of Industrial and Engineering Chemistry

P. Smith and M. Moore, *Program Chairs*

OTHER SYMPOSIA OF INTEREST:

Nanostructured Porous Polymers: Synthesis, Properties and Applications *(see PMSE, Sun, Mon)*

Drug Delivery and Drug Device Combination Product *(see PMSE, Tue, Wed, Thu)*

Advances in Analytical Separations *(see ANYL, Mon)*

50th Anniversary of the NUCL Division *(see NUCL, Tue, Wed)*

Glenn T. Seaborg Award: Symposium in Honor of Heino Nitsche *(see NUCL, Sun, Mon)*

Chemical Angel Network: Chemists Investing in Chemical Companies *(see PROF, Mon)*

SOCIAL EVENTS:

Luncheon, 12:00 PM: Tue

BUSINESS MEETINGS:

Business Meeting, 12:00 PM: Sun
Business Meeting, 6:30 PM: Mon

SUNDAY MORNING

Section A

Embassy Suites Denver–Downtown Convention Center
Crystal Ballroom A

ACS Award in Separations Science & Technology: Symposium in Honor of Richard D. Noble

D. L. Gin, *Organizer, Presiding*

8:30 I&EC **1.** Double salt ionic liquids with unique chemical environments for separations. **R.D. Rogers**, H. Wang, S.P. Kelley

9:05 I&EC **2.** Phase change ionic liquids for post-combustion CO_2 capture. **J.F. Brennecke**, S. Seo, L.D. Simoni, M.A. Stadtherr

9:40 I&EC **3.** Reverse osmosis membranes research-current development and future directions. **N.N. Li**, M. Tsai, J. Li

10:15 I&EC **4.** Materials and devices to enable low-energy-intensive gas separations. **W. Koros**

10:50 I&EC **5.** Improving distillation: Not an oxymoron. **P. Wankat**

Section B

Embassy Suites Denver–Downtown Convention Center
Crystal Ballroom B

Uranium in Seawater

The Chemistry

Cosponsored by CEI and MPPG‡

P. F. Britt, *Organizer*
R. D. Rogers, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 I&EC **6.** Uranium and U. **C.H. Middlecamp**

Technical program information known at press time.
The official technical program for the 249th ACS National Meeting is available at: www.acs.org/denver2015

8:25 I&EC **7.** Design and synthesis of pyridine-based and amidoxime-based ligands for uranium adsorption. **C. Zhang**, S. Dai

8:45 I&EC **8.** Polymer-supported amines and aminophosphonates as uranyl-selective extractants. **S. Alexandratos**, R.C. Sellin, M. Florent, X. Zhu

9:05 I&EC **9.** Complexation of glutarimidedioxime with V(V), a major competing ion for the extraction of U(VI) from seawater. **C. Leggett**, L. Rao

9:25 Intermission.

9:45 I&EC **10.** Accelerating extraction of uranium from seawater through high-performance computational science: Challenges and advances. **D.A. Penchoff**, D.M. Jenkins, G.K. Schweitzer, R.J. Harrison

10:05 I&EC **11.** Development of bifunctional chelators for selective extraction of uranium from seawater. **C.W. Abney**, J.C. Gilhula, W. Lin

10:25 I&EC **12.** Density functional theory methods to predict ligands pKa's, and stability constants for uranyl complexes. **V. Bryantsev**, N. Mehio

10:45 I&EC **13.** Combinatorial peptoid screening to discover new ligands for uranyl binding. **B. Parker**, A. Knight, S. Vukovic, M.B. Francis, J. Arnold

11:05 I&EC **14.** Determination of formation constants for Uranyl(VI) complexes in aqueous solution by spectroscopic techniques. **R.D. Hancock**

11:25 I&EC **15.** Nanofiber chitin mats for coextraction of value added metals from seawater: Improving the economics of uranium recovery. **R.D. Rogers**, S.P. Kelley, G. Gurau, J.L. Shamshina

SUNDAY AFTERNOON

Section A

Embassy Suites Denver–Downtown Convention Center

Crystal Ballroom A

ACS Award in Separations Science & Technology: Symposium in Honor of Richard D. Noble

D. L. Gin, *Organizer, Presiding*

2:00 I&EC **16. Award Address** (ACS Award is Separations Science & Technology). Recent advances in the design of functional room-temperature ionic liquid-based materials for selective gas separations. **D.L. Gin**, Y. Kohno, M.G. Cowan, W.M. McDanel, Z.V. Singh, Z. Shi, R.D. Noble

2:35 I&EC **17.** Influence of propane on CO_2/CH_4 and N_2/CH_4 separations in CHA zeolite membranes. **J.L. Falconer**, H.H. Funke, R.D. Noble, T. Wu, M. Diaz, R. Zhou

3:10 I&EC **18.** Properties of membrane materials for solar fuels generators. **C.A. Koval**

3:45 I&EC **19.** Ionic polyimides: New dimensions in the design of polymer materials for membrane separations. **J. Bara**, J.D. Roveda, M. Shannon, D. Wallace

4:20 I&EC **20.** Composite Pd alloy membranes for high temperature hydrogen production with CO_2 capture. **J.D. Way**, H. Abu El Hawa, S.N. Paglieri, S. Lundin, N. Patki

The use of any device to capture images (e.g., cameras and camera phones) or sound (e.g., tape and digital recorders) or to stream, upload or rebroadcast speakers or presentations is strictly prohibited at all official ACS meetings and events without express written consent from ACS.

Section B

Embassy Suites Denver–Downtown Convention Center

Crystal Ballroom B

Uranium in Seawater

The Sorbents

Cosponsored by CEI and MPPG‡

R. D. Rogers, *Organizer*

P. F. Britt, *Organizer, Presiding*

1:00 I&EC **21.** Improvements of radiation grafting of selective ligands onto polymeric substrates to produce high-capacity adsorbents for harvesting uranium from seawater. T.C. Dietz, C. Tomaszewski, M.A. Adel-Hadadi, A. Barkatt, **M. Al-Sheikhly**

1:20 I&EC **22.** Advanced fiber adsorbents for recovery of uranium from seawater prepared via controlled radical polymerization. S. Brown, S. Chatterjee, J.C. Johnson, L. Kuo, G.A. Gill, **T. Saito**

1:40 I&EC **23.** Fibrous adsorbents prepared by SI-ATRP for the recovery of uranium from seawater. **S. Brown**, L. Kuo, S. Chatterjee, J.C. Johnson, Y. Yue, G.A. Gill, T. Saito, S. Dai

2:00 I&EC **24.** Preparation of uranium adsorbents by radiation-induced graft polymerization. **C. Janke**, S. Das, R. Mayes, C. Tsouris, S. Dai

2:20 I&EC **25.** Nanofiber absorbents for uranium extraction from seawater. S. Xie, X. Liu, B. Zhang, H. Ma, C. Ling, M. Yu, **J. Li**

2:40 Intermission.

3:00 I&EC **26.** Performance enhancing amidoxime adsorbent for uranium recovery from seawater. **S. Das**, C. Janke, R. Mayes, C. Tsouris, S. Dai

3:20 I&EC **27.** Development of novel porous sorbents for extraction of uranium from seawater. W. Lin

3:40 I&EC **28.** Carbon materials for seawater uranium extraction. **R.T. Mayes**, J. Gorka, Y. Yue, S. Dai, G. Gill, L. Kuo, J. Wood

4:00 I&EC **29.** Novel nanostructured sorbent materials for the collection and recovery of uranium from seawater and other solutions. **R.S. Addleman**, W. Chouyyok, J.W. Pittman, K.M. Nell, S. Peterson, M.G. Warner, C. Warner

4:20 I&EC **30.** Uranium-from-seawater sorbents from fishing industry waste – from batch to continuous production. **G. Gurau**, J.L. Shamshina, S.P. Kelley, R.D. Rogers

4:40 I&EC **31.** Porous polymeric adsorbents for the recovery of uranium from seawater. **Y. Yue**

MONDAY MORNING

Section A

Embassy Suites Denver–Downtown Convention Center

Crystal Ballroom A

Uranium in Seawater

Sorbents and Analysis

Cosponsored by CEI, MPPG‡ and NUCL

P. F. Britt, R. D. Rogers, *Organizers*

S. Dai, *Presiding*

8:00 I&EC **32.** Fiber functionalization via novel ligand for uranium recovery from seawater. **S. Chatterjee**, S. Brown, J. Johnson, R.T. Mayes, C.A. Grant, B.P. Hay, T. Saito

8:20 I&EC **33.** Synthesis and properties of amidoxime-based fibrous adsorbents for extraction of uranium from seawater by radiation-induced graft polymerization. **G. Wu**, J. Hu, Z. Xing, **L. Xu**, R. Li, S. Li

8:40 I&EC **34.** Effects of crosslinking in polymer brush uranium adsorbents. **J. Johnson**, S. Brown, S. Chatterjee, T. Saito

9:00 I&EC **35.** Application of synchrotron radiation technique in extraction uranium from seawater. **L. Zhang**, C. Jin, J. Zhou, J. Wang

9:20 I&EC **36.** Adsorption behavior of uranium from seawater on amidoxime-based UHMWPE prepared by radiation induced graft polymerization. **H. Ma**, X. Liu, C. Ling, X. Yang, J. Hu, S. Li, Z. Xing, J. Li, G. Wu

9:40 Intermission.

10:00 I&EC **37.** Chemical and structural characterization of high density polyethylene (HDPE) based sorbents developed for the binding of uranium from seawater. **M.G. Warner**, S.M. Peterson, B. Arey, I. Arslan, M.H. Engelhard, B. Naes, D. Willingham, C. Barrett, R.S. Addleman

10:20 I&EC **38.** Uranium from seawater marine testing program at the Pacific Northwest National Laboratory: Overview. **G.A. Gill**, L. Kuo, J. Wood, J.E. Strivens, M.E. Cobb, G. Bonheyo, R. Jeters, J. Park, T. Khangaonkar, R.S. Addleman, M.G. Warner, S.M. Peterson, K. Buesseler, C. Breier, E. D'Alessandro

10:40 I&EC **39.** Elution of uranium and transition metals from amidoxime-based sorbents for sequestering uranium from seawater. H. Pan, L. Kuo, G.A. Gill, **C.M. Wai**

11:00 I&EC **40.** Separation and concentration of Uranium from sea water using aptamer receptors. **R.F. Williams**

11:20 I&EC **41.** Matrix elimination for the determination of uranium in seawater using inductively coupled plasma mass spectrometry. **J. Wood**, G.A. Gill, K. Choe

11:40 I&EC **42.** Adsorbent pretreatment and batch kinetic experiments for uranium adsorption testing and modeling. S. Das, W. Liao, R. Mayes, C.J. Janke, S. Dai, **C. Tsouris**

ACS Award in Industrial Chemistry: Symposium in Honor of Thomas J. Colacot

Sponsored by BMGT, Cosponsored by ANYL and I&EC

MONDAY AFTERNOON

Section A

Embassy Suites Denver–Downtown Convention Center

Crystal Ballroom A

Uranium in Seawater

Analysis and Toxicity/Cost

Cosponsored by CEI and MPPG‡

P. F. Britt, R. D. Rogers, *Organizers*

G. A. Gill, *Presiding*

1:00 I&EC **43.** Characterization and testing of adsorbent materials to extract uranium from natural seawater. **L. Kuo**, G.A. Gill, J. Wood, J.E. Strivens, M.E. Cobb, C. Janke

1:20 I&EC **44.** Selectivity and kinetic behavior of heavy metal and radionuclides on supported ion-exchange adsorbant. **W.T. Honeycutt**, E.B. Kadossov, A.W. Apblett, N.F. Materer

1:40 I&EC **45.** Toxicity of the adsorbent materials used to extract uranium from seawater. **J. Park**, R. Jeters, G.A. Gill, L. Kuo, G. Bonheyo

2:00 I&EC **46.** How biofouling impacts uranium sorbent material performance and what can be done to mitigate the effect. **G.T. Bonheyo**, J. Park, R. Jeters, E.M. Winder, L. Kuo, G.A. Gill

2:20 I&EC **47.** Homogeneous blending of chitin with biopolymers for advanced biodegradable sorbents for uranium extraction from seawater. **J. Bandomir**, S.P. Kelley, J.L. Shamshina, G. Gurau, R.D. Rogers

2:40 I&EC **48.** Dual functional chitin based sorbents for coextraction of aqueous copper and uranium. **S.P. Kelley**, J.L. Shamshina, G. Gurau, R.D. Rogers

3:00 Intermission.

3:20 I&EC **49.** Cost assessment for the recovery of uranium from seawater via a textile adsorbent. **E. Schneider**, M. Flicker, X. Chen, H. Lindner

3:40 I&EC **50.** Uranium-from-seawater sorbents from fishing industry waste – cost reduction through solvent recycle. **J.L. Shamshina**, G. Gurau, S.P. Kelley, R.D. Rogers

4:00 I&EC **51.** Impacts of seawater uranium extraction on oceanic circulation and transport. **T. Khangaonkar**, T. Wang, G.A. Gill

4:20 I&EC **52.** Green process for extraction and recovery of uranium from ground water and seawater. **A.W. Apblett**, C. Perkins, H. Albusaidi

4:40 Panel Discussion.

5:00 Concluding Remarks.

ACS Award in Industrial Chemistry: Symposium in Honor of Thomas J. Colacot

Sponsored by BMGT, Cosponsored by ANYL and I&EC

MONDAY EVENING

Section A

Colorado Convention Center

Halls C/D

Sci-Mix

P. Smith and M. Moore, *Organizer*

8:00 - 10:00

10, 24, 44. See previous listings.
67, 69, 71, 73-74, 82, 98. See subsequent listings.

TUESDAY MORNING

Section A

Embassy Suites Denver–Downtown Convention Center

Crystal Ballroom A

E.V. Murphree Award in Industrial & Engineering Chemistry: Symposium in Honor of Joseph R. Zoeller

Cosponsored by CATL

Financially supported by ExxonMobil Research and Engineering Co

M. Moore, *Organizer*

J. S. Witzeman, *Organizer, Presiding*

8:30 I&EC **53.** Amido fluorophosphite ligands for the rhodium catalyzed low pressure hydroformylation reaction. **T.A. Puckette**

8:55 I&EC **54.** Selective aerobic C-C bond cleavage in lignin models and extracts using oxovanadium complexes. **R. Baker**

9:20 I&EC **55.** Epoxybutene: The development of a selective process from butadiene. **J.L. Stavinoha**

9:45 I&EC **56.** Acetylene from shale gas. **N. Collins**, T. Upshaw

10:10 I&EC **57.** Measuring kinetics of hydrocarbon and oxygenate pyrolysis. **P.R. Westmoreland**

10:35 I&EC **58.** Catalytic conversion of C1 reactants to higher value oxygenates. **J.J. Spivey**

11:00 I&EC **59.** Tailored transition metal oxides for carbonaceous fuel conversion. **F. Li**

TUESDAY AFTERNOON

Section A

Embassy Suites Denver–Downtown Convention Center

Crystal Ballroom A

E.V. Murphree Award in Industrial & Engineering Chemistry: Symposium in Honor of Joseph R. Zoeller

Cosponsored by CATL

Financially supported by ExxonMobil Research and Engineering

M. Moore, *Organizer*

J. S. Witzeman, *Organizer, Presiding*

1:30 I&EC **60.** Bimetallic cooperativity in homogeneous catalysis: Takes two to tango. G.G. Stanley

1:55 I&EC **61.** Active state of gold catalysts for carbonylation reactions. C. Hardacre, M.J. Muldoon, J. Sa', K. Morgan, Q. Cao, A. Goguet, S. Taylor

2:20 I&EC **62.** Molecular active sites in heterogeneous Ir-La/C catalyzed carbonylation of methanol to acetates. Y. Wang

2:45 I&EC **63.** Pincer-crown ether catalysts for Lewis acid-promoted transformations. A.J. Miller, J.B. Smith, J. Grajeda, L.C. Gregor

3:10 I&EC **64.** Neutron scattering studies of molecular interactions with pure and decorated metal nanomaterials. J.Z. Larese

‡ *Cooperative Cosponsorship*

3:35 I&EC **65.** Carbonylation of methanol without alkyl halide. A.J. Vetter, J.R. Zoeller, T. Smith, **M. Moore**, M.K. Wiedmann

4:00 I&EC **66. Award Address** (E. V. Murphree Award in Industrial and Engineering Chemistry sponsored by ExxonMobil Research and Engineering). Role of mechanistic studies in industrial processes. **J.R. Zoeller**

TUESDAY EVENING

Section A

Colorado Convention Center
Halls C/D

General Posters

P. M. Smith, *Organizer*

5:00 - 6:30

I&EC **67.** Click chemistry-mediated synthesis of novel functionlized ionic liquids containing TMS moiety. **M. Sanchez Zayas**, S. Nestor, J.C. Gaitor, A. Mirjafari

I&EC **68.** Adsorption performance of carbon molecular sieve prepared by carbon deposition with several depositing agents. **F. Jin, X. Zhang**, M. Gao, J. Zhang, H. Xu, D. Hua

I&EC **69.** Uranium extraction from seawater using amidoxime modified mesoporous silica. **C. Gunathilake**, M. Jaroniec, J. Gorka, S. Dai

I&EC **70.** LbL (layer-by-layer) multilayering on cellulose nanofibrils and its effects on surface charge and suspension dewatering. K. Sim, **H. Youn**, J. Lee, H. Lee

I&EC **71.** Withdrawn.

I&EC **72.** Spectroscopic identifications of inhibition effect by an ionic liquid as a synergist on gas hydrate formation. S. Han, J. Shin, **S. Kang**

I&EC **73.** Distinguishing the Rosary and Island form of asphaltene with solid state nuclear magnetic resonance. **M. Verma**, S. Pradhan, P. Venkataraman, Y. Fang, M. Shammai, S.L. Wellington, W.E. Billups, L. Alemany

I&EC **74.** Predicting the acid dissociation constants of aqueous amidoximes. **N. Mehio**, M. Lashley, J. Nudgent, L. Tucker, B. Correia, C. Do-Thanh, S. Vukovic, S. Dai, R.D. Hancock, V. Bryantsev

I&EC **75.** Nanoparticle tracers for measurement of degree of preferential flow in shale. N. Yang, G. Jiang, E. Zheng, A. Wang, Y. Xu, **X. Guo**

I&EC **76.** Polymerized imidazolium ionic liquids containing flexible pendant groups and their properties. **J. Lee**, H. Kim, J. Lee, H. Kim

I&EC **77.** Ionic liquids containing ether-functionalized anion and their properties. **J. Lee**, Y. Kim, S. Park, J. Hwang

I&EC **78.** Nitrile-functionalized tertiary amines for SO_2 absorption. **J. Lee**, S. Hong, M. Cheong, H. Kim

I&EC **79.** Isolation and structural characterization of bicarbonate and carbonate species formed during CO_2 absorption/desorption. **J. Lee**, J. Im, M. Cheong, H. Kim

I&EC **80.** Porous carbons derived from biomass for carbon capture. **J. Lee**, S. Park

I&EC **81.** Ground calcium carbonate modified by polyelectrolytes multilayering at various salt concentrations for high filler loading in papermaking process. **J. Lee**, H. Youn, K. Sim, H. Lee, H. Lee

I&EC **82.** Removal of acid yellow 25 dye onto chitin extracted from waste crab legs. **D.D. Wright**, L. O'Brien, I. Pathiraja, C. Wei, L. Norcio

I&EC **83.** Guest gas enclathration in the tetra-n-butyl ammonium chloride (TBAC) semiclathrates: potential application to CO_2 capture. **Y. Seo**, S. Kim, S. Kang

WEDNESDAY MORNING

Section A

Embassy Suites Denver–Downtown Convention Center
Rexford Room

General Papers

C. J. Murphy, *Organizer, Presiding*

8:30 I&EC **84.** Development of flexible alkaline batteries with carbon nanotube and polymers. **Z. Wang**, Z. Wu, N. Bramnik, S. Mitra

8:50 I&EC **85.** Two step process for extraction of graphene quantum dots and chemicals/fuels from coal. **K. Mondal**, A. Sims, K. Tsai, T. Hasan

9:10 I&EC **86.** Amine based mesoporous silica with incorporated metal oxide for carbon dioxide sorption. **C. Gunathilake**, M. Jaroniec

9:30 I&EC **87.** Study of a novel depressant for reverse cation flotation of iron ore with focused beam reflective measurement. **S.A. Kofsky Wofford**, X. Yin

9:50 Intermission.

10:05 I&EC **88.** Effects of alkyl chain length on lithium salt solubilities in ammonium Tf_2N based ionic liquids. **D.P. Fagnant**, J.F. Brennecke

10:25 I&EC **89.** Influence of the use of film forming amines in condensate polishing systems on the properties of ion exchange resins. **A. Kabir**, A. Apblett

10:45 I&EC **90.** Robust block copolymer based RTIL-gel membrane materials for CO_2 separation. **D. Wijayasekara**, T.S. Bailey

11:05 I&EC **91.** Carbonyl sulfide formation during wide temperature reformate desulfurization on ZnO/SiO_2 and Cu promoted ZnO/SiO_2 adsorbents. **A.R. Sujan**, B. Tatarchuk, H. Yang

WEDNESDAY AFTERNOON

Section A

Embassy Suites Denver–Downtown Convention Center
Rexford Room

General Papers

C. J. Murphy, *Organizer, Presiding*

1:30 I&EC **92.** Improved kinetic model for ethane pyrolysis at high conversions and high pressures. **K. Wang**, M.H. Saldana, S. Villano, G. Bogin, A.M. Dean

1:50 I&EC **93.** Electrical discharge enabled plasmachemical activation of methane in microscale reactors. **P. Kreider**, J. Pommerencck, A.F. Yokochi

2:10 I&EC **94.** Diffusion and aging of wood preservatives in softwood under environmental exposure. **K. Ondrusova**, V. Martinska, A. Kubatova, E.I. Kozliak

2:30 I&EC **95.** Smoother ride: Paving the voids in thermophysical property data using QSPR. **W.H. Carande**, A. Kazakov, C. Muzny

2:50 Intermission.

3:05 I&EC **96.** Concatenated gas saturation method for vapor pressure measurement: A technique for oxidatively unstable compounds. **J.A. Widegren**, A.E. Tolbert, T.J. Bruno

3:25 I&EC **97.** Highly selective cation separations in electrodialysis through cation-exchange membranes coated with polyelectrolyte multilayers. **N. White**, M.L. Bruening, M. Misovich

3:45 I&EC **98.** Extraction of the protein fraction of dry distillers grains with solubles (DDGS), implementing chemical methods. **M.F. Villegas Torres**, J. Ward, G.J. Lye

4:05 I&EC **99.** Coating for biofouling prevention. **Y. Li**, H. Yu, K.L. Yeung

4:25 I&EC **100.** Conversion of biodiesel-derived crude glycerol into acrolein. R. Liu, Y. Jin, **T. Wang**

INOR

Division of Inorganic Chemistry

S. A. Koch and N. S. Radu, *Program Chairs*

OTHER SYMPOSIA OF INTEREST:

Alfred Bader Award in Bioinorganic or Bioorganic Chemistry: Symposium in Honor of Michael A. Marletta *(see BIOL, Sun)*

ACS Award for Creative Research and Applications of Iodine Chemistry: Symposium in Honor of Karl O. Christe *(see FLUO, Tue)*

Convergence of Theory & Experiment in Heavy Element Chemistry *(see NUCL, Wed, Thu)*

SOCIAL EVENTS:

Reception: Dow Chemistry of the Energy Water Nexus Reception, 4:30 PM: Tue

SUNDAY MORNING

Section A

Colorado Convention Center
Room 105

Undergraduate Research at the Frontiers of Inorganic Chemistry

Coordination Chemistry

C. Nataro, S. R. Smith, *Organizers*
C. Hamaker, *Presiding*

9:00 Introductory Remarks.

9:05 INOR **1.** Investigating the oxidation of olefins using derivatives of the non-heme iron catalyst [Fe(BPMEN)](OTf)$_2$]. **C.A. Lidston**, M.R. Davies, R.D. Pike, **C. Goh**

9:25 INOR **2.** Metal cation detection using a novel small molecule chemosensor. D.T. de Lill, A.M. Gagnon, M. Brown, **K. Shelley**, M. DeLuca

9:45 INOR **3.** Tripodal carbamoylmethylphosphine oxide (CMPO) ligands for f-element chelation: Solution photophysical studies and lanthanide/actinide extraction properties. **E.J. Werner**, S.M. Biros, S.N. McGraw, D.A. Hardy, H.T. Sartain

10:05 INOR **4.** Synthesis of a series of first row transition metal complexes containing a tetradentate ligand. **H.F. Drake**, A. Blake, C.M. Donahue, S.R. Daly, **B.J. Bellott**

10:25 Intermission.

10:35 INOR **5.** Lanthanides, chirality, and ionic liquids: Finding a niche with undergraduates. **T. Hopkins**

10:55 INOR **6.** Interconversion of eight-coordinate, dodecahedral, rhenium(V) isomers supported by a single chelating ligand. H. Sodhi, C.P. Bosko, S. Rashid, **G.A. Moehring**

11:15 INOR **7.** Methanobactin-inspired coordination chemistry with new mixed-donor ligands. **D. Rabinovich**

11:35 INOR **8.** Utilization of sulfonamides in crystal engineering. **C. Hamaker**, Z.E. Lawton, M. Oblazny

Section B

Colorado Convention Center
Room 301

2015 Priestley Medalist: Symposium in Honor of Jacqueline K. Barton

E. Boon, M. C. Buzzeo, S. Delaney, *Organizers*
V. C. Pierre, *Organizer, Presiding*

8:30 Introductory Remarks.

8:40 INOR **9.** Road to genome expansion is paved with good intentions: When DNA repair goes awry. **S. Delaney**

9:10 INOR **10.** Snapshots of metallobleomycin-DNA recognition and binding: A tale of two tails. **E.C. Long**, M.M. Georgiadis

9:40 INOR **11.** Scrutinizing DNA damage. **M. Nunez**

10:10 Intermission.

10:20 INOR **12.** Formation and characterization of platinum adducts on ribosomal RNA. X. Bao, **C.S. Chow**

10:50 INOR **13.** Enhancing extracellular proteostasis through the unfolded protein response. **J. Genereux**, J.W. Kelly, R. Wiseman

11:20 INOR **14.** Molecular shape control applied to the dynamic capture and release of biorelevant substrates. **A. Petitjean**

11:50 INOR **15.** Systematic material design using biomolecules. **T. Tamaki**

Section C

Colorado Convention Center
Room 302

ACS Award in Organometallic Chemistry: Symposium in Honor of William J. Evans

J. R. Walensky, *Organizer*
J. W. Ziller, *Presiding*

8:30 INOR **16.** Measuring hydride donor ability to guide catalyst design for reduction reactions. **J. Yang**, C. Tsay, J. Khosrowabadi Kotyk, B. Livesay

8:50 INOR **17.** Next generation redox-active "ligands" from non-innocent coordination complexes. **A.F. Heyduk**

9:10 INOR **18.** Synthetic chemistry as a wIndow into biology: Probing molecular complexity with small molecular species. **A. Borovik**

9:30 INOR **19.** Evaluating metal–carbon orbital mixing in metallocene dichlorides. **S.A. Kozimor**, E.R. Batista, J.N. Cross, D.L. Clark, J.M. Keith, R.L. Martin, S.G. Minasian, D.K. Shuh, C.S. Stieber, J.A. Trujillo, T. Tyliszczak

9:50 Intermission.

10:00 INOR **20.** Covalency in actinide metallocene complexes. **D.L. Clark**

10:20 INOR **21.** Bond strength in molecular f element compounds from the quantum theory of atoms in molecules. Q. Huang, J.R. Kingham, A. Mountain, **N. Kaltsoyannis**

10:40 INOR **22.** Group 11 cluster chemistry: What I didn't learn in the Evans Lab. **J.R. Walensky**, A. Lane, P. Rungthanapathsophon

11:00 INOR **23.** Practical models for organometallic chemistry. **W. Hehre**

Section D

Colorado Convention Center
Room 303

Chemical Approaches to Spintronics Research

R. Beaulac, *Organizer*
K. R. Kittilstved, *Presiding*

8:30 INOR **24.** Spin coherence transfer using photogenerated spin-correlated radical pairs. **M.R. Wasielewski**, N.E. Horwitz, B.K. Rugg

9:00 INOR **25.** Spin transport in organic materials: From single molecules to crystals. **S. Sanvito**

9:30 INOR **26.** Probing spin-exciton and spin-charge interactions in open-shell organic semiconductors. **T.L. Andrew**

10:00 Intermission.

10:30 INOR **27.** Evaluating magnetic properties of molecules with strong anisotropy based on electronic configuration and geometry. **K.R. Dunbar**, M. Ballesteros, S. Hill, D. Pinkowicz, M.R. Saber, T.J. Woods, Y. Zhang, H. Zhao

11:00 INOR **28.** Magnetic ordering and conductivity in heavy atom and multiband radicals. A. Mailman, S.M. Winter, J.W. Wong, D. Tian, C.M. Robertson, P.A. Dube, S.R. Julian, S. Hill, **R.T. Oakley**

11:30 INOR **29.** Spin-selective charge recombination in complexes of CdS quantum dots and organic hole acceptors. **D.J. Weinberg**, S.M. Dyar, Z. Khademi, M. Malicki, S.R. Marder, M.R. Wasielewski, E.A. Weiss

Section E

Colorado Convention Center

Room 201

ACS Award in Inorganic Chemistry: Symposium in Honor of John T. Groves

P. J. Chirik, *Organizer*

R. N. Austin, *Organizer, Presiding*

9:00 INOR **30.** Base metal catalysis for hydrocarbon manipulation. **P.J. Chirik**

9:30 INOR **31.** Tandem catalytic hydrogenation of carbon dioxide to methanol. **M.S. Sanford**

10:00 INOR **32.** Functionalization of C–H bonds by iodate and chloride: Mechanistic studies. **T.B. Gunnoe**, J.T. Groves, G.C. Fortman, N.C. Boaz, S.E. Kalman, R.A. Periana, M.M. Konnick

10:30 Intermission.

10:45 INOR **33.** Amazing nonheme high-valent iron-oxo reactivity landscape. **L. Que**

11:15 INOR **34.** Concerted multiple-site proton-coupled electron transfer (PCET): Effects of separating the proton and electron. **J.M. Mayer**, M.A. Bowring, V. Manner, J.J. Warren, J. Wittman, L.R. Bradshaw, D.R. Gamelin, W.D. Morris, T.F. Markle

Section F

Colorado Convention Center

Room 304

Harry Gray Award for Creative Work in Inorganic Chemistry by a Young Investigator: Symposium in Honor of Emily A. Weiss

Cosponsored by WCC

M. R. Hartings, *Organizer, Presiding*

8:30 INOR **35.** Harry Gray as a young investigator: Paradigms lost, found, and going up in gas. **R. Eisenberg**

8:55 INOR **36.** Gray nation: Out of this world. **M.L. Cable**, J.P. Kirby, A. Ponce, A.M. Stockton, M.F. Mora, P. Willis, T.H. Vu, P.M. Beauchamp, H.B. Gray

9:20 INOR **37.** Molecular systems for photocatalytic hydrogen oxidation. **M.D. Hopkins**, H.B. Vibbert, M. Westwood, N.T. La Porte

9:45 Intermission.

9:55 INOR **38.** Artificial hydrogenases for solar hydrogen production. **K.L. Bren**, B. Kandemir, J.G. Kleingardner, L. Kubie

10:20 INOR **39.** Designing metalloproteins with tunable redox potentials and reorganization energies for efficient long-range electron transfer. **Y. Lu**, N.M. Marshall, P. Hosseinzadeh, O. Farver, S.E. Wherland, I. Pecht

10:45 INOR **40.** Time-resolved spectroscopic studies of electron and proton transfer in biologically relevant systems. **M.E. Ener**, H.B. Gray, T.G. Spiro

11:10 INOR **41.** Understanding plasticity in molecular recognition. **D.S. Wuttke**, T.H. Dickey, M. McKercher

11:35 INOR **42.** Bioinorganic chemistry in a gray area. **F.A. Tezcan**

Section G

Colorado Convention Center

Room 401

Earth-Abundant Materials for Sustainable Hydrogen Production and Storage

Cosponsored by MPPG

A. L. Prieto, *Organizer*

C. Ban, Y. Yang, *Organizers, Presiding*

8:00 INOR **43.** Sunlight-driven hydrogen formation by membrane-supported photoelectrochemical water splitting. **N.S. Lewis**

8:40 INOR **44.** Challenges in photoelectrochemical water splitting materials. **J.A. Turner**

9:20 INOR **45.** Enabling solar fuels technology by high throughput discovery of earth abundant oxygen evolution reaction catalysts. **J. Haber**, D. Guevarra, R. Jones, A. Shinde, N. Becerra, C. Xiang, S. Mitrovic, S. Jung, C. Kisielowski, J. Yano, J. Jin, J. Gregoire

9:40 Intermission.

9:50 INOR **46.** Tin nitride spinel semiconductor for photoelectrochemical water oxidation. C. Caskey, J.A. Seabold, V. Stevanovic, D.S. Ginley, N. Neal, R.M. Richards, S. Lany, **A. Zakutayev**

10:10 INOR **47.** Electrolysis of urea for the sustainable production of hydrogen. **G. Botte**

10:50 INOR **48.** Sulfur Sulfur thermochemical hydrogen production cycle: A new thermochemical cycle employing only earth abundant elements. N. AuYeung, K. Caple, P. Kreider, **A.F. Yokochi**

11:30 INOR **49.** Lithium metalorganic complex used to clean hydrogen sulfide for hydrogen production and/or storage. **X. Li**, R. Morrish, C.A. Wolden, **Y. Yang**

Section H

Colorado Convention Center

Room 203

Organometallic Chemistry

Catalysis

N. S. Radu, *Organizer*

G. Dobereiner, C. Hahn, *Presiding*

9:00 INOR **50.** Tetracarbene iron(IV) intermediates for catalytic aziridination. S.A. Cramer, R. Hernandez Sanchez, P.P. Chandrachud, D.F. Brakhage, **D.M. Jenkins**

9:20 INOR **51.** Synthesis and reactions of (^{C_2F_5}PCP)Ru(cod)H. **B. Thapaliya**, G.A. Venegas, N. Arulsamy, D.M. Roddick

9:40 INOR **52.** Synthesis and metal coordination chemistry of (^{iPr_2})(PNP) and (^{R_2})(PONOP) (R_f = CF_3, C_2F_5) chelates. **P. Miller**, D.M. Roddick

10:00 INOR **53.** Experimental and computational investigation of Csp3-N, Csp3-F, and Csp3- Csp2 reductive elimination from model palladium (IV) complexes. **I.M. Pendleton**, P.M. Zimmerman, M.S. Sanford, M. Perez-Temprano

10:20 INOR **54.** Investigation of acid and base co-catalysts for the palladium(II) and platinum(II) catalyzed hydroarylation of acetylene. **C. Hahn**, M. Manjahi

10:40 INOR **55.** Synthesis and metal (M = Ir, Ru) coordination chemistry of (^{t}Bu)(R_f)(PCP) (R_f = CF_3, C_2F_5) chelates. **S. Debnath**, D.M. Roddick

11:00 INOR **56.** Influence of Lewis acids on migratory insertion: Applications to C-C bond formations. **G. Dobereiner**

11:20 INOR **57.** Cross-coupling catalysis in water – a versatile approach. **J. Eppinger**, D. Sawant, A.V. Zernickel

Section I

Colorado Convention Center

Room 205

Chemistry of Materials

Materials for Energy and Catalytic Applications

C. G. Lugmair, *Organizer*

N. C. Anderson, F. Jiao, *Presiding*

8:30 INOR **58.** Synthesis of silicon-germanium alloy nanoparticles for thermoelectric applications. A. Hochbaum, **T. Cornell**

8:50 INOR **59.** Energy transfer by demand in well-defined hybrid materials. **N.B. Shustova**, D.E. Williams, E.A. Dolgopolova

9:10 INOR **60.** CdSe sensitized photocathodes on a mesoporous transparent conducting oxide scaffold. **M.R. Norris**, B.M. Cossairt

9:30 INOR **61.** Exploring the potential of nanostructured black silicon toward catalyst-assisted photoelectrochemical reduction of water. **N.C. Anderson**, Y. Zhao, N.R. Neale, H. Branz, P.W. King

9:50 INOR **62.** Zeolite protected nanocatalysts; Using a hard framework for selection and protection. **J. Palomba**, J.V. Morabito, C. Tsung

10:10 INOR **63.** Mesoporous metal sulfides: Synthesis and photocatalysis. **F. Jiao**

10:30 INOR **64.** Control of doping in Cu_2SnS_3, a novel photovoltaic absorber, through defects, alloying, and annealing. **L. Baranowski**, P. Zawadzki, S. Christensen, S. Lany, L. Gedvilas, E. Toberer, A. Zakutayev

10:50 INOR **65.** Symmetry breaking charge transfer in zinc dipyrrins for OPVs with open circuit voltage in excess of 1.3 V. **A. Bartynski**, M.E. Thompson

11:10 INOR **66.** Charge storage in cation incorporated α-MnO_2. **M. Young**, A. Holder, S.M. George, C. Musgrave

11:30 INOR **67.** $(Cr_xFe_{1-x})_7C_3$ Solid solution as an efficient electrocatalyst for oxygen reduction and evolution reactions in both acidic and alkaline media. **C. Wan**, B.M. Leonard

Section J

Colorado Convention Center

Room 402

Environmental and Energy-Related Inorganic Chemistry

S. A. Koch, *Organizer*

A. J. Morris, *Presiding*

8:30 INOR **68.** Production of chemical feedstocks from pyrolytic lignin using transition metal oxidation catalysts. M.S. Fortin, M.D. Mohadjer Beromi, A. Lai, C.A. Mullen, A.A. Boateng, **N.M. West**

8:50 INOR **69.** On the use of cobalt complexes as mediators in dye sensitized solar cells: Instability of high-potential complexes. **J.T. Kirner**, C.M. Elliott

9:10 INOR **70.** Dipyridyl ketone based catalysts for carbon dioxide reduction. **H. Meylemans**, P. Goodman

9:30 INOR **71.** Enhancement of CO_2 absorption utilizing zinc-based homogenous catalysts in primary amine solution. M. Sarma, C. Lippert, R.A. Burrows, **L.R. Widger**, C. Brandewie, S. Parkin, K. Liu

9:50 Intermission.

10:00 INOR **72.** Exploring charge transfer induced spin cross-over redox mediators in quantum dot sensitized solar cells. A.J. Haring, J.D. Godward, M.E. Pomatto, **A.J. Morris**

10:20 INOR **73.** Controlling interfacial energetics for efficient hybrid bulk heterojunction solar cells. A.J. Haring, **A.J. Morris**

10:40 INOR **74.** Oxidation of carbon monoxide in basic solution catalyzed by nickel cyano carbonyls at ambient condition and the prototype of a CO-powered alkaline flow battery type fuel cell. W. Lo, T. Berenson, N. Tracer, D. Shlian, M. Khaloo, **J. Jiang**

11:00 INOR **75.** Unassisted energy storage using layered chalcogenide semiconductors. **J.R. McKone**, R.A. Potash, F.J. DiSalvo, H.D. Abruna

11:20 INOR **76.** Heterometallic mixed-valent molecular precursors for the synthesis of transition metal oxides. **E. Dikarev**, C.M. Lieberman, Z. Wei, A.S. Filatov

SUNDAY AFTERNOON

Section A

Colorado Convention Center

Room 105

Undergraduate Research at the Frontiers of Inorganic Chemistry

Organometallic Chemistry

C. Nataro, S. R. Smith, *Organizers*

M. Guino-o, *Presiding*

1:30 Introductory Remarks.

1:35 INOR **77.** Ruthenium(II) complexes supported by electron-rich aromatic ligands for small molecule activation and catalysis. **J.P. Lee**, M.J. Hankins, A.D. Riner

1:55 INOR **78.** Investigating the mechanism of N-H bond activation by a sterically congested PCP-iridium complex. **D.A. Laviska**

2:15 INOR **79.** Progress toward the synthesis, characterization, and catalysis of iridium complexes containing [N,N,N]-dianionic pincer ligands. **H. Sajjad**, A.R. O'Connor

2:35 INOR **80.** Copper-catalyzed acyloxylation of aromatic halides. **F. Barrios-Landeros**, B. Ben-Zvi, A.E. Kessler, B.W. Goodman, D.Y. Drory, D.L. Levine

2:55 Intermission.

2:55 INOR **81.** Microwave-assisted copper-catalyzed reactions of aryl halides via concurrent tandem catalysis. D.J. Brown, S. Lin, **A.H. Roy MacArthur**

3:15 INOR **82.** Ambiphilic late-metal silyl and silylene complexes for cooperative activation of small molecules. **A. Deetz**, M.T. Whited

3:35 INOR **83.** Modulation of tris(diphenylphosphinomethyl)phenylborate donor ability via introduction of $M(CO)_3$ units at the boron-bound phenyl substituent. **P.J. Fischer**, A.B. Weberg, T.D. Bohrmann, H. Xu

3:55 INOR **84.** Cyclic hydroboration using azaferrocene-stabilized borenium cations. T.J. Brunker, **S. Krause**, A.L. Rheingold

4:15 INOR **85.** Trends observed during the nickel-catalyzed dehydrogenation of ammonia-borane utilizing asymmetrical triazolylidene ligands. **M.O. Talbot**, M. Guino-o

Section B

Colorado Convention Center

Room 301

2015 Priestley Medalist: Symposium in Honor of Jacqueline K. Barton

E. Boon, M. C. Buzzeo, V. C. Pierre, *Organizers*

S. Delaney, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 INOR **86.** Roles for metal cofactors of MutY enzymes in preventing DNA mutations. **S.S. David**

2:05 INOR **87.** New ROS-activated agents that specifically targert AML cancer cells. **E.J. Merino**

2:35 INOR **88.** Evidence of histidine and aspartic acid phosphorylation in human prostate cancer cells. **A.E. Friedman**

3:05 Intermission.

3:15 INOR **89.** Nitric oxide regulation of bacterial biofilms. **E.M. Boon**

3:45 INOR **90.** DNA-protein self assemblies on millimeter length scales: Artificial light antenna systems. **C.V. Kumar**

4:15 INOR **91.** Assay and mechanistic investigations of iron oxidation catalysts. **C.M. Dupureur**, Y. Song, H. Mayes, E.B. Bauer

Section C

Colorado Convention Center

Room 302

ACS Award in Organometallic Chemistry: Symposium in Honor of William J. Evans

J. R. Walensky, *Organizer*

J. W. Ziller, *Presiding*

1:30 INOR **92.** Synthesis without the solvent: Mechanochemical approaches to organometallic complexes. N.R. Rightmire, D.L. Bruns, **T.P. Hanusa**

1:50 INOR **93.** f-Element single-molecule magnets. K.R. Meihaus, S. Demir, J.D. Rinehart, M. Nippe, J.M. Zadrozny, **J.R. Long**

2:10 INOR **94.** Withdrawn.

2:30 INOR **95.** RE-cycle efforts for nationally critical elements: Fundamental coordination chemistry of scandium. **T.J. Boyle**, J.M. Sears, M.L. Neville, D.T. Yonemoto, R. Cramer, T.N. Lambert, R.F. Hess, L.J. Small

2:50 INOR **96.** Role of lanthanide ions in metal-seamed organic nanocapsules. **J.L. Atwood**, H. Kumari, K. Feaster

3:10 Intermission.

3:20 INOR **97.** To cluster or not to cluster. **G. Meyer**

3:40 INOR **98.** iPhone glues: An introduction to the chemistry of reliable *and reworkable* capillary-flow underfills. **T. Champagne**

4:00 INOR **99.** Synthesis of sodium borohydride without sodium metal. **N. Allen**, R. Butterick, D.M. Millar, D.C. Molzahn

4:20 INOR **100.** Multi-metallic materials containing *f*-elements. **J.H. Farnaby**, P.L. Arnold, W.J. Evans, F.N. Cloke

‡ *Cooperative Cosponsorship*

Section D

Colorado Convention Center
Room 303

Chemical Approaches to Spintronics Research

R. Beaulac, *Organizer*
D. J. Weinberg, *Presiding*

1:30 INOR **101.** Aggregates of Mn_3 single-molecule magnets: Synthesis, properties, and quantum effects. **G. Christou**, T.N. Nguyen, M. Shiddiq, A.M. Mowson, K.A. Abboud, S. Hill

2:00 INOR **102.** Theoretical approaches to the control of spin states in molecules. **C. Herrmann**

2:30 INOR **103.** Development of redox and environmental switches for control of magnetic communication in molecular complexes. **M.P. Shores**, R. Higgins, C. Klug, i. bhowmick, S. Fiedler, A.K. Rappe

3:00 Intermission.

3:30 INOR **104.** Metal silicide nanowires for detection and manipulation of magnetic skyrmions. **S. Jin**

4:00 INOR **105.** Monolayer-protected nanoclusters: Structurally precise building blocks for spintronic applications. **K.L. Knappenberger**, T.D. Green, C. Yi

4:30 INOR **106.** Mechanism of dopant incorporation in $SrTiO_3$ bulk powders and colloidal nanocrystals. K.A. Lehuta, W. Harrigan, **K.R. Kittilstved**

5:00 INOR **107.** Photomagnetic switching in highly conductive Fe(II) spin-crossover complexes with organic radicals. H. Phan, S. Benjamin, E. Steven, J. Brooks, **M. Shatruk**

Section E

Colorado Convention Center
Room 201

ACS Award in Inorganic Chemistry: Symposium in Honor of John T. Groves

P. J. Chirik, *Organizer*
R. N. Austin, *Organizer, Presiding*

1:30 INOR **108.** Inorganic chemistry of biological nitrogen fixation. D. Dean, **B.M. Hoffman**, D. Lukoyanov, L.C. Seefeldt, S. Shaw, Z. Yang

2:00 INOR **109.** Thermodynamics and mechanism of C-H bond activation by the Cu(III)-OH core. **W.B. Tolman**

2:30 INOR **110.** Ligand switching in the control of cytochrome *c* redox function. **E.V. Pletneva**

3:00 Intermission.

3:15 INOR **111.** Raman spectroscopy and computation reveal how hemoglobin controls oxygen affinity. **T.G. Spiro**

3:45 INOR **112.** Structure/function correlations over non-heme iron enzymes. **E.I. Solomon**

Section F

Colorado Convention Center
Room 304

Harry Gray Award for Creative Work in Inorganic Chemistry by a Young Investigator: Symposium in Honor of Emily A. Weiss

Cosponsored by WCC

M. R. Hartings, *Organizer, Presiding*

1:30 INOR **113.** Singlet fission in carotenoid aggregates and dimers. M.J. Tauber

1:55 INOR **114.** Probing pathways of excited-state proton-coupled electron transfer reaction. **J.L. Dempsey**, T.T. Eisenhart, J.C. Lennox, W.C. Howland

2:20 INOR **115.** New sensitizers for solar hydrogen production. **R. Sabatini**, B. Zheng, W.T. Eckenhoff, A. Orchard, K. Liwosz, D. Watson, M. Detty, R. Eisenberg, D.W. McCamant

2:45 INOR **116.** Toward spying on individual working catalyst molecules. **R.H. Goldsmith**

3:10 Intermission.

3:20 INOR **117.** Exploring the mechanism of small molecule metal ion chelators as chemotherapeutic agents against pathogenic bacteria. T. Santos, M. Zhou, M. Lammers, M. Rajendran, K. Hurley, Y. Eun, **D.B. Weibel**

3:45 INOR **118.** Thermodynamic and kinetic measurements of cation exchange in chalcogenide nanocrystals by isothermal titration calorimetry. N. Sturgis, **R.M. Rioux**

4:10 INOR **119.** Luminescent copper-doped semiconductor nanocrystals. **K.E. Knowles**, H.D. Nelson, P.J. Whitham, D.R. Gamelin

4:35 INOR **120.** Metal nanoparticles trapped in unfolded proteins: Synthesis, characterization, and unique materials properties. **M.R. Hartings**, D. Fox, A.E. Miller

Section G

Colorado Convention Center
Room 401

Earth-Abundant Materials for Sustainable Hydrogen Production and Storage

Cosponsored by MPPG

C. Ban, Y. Yang, *Organizers*
A. L. Prieto, *Organizer, Presiding*
Y. Zhao, *Presiding*

1:30 INOR **121.** Molecular studies of gas clathrate hydrates. **C.A. Koh**

2:10 INOR **122.** Fueling the future: Safe, dense, reversible hydrogen storage in hybrid nanomaterials. **J. Urban**

2:40 INOR **123.** Development of metal hydrides for high temperature thermochemical energy storage. **E. Ronnebro**

3:20 Intermission.

3:30 INOR **124.** Water-mediated cooperative migration of chemisorbed hydrogen on graphene. **Y. Zhao**, T. Gennett

3:50 INOR **125.** Spectroscopic studies of proton-coupled electron transfer in the mechanism of H_2 activation by [FeFe]-hydrogenases. D.W. Mulder, M.W. Ratzloff, M. Bruschi, C. Greco, Y. Guo, E. Koonce, J.W. Peters, **P.W. King**

4:30 INOR **126.** Molecular electrocatalysts for the oxidation of hydrogen: Pendant amines as proton relays. R. Bullock, T. Liu, J.M. Darmon, E.B. Hulley, M. Helm

5:10 INOR **127.** Hydrogen fuel cell electric vehicles: new possibilities? **Y. Shao**

Section H

Colorado Convention Center
Room 203

ACS Award in the Chemistry of Materials: Symposium in Honor of Mark E. Thompson

R. L. Brutchey, *Organizer, Presiding*

1:30 INOR **128.** Efficient cyclometalated platinum and palladium complexes for displays and lighting applications. **J. Li**

1:50 INOR **129.** Solvent-dependent fluorescence of substituted quinoxalines. **S.P. Sibley**

2:10 INOR **130.** Excitons and OLEDs: You can't live with them and you can't operate without them. **S. Forrest**

2:30 INOR **131.** Synthetic control of photoinduced structural change and dual emission of phosphorescent molecular butterflies. **B. Ma**

2:50 INOR **132.** Exploiting nonradiative decay of cyclometalated iridium complexes to perform in situ analysis of degradation products in OLEDs. **P.I. Djurovich**

3:10 Intermission.

3:25 INOR **133.** High efficiency phosphorescent OLEDs. **J. Brooks**

3:45 INOR **134.** Stoichiometric and catalytic reactivity based on late-metal/main-group cooperation. **M.T. Whited**

4:05 INOR **135.** Investigating the trap state landscape of cadmium halide-treated CdSe nanocrystals. **R.L. Brutchey**

4:25 INOR **136.** Charge dynamics in next-generation energy conversion materials. **C.W. Schlenker**

4:45 INOR **137.** Photon upconversion and photocurrent generation via self-assembled bilayers on metal oxide surfaces. **K. Hanson**, S.P. Hill, T. Banerjee

Section I

Colorado Convention Center
Room 205

Division of Inorganic Chemistry Celebration of the Gabor A. Somorjai Award: Symposium in Honor of Maurice Brookhart

K. I. Goldberg, *Organizer*
A. Goldman, *Organizer, Presiding*

1:30 INOR **138.** Thermal and photochemical reactions mediated by water-soluble host-guest supramolecular systems. **R.G. Bergman**

1:50 INOR **139.** Cation-modulated hemilability in pincer-crown ether complexes. **A.J. Miller**, M.R. Kita, J.B. Smith

2:10 INOR **140.** Redox reactions of nanoscale oxide materials: Thermodynamics and kinetics of hydrogen-atom and proton-coupled electron transfer processes. **J.M. Mayer**, C.N. Valdez, M.N. Braten, J. Peper, A. Soria, J.A. Johnson, D.R. Gamelin, A.M. Schimpf, M. Ryoji, C. Tsou, D. Damatov, H. Larson

2:30 INOR **141.** Relative reactivity scale of alkanes from C-H bond functionalization reactions. A. Olmos, R. Gava, B. Noverges, D.R. Enrique, K. Jacob, T. Varea, A. Caballero, M. Etienne, G. Asensio, **P.J. Perez**

2:50 INOR **142.** Synthesis and reactivity of high valent organometallic Ni complexes. **M.S. Sanford**

3:10 INOR **143.** Small molecule activation mediated by an iron half-sandwich complex, $[Cp'FeX]_2$. **M.D. Walter**, M. Reiners, M. Maekawa, P.G. Jones, J. Hohenberger, J. Sutter, K. Meyer

3:30 Intermission.

3:40 INOR **144.** Promoting alkane dehydrogenation by C-H activation at **Ir**III. A.M. Wright, K. Allen, D. Pahls, T.R. Cundari, A.S. Goldman, D.M. Heinekey, **K.I. Goldberg**

4:00 INOR **145.** Chelate complexes of 1st row transition metals: Redox non-innocence and multiple metal-ligand bonds. **P.T. Wolczanski**, A. Swidan, B.M. Lindley, S.P. Heins, W.D. Morris, N. Livezey, B.P. Jacobs, R. Agarwal

4:20 INOR **146.** Low temperature oxidations of iridium(Cp*) complexes. C. Turlington, M. Brookhart, **J.L. Templeton**

4:40 INOR **147.** Hydrogenolyis reactions catalyzed by iridium pincer complexes. J.M. Goldberg, G.W. Wong, T. Lekich, K.I. Goldberg, **D.M. Heinekey**

5:00 INOR **148.** Well-defined iron catalysts for the acceptorless reversible dehydrogenation of alcohols and N-heterocycles. S. Chakraborty, W. Brennessel, **W.D. Jones**

5:20 INOR **149.** First row transition metals and Lewis acid co-catalysts for carbon dioxide reduction. **W.H. Bernskoetter**, N. Hazari

5:40 INOR **150.** Applications of tripodal ligands in bioinorganic and organometallic chemistry. **G.F. Parkin**

Section J

Colorado Convention Center
Room 402

Lanthanide and Actinide Chemistry

A. De Bettencourt Dias, *Organizer*
M. Fieser, M. Murugesu, *Presiding*

1:30 INOR **151.** Isolation of a terminal organocerium acetylide complex and its reactivity with enolizable ketones. **J. Kim**, **D. Weinberger**, P. Carroll, E.J. Schelter

1:50 INOR **152.** Ligand effects in the synthesis of Ln2+ complexes by reduction of tris(cyclopentadienyl) rare earth precursors including C–H bond activation of an indenyl ligand. **J.F. Corbey**, C.T. Palumbo, D. Woen, J.W. Ziller, W.J. Evans

2:10 INOR **153.** Reactivity of the Ln^{2+} complexes $[K(2.2.2\text{-cryptand})][(C_5H_3SiMe_3)_3Ln]$: Reduction of aromatic hydrocarbons. **C. Kotyk**, M.R. MacDonald, J.W. Ziller, W.J. Evans

2:30 Intermission.

2:40 INOR **154.** Investigation on charge-transfer absorptions of uranyl UO_2^{2+}(VI) and chemical reduction of UO_2^{2+}(VI) to UO_2^{+}(V) by UV-visible and EPR spectroscopies. **X. Sun**, D. Kolling, H. Mazagri, B. Karawan

3:00 INOR **155.** Facile synthesis of NpI_4 in solution. **A.T. Johnson**, J.K. Pfeiffer, M.R. Finck, K.P. Carney, L.R. Martin

3:20 INOR **156.** Lanthanide ions in molecular magnets. **M. Murugesu**

3:40 INOR **157.** Lanthanides-TTF complexes: Correlation between single molecule magnet behavior and luminescence. **L. Ouahab**, F. Pointillart, O. Cador, S. Golhen

4:00 Intermission.

4:10 INOR **158.** Ionothermal effects on actinyl coordination chemistry using task-specific ionic liquids. **P.A. Smith**, P.C. Burns

4:30 INOR **159.** Synthesis, structure, and electronic spectroscopy of *f*-element thiocyanates. **J.N. Cross**, S.A. Kozimor, C.S. Stieber, J.A. Trujillo, E.R. Batista, R.L. Martin, S.R. Daly

4:50 INOR **160.** Unconventional metal-organic frameworks (UMOFs) for separation of lanthanides from actinides and americium from curium. **R.M. Silbernagel**, J.D. Burns, D.T. Reed, D.T. Hobbs, A. Clearfield

Department, University, and National Models for Faculty Development to Support Adoption of Evidence-Based Teaching

Sponsored by CHED, Cosponsored by INOR, ORGN and PRES

SUNDAY EVENING

Section A

Colorado Convention Center
Hall C

Undergraduate Research at the Frontiers of Inorganic Chemistry

General Posters

C. Nataro, *Organizer*

6:00 - 8:00

INOR **161.** Mg deficient IONiC/VIPEr: An online community for inorganic chemists. M.J. Geselbracht, **A.K. Bentley**, **H.J. Eppley**, **E.R. Jamieson**, **A.R. Johnson**, **C. Nataro**, **B.A. Reisner**, **J.L. Stewart**, **S.R. Smith**, **N. Williams**, **L.A. Watson**

INOR **162.** IONiC VIPEr workshops at the frontiers of inorganic chemistry. **S.R. Smith**, **L.G. Habgood**, **S.E. Schmidt**, **K. Young**

Section B

Colorado Convention Center
Hall C

Bioinorganic Chemistry

DNA, RNA and Inorganic Drugs

S. A. Koch, *Organizer*

6:00 - 8:00

INOR **163.** Effect of oxidation state on the anticancer activity of several gold polypyridyl complexes. **D. Gibler**, A.C. Ontko

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INOR **164.** Novel gold(III) chelates of 7-substituted dipyrido[3,2-a:2',3'-c] phenazine and their evaluation as antitumor agents. K. Palanichamy, **C. Gatewood**, A.C. Ontko

INOR **165.** Withdrawn.

INOR **166.** Synthesis and photolysis of a novel family of photoactivatable HNO donors using the (3-hydroxy-2-naphthalenyl)methyl photolabile protecting group. **Y. Zhou**, R.S. Dassanayake, N.E. Brasch, P. Sampson

INOR **167.** Correlating cytotoxicity of ruthenium(II) polypyridyl complexes with activation wavelength. **E. Wachter**, D.K. Heidary, A. Effinger, E.C. Glazer

INOR **168.** E. coli as a screening system to study potential anti-cancer agents with different mechanisms of action. **Y. Sun**, Z. Zhang, D. Heidary, C.I. Richards, E. Glazer

INOR **169.** New family of rhodium metalloinsertors with improved selectivity and potency against DNA mismatch repair deficient cell lines. **K.M. Boyle**, A. Komor, J.K. Barton

INOR **170.** Development of light activated Ru(II) complexes applicable in photodynamic therapy. **A.M. Kishlock**, E.A. Stimmell, **A. Jain**

INOR **171.** Transition metal complexes used for the detection of mismatched DNA base pairs. **T.N. Rohrabaugh**, C. Turro

Section B

Colorado Convention Center

Hall C

Bioinorganic Chemistry

Proteins and Enzymes and Model Systems

S. A. Koch, *Organizer*

6:00 - 8:00

INOR **172.** Spectroscopic studies of the biologically active peptide of low-molecular-weight chromium-binding substance. H. Arakawa, E. Love, **J.B. Vincent**

INOR **173.** Modeling matrix metalloproteinase inhibition with carbonic anhydrase. **W.A. Richert**, D. DeGenova, A. Forchonie, R. Patel, A. Plonski, R. Venna, Z. Higgins, M. Morris, S. Al-Abdul-Wahid, D.L. Tierney

INOR **174.** Toxic carbon monoxide removal by the soil bacteria *Oligatropha carboxidavorans*: Insights from *In silico* models. **M.C. Dienst**, T.A. Large, D. Rokhsana, M. Retegan, F. Neese

INOR **175.** Overlap of protein inhibition and metal chelation: A case study. **R. Gautam**, E. Akam, E. Tomat

INOR **176.** Structural insights of a mononuclear iron center in 2,6-dichlorohydroquinone-1,2-dioxygenase (PcpA) from in silico models. **P.R. Carmichael**, D. Rokhsana, T.E. Machonkin

INOR **177.** Synthesis and reactivity of manganese(III) complexes with tetradentate ligands that mimic superoxide dismutase enzymes. **S.T. Frey**, **H.A. Cirka**, W.A. Gallopp, P.B. Moses

INOR **178.** Biochemical, kinetic, and spectroscopic characterization of a promiscuous metal-dependent DMSP-lyase. **A. Brummett**, M. Dey

INOR **179.** Effect of mutations on the stability of $P450_{BM3}$ as determined by chemical and thermal denaturation. **C. Denning**, D.K. Heidary, E. Glazer

INOR **180.** Synthesis, characterization, and applicability of reactive biomimetic model complexes toward important biological reactions. **K.J. Meise**, E.M. Brandes, R. Theisen

INOR **181.** Reduction of copper(II) by thioether sulfur: A synthetic model for the amyloid beta peptide. **M. Wallace**, R.P. Houser

Section C

Colorado Convention Center

Hall C

2015 Priestley Medalist: Symposium in Honor of Jacqueline K. Barton

E. Boon, M. C. Buzzeo, S. Delaney, V. C. Pierre, *Organizers*

6:00 - 8:00

INOR **182.** Reactivity and electrostatics of ribosomal RNA hairpins with modified nucleotides determined by cationic metal complexes. **G. Dedduwa-Mudalige**, S. Elmroth, C.S. Chow

INOR **183.** Fluorescently-labeled bioactive protein nanoparticles (prodots) for improved uptake by oral cancer cells. **B. Stromer**, I. Deshapriya, A. Pattammattel

INOR **184.** New fluorescent probes for peptide nucleic acid (PNA) based diagnostics. S. Naik, **E. Yavin**

INOR **185.** Efficient DNA photo modulation by PNA-Rose Bengal conjugates. Y. Shemesh, **S. Naik**, E. Yavin

INOR **186.** Nanoconfinement of gold on the spatial location of titania nanotubes. **S.A. Ferdousi**, K.L. Yeung

INOR **187.** Lipid signaling through NM23-H1 as a possible suppressor of metastasis. **M.R. Friedman**, J.D. Lapek, A.E. Friedman

Section C

Colorado Convention Center

Hall C

Undergraduate Research at the Frontiers of Inorganic Chemistry

Bioinorganic Chemistry

C. Nataro, *Organizer*

6:00 - 8:00

INOR **188.** Probing the effects of environments on pK_a values: Interaction of aniline with reverse micelles as monitored using by 1H NMR spectroscopy. J. Sripradite, S.A. Miller, A. Tongraar, M.D. Johnson, **D.C. Crans**

INOR **189.** Electron withdrawing capability of ligating histidine adducts influence the reduction potential of the [2Fe-2S] cluster of the Rieske protein. L.M. Hunsicker Wang, **C. Hertz**, N. Karagas

INOR **190.** Semiquinone stabilization via de novo designed protein scaffolds. **I. Sokirniy**, G. Ulas, W.F. Degrado, A.J. Reig

INOR **191.** Structural and functional characterizations of 4-His/3-carboxylate G4DFsc proteins. **K. O'Shea**, K. Biernat, A.J. Reig

INOR **192.** Creation and characterization of rubrerythrin and symerythrin model proteins. **J. Pellegrino**, R.Z. Polinski, S.N. Cimerol, A. Jacobs, E.I. Solomon, A.J. Reig

INOR **193.** Modeling the activity of the tungsten-containing nitrate reductase of *Pyrobaculum aerophilium*. **K. Scott**, R. Page, B. Trujillo, M.A. Cranswick

INOR **194.** Toward understanding the reaction mechanism of the tungstoenzyme, acetylene hydratase. **E. Vergunst**, B. Trujillo, M.A. Cranswick

INOR **195.** Interactions of acrylamide with heme models. C. Lingafelt, **N. Xu**

INOR **196.** Derivatives of a metallopeptide-based mimic of nickel-containing superoxide dismutase. **T. Detomasi**, J. Schmitt, J.M. Shearer

INOR **197.** Investigation of sugar-Cu(II) and Zn(II) complexes' interactions in aqueous alkaline media. **M.A. Pedraza**, C. Stewart, H. Arman, G.T. Musie

Section F

Colorado Convention Center

Hall C

Undergraduate Research at the Frontiers of Inorganic Chemistry

Coordination Chemistry

C. Nataro, *Organizer*

6:00 - 8:00

INOR **198.** Synthesis and characterization of BIAN iron dihalide complexes. **M.J. Supej**, K.A. Wheeler, C.E. Schulz, H.M. Hoyt

INOR **199.** Synthesis and reactivity of iron compounds containing acid functionalized 1,4,7-triazacyclononane ligands. **E. Foerster**, G. Rowe

INOR **200.** Ligand donor effects in copper(I) and copper(II) complexes of polydentate heteroaromatic-amine ligands in the ATRP of styrene. **T. Chidanguro**, L. Ma, S.L. Guillot, R.D. Pike, **C. Goh**

INOR **201.** Isolation and characterization of group 13 bis(2-(1-methylimidazolyl)methyl) amine complexes. **N.B. Kingsley**, T.J. Doyon

INOR **202.** Tuning the photophysical properties in a series of Re(I) charge transfer complexes. **J. Breaux**, A. Leeds, J. Yarnell

INOR **203.** Bidirectional "ping-pong" energy transfer in a Ir(III) charge transfer complex. **A. Leeds**, J. Breaux, J. Yarnell

INOR **204.** Development of gold(III) complexes containing ligands designed for chelation-assisted functionalization of strong, sp3-hybridized C-H bonds. **R. Miller**, J.E. Thompson, M. Sleck, A. Brown, S. Summi, D. Ohlson, B. Williams, I. Brown, E. Nissen, T. Stutzriem, A.L. Rheingold, D.R. Weinberg

INOR **205.** Gold(I) complexes of 2- and 6-mercaptoazulenes: Syntheses, molecular and electronic structures, and reactivity profiles. **B.A. Tappan**, A.D. Spaeth, O. Torres-texidor, N. Gerasimchuk, M.V. Barybin

INOR **206.** Molybdate hydrolysis of phosphonothioate neurotoxin. **K.M. Dill**, L.Y. Kuo, Y. Shari'ati

INOR **207.** Withdrawn.

INOR **208.** Developing a method of copper(II) oxidation catalyst synthesis. **C. Anderson**, J. Rumreich, J. Bodwin

INOR **209.** Probing the selectivity of luminescent lanthanide complexes toward biologically relevant anions. **K.R. Johnson**, K.H. Felix, E.J. Werner

INOR **210.** Rational design of catalysts for water-gas shift reaction. J. Fox, **A. Dinescu**

INOR **211.** Luminescence and extraction properties of novel tripodal CMPO ligands. **D.A. Hardy**, M.T. Peruzzi, S.N. McGraw, S.M. Biros, E.J. Werner

INOR **212.** Utilizing diphenylacetate lability in the synthesis of mixed ligand copper (II) dimers. **M. Chen**, T.W. Clayton

Section G

Colorado Convention Center

Hall C

ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry: Symposium in Honor of Kim R. Dunbar

Cosponsored by WCC

C. P. Berlinguette, D. J. Mindiola, E. J. Schelter, M. Shatruk, *Organizers*

6:00 - 8:00

INOR **213.** Synthesis, characterization, and photochemical studies of solvated dinuclear Ru(II) compounds with quinoxaline and pyrazine based bridging ligands. **S. Saha**, B. Pena, B.A. Albani, C. Turro, K.R. Dunbar

INOR **214.** Computational exploration of the noncovalent interactions involved in the inhibition of malate synthase for treatment of tuberculosis. **J.F. Ellenbarger**, S.E. Wheeler, J.C. Sacchettini, K.R. Dunbar

INOR **215.** "Reinventing the wheel" with heptacyanomolybdate(III). **D.K. Kempe**, H. Zhao, T.J. Woods, M.R. Saber, K.R. Dunbar

INOR **216.** Cyanide-bridged single chain magnets with hexacyanomanganate. **Y. Zhang**, H. Zhao, E.S. Funck, K.R. Dunbar

INOR **217.** Ligand effects and geometrical control of the magnetic anisotropy in mononuclear SMMs. **M.R. Saber**, K.R. Dunbar

INOR **218.** Semiconducting and magnetic properties in metal-TCNQ-based functional materials. **X. Zhang**, H. Zhao, Z. Wang, Y. Zhang, K.R. Dunbar

INOR **219.** Series of trigonal bipyramidal Co(II) complexes that display SMM behavior. **M.F. Ballesteros-Rivas**, T.J. Woods, K.R. Dunbar

INOR **220.** Dinuclear lanthanide complexes containing a radical bridging ligand. **T.J. Woods**, M.F. Ballesteros-Rivas, K.R. Dunbar

INOR **221.** Biological studies of dirhodium(II,II) based compounds and their applications as photochemotherapeutic agents. **A. David**, Z. Li, B. Pena, J. Pellois, K.R. Dunbar

INOR **222.** Structural study of Prussian blue. **A. Brown**, H. Zhao, K.R. Dunbar

INOR **223.** Solvent effects on the spin transitions in discrete cyanide-based magnetic material. **C. Sanders**, H. Stout, C. Achim, D. Petasis, K.R. Dunbar

INOR **224.** Exploring and enhancing the functionality of tetrazine molecular switches. **C. Benson**, A.H. Flood

INOR **225.** Imaging studies of metal-containing nanoparticle as multimodal platforms for biomedical applications. **P. Promdet**, B. Rodríguez-García, A. Henry, C. Blumenfeld, R.A. Moats, R.H. Grubbs, H.B. Gray, J. Galán-Mascarós, K. Sorasaenee

INOR **226.** Investigating the magnetic properties of metal complexes containing a tris(amido)amine ligand. **F.J. Birk**, K. Schulte, D. Pinkowicz, K.R. Dunbar

INOR **227.** Anion-π contacts in supramolecular architectures. **H.T. Chifotides**

Section H

Colorado Convention Center

Hall C

Coordination Chemistry

Characterization and Applications

D. C. Crans, *Organizer, Presiding*

6:00 - 8:00

INOR **228.** Heteroleptic polypyridyl ligand cobalt(III) complexes. **S.E. Hightower**, B.A. Frenzel, C.T. Kuester

INOR **229.** Transition metal complexes as paraSHIFT and paraCEST MRI contrast agents. **P.B. Tsitovich**, J.M. Cox, J.B. Benedict, J.R. Morrow

INOR **230.** Carbonato-bridged copper(II) complexes formed via fixation of atmospheric CO_2. **F. Louka**, F.A. Mautner, S.S. Massoud

INOR **231.** Synthesis and structural characterization of PTA derivative modified transition metals. **J.M. Sears**, T.J. Boyle, B.J. Frost, W. Lee, M.L. Neville

INOR **232.** Investigation of isomeric single amino acid chelate (SAAc) rhenium series. **N.J. Azzarelli**, M.P. Coogan, J.A. Platts, R.P. Doyle, J.A. Zubieta

INOR **233.** Electronic structure and reactivity of *d*0 Mo and Ti complexes of a tris-aminophenolate ligand. **T. Marshall-Roth**, S.N. Brown

INOR **234.** Syntheses and characterizations of luminescent rare earth metals complexes. P.K. Yuen, C.D. Lau

INOR **235.** Designing artificial monoamine transporters based on synthetic supercontainers. **U. Sambasivam**, Z. Wang

INOR **236.** Interactions of coordination complexes with reverse micellar interfaces: The effects on MLCT bands and coordinated ligand pKa values. **A.A. Cadena**, **M.D. Johnson**, J. Sripradite, S.A. Miller, D.C. Crans

INOR **237.** Study of glutathione interactions with anticancer Gold(III) diammines complexes using NMR, UV-VIS and electrochemistry. **A. Isab**

INOR **238.** Photocatalytic NADH regeneration and hydrogen production using Rh complexes and Pt nanoparticles. **J. Kim**, S. Kim

INOR **239.** Mechanistic studies of oxidative aliphatic carbon-carbon bond cleavage in Cu(II) chlorodiketonate complexes. **S.L. Saraf**, J.R. Argue, L.M. Berreau

INOR **240.** Coordination chemistry of cyanopyrazoles and cyanoscorpionates. **D.M. Eichhorn**

INOR **241.** Single and multiphoton turn-off fluorescent sensor for tin and iron. **R.M. Madawala**, E. Sinn

‡ *Cooperative Cosponsorship*

INOR **242.** Synthesis, NMR characterization, and MIC studies of a new series of alpha-(N)-heterocyclic thiosemicarbazone ligands and their Pd2+ and Cu2+ metal complexes. **J.D. Conner**, S.D. Simpson, A.L. Koch, E.C. Lisic

Section I

Colorado Convention Center
Hall C

Organometallic Chemistry

Applications to Organic Transformations

N. S. Radu, *Organizer*

6:00 - 8:00

INOR **243.** Borates in biomass conversion processes. **D.M. Schubert**, M.K. McCray

INOR **244.** Late transition metal complexes for industrially relevant catalysis. **N.A. Swisher**, P. Romero, R.H. Grubbs

INOR **245.** Cobalt-induced B-H and C-H Activation Leading to Facile B-C Coupling of Carboranedithiolate and Cyclopentadienyl. **H. Yan**

Section J

Colorado Convention Center
Hall C

Organometallic Chemistry

Catalysis

N. S. Radu, *Organizer*

6:00 - 8:00

INOR **246.** Polynuclear iridium-bismuth carbonyl clusters: Synthesis, chemistry, and applications. **G. Elpitiya**, R.D. Adams, M. Chen, Q. Zhang, R. Raja

INOR **247.** Alkene vs. alkyne hydroarylation catalyzed by electrophilic palladium(II) and platinum(II) complexes. **M. Manjahi**, C. Hahn

INOR **248.** Theoretical studies of hydroformylation of butadiene. **C.H. Mendis**, T. Maji, J.A. Tunge, W.H. Thompson

INOR **249.** Control of *cis*-selectivity and tacticity in ring opening metathesis polymerization using ruthenium metathesis catalysts. **L.E. Rosebrugh**, V.M. Marx, T.S. Ahmed, J. Hartung, R.H. Grubbs

INOR **250.** Enantioselectivity and substitution effects in rhodium catalyzed intramolecular hydroacylation. **B.P. Schumacher**, L.M. Stanley, J. Scanlon

INOR **251.** Electrocatalytic reduction of CO_2 to formate using iridium pincer complexes. **P. Kang**, S. Zhang, Z. Chen, C. Chen, T.J. Meyer, M. Brookhart

INOR **252.** Oxygen atom transfer to iridium(Cp*) complexes. **C. Turlington**, M. Brookhart, J.L. Templeton

INOR **253.** Synthesis of branched ultra-high-molecular-weight polyethylene using highly active neutral, single-component Ni(II) catalysts. **Z. Chen**, M. Mesgar, P.S. White, O. Daugulis, M. Brookhart

INOR **254.** Living polymerization of ethylene and copolymerization of ethylene/methyl acrylate using "sandwich" diimine palladium catalysts. **K. Allen**, J. Campos Manzano, O. Daugulis, M. Brookhart

INOR **255.** Selective cross-dimerization of ethylene with substituted olefins. **P.R. Payne**, M. Brookhart, M.R. Gagne

INOR **256.** Applications of PC(sp3)P iridium complexes in transfer dehydrogenation of alkanes and ethers. **D. Bezier**, M. Brookhart

INOR **257.** Regioselective palladium-catalyzed hydrodebromination of 2,3,5-tribromothiophene. **K.L. Konkol**, S.C. Rasmussen

INOR **258.** Ligand modification at a remote site to regulate iron-catalyzed olefin hydroboration. **K.T. Tseng**, J. Kampf, N.K. Szymczak

INOR **259.** Catalytic carbonylation of icosahedral dodecaborates. **K.R. Kamp**, R.J. Staples, J.A. Dopke

INOR **260.** Copper-catalyzed addition of phenols to icosahedral dodecaborates. **C. Barnhart**, R.J. Staples, A.J. Ramirez, J.A. Dopke

INOR **261.** Ruthenium-catalyzed substitutions of icosahedral dodecaborates. **L.R. Bent**, A.J. Ramirez, J.A. Dopke

INOR **262.** Electrocatalytic oxidation of methylrhenium trioxide to methanol by an electrode-immobilized ruthenium(II) polypyridyl catalyst. **M.K. Coggins**, T.J. Meyer, R.A. Periana

Section K

Colorado Convention Center
Hall C

Undergraduate Research at the Frontiers of Inorganic Chemistry

Organometallic Chemistry

C. Nataro, *Organizer*

6:00 - 8:00

INOR **263.** Twists and turns: WGS "catalysts" of Fe, Ru, and Os. A. Eschmann, E. Wulff-Fuentes, D. Cunningham, B. Schreiber, L. Burgan, Z. Hecht, G. Seichter, A.L. Rheingold, **J.S. D'Acchioli**

INOR **264.** Selective hydrogenation of phenylacetylene over supported gold catalysts. **E. Purdy**, B.D. Chandler

INOR **265.** Experimental and theoretical studies investigating the effect of solvent on ^1JWH in Cp_2WH_2. **C.I. Viquez Rojas**, T.A. Mobley

INOR **266.** Low valent metal complexes of tris(diphenylphosphinomethyl)phenylborate. **A.B. Weberg**, T.D. Bohrmann, H. Xu, P.J. Fischer

INOR **267.** Redox-active NHC pincer ligands for Ni-catalyzed aerobic dehydrogenative C–C cross coupling. **J.E. Hertzog**, C.F. Harris, J.D. Soper

INOR **268.** Synthesis of palladium(II)-NHC compounds and their employment as cross-coupling catalysts. **D. Colosimo**, **M. Dominguez**, G. Rowe

INOR **269.** Sulfur-hydrogen bond activation by novel iridium diphosphine complexes. **H.N. Russ**, S.H. Schreiner

INOR **270.** Synthesis of molybdenum carbon dioxide complexes via oxidation of a carbonyl ligand. **M.A. Pogash**, G.R. Lorzing, J.R. Vasta, X. Duan, R.G. Carden, J.J. Ohane, P.M. Graham

INOR **271.** Microwave-assisted concurrent tandem catalysis (CTC) methodology for the copper-catalyzed amidation of aryl halides. E. Shields, M. Lee, D.J. Brown, **S. Lin**, A.R. MacArthur

INOR **272.** Catalytic transfer hydrogenation of aryl-alkyl ketones using Cp*Ir(III)Cl pyridinesulfonamide complexes. **A. Ruff**, B.C. Chan, A.R. O'Connor

INOR **273.** Catalytic transfer hydrogenation of aryl aldehydes using Cp*Ir(III) pyridinesulfonamide complexes. **C. Kirby**, A.R. O'Connor

Section L

Colorado Convention Center
Hall C

Chemistry of Materials

C. G. Lugmair, *Organizer*

6:00 - 8:00

INOR **274.** pH-dependent ceria-doped titanate nanotubes. Y. Fam, **S.A. Ferdousi**, K.L. Yeung, Y. Du

INOR **275.** Sythesis and characterization of quaternary misfit-layer-compound-like ferecrystals. **R. Westover**, D.C. Johnson, J. Ditto

INOR **276.** Self-assembly of organometallic molecular films based on the azulenic scaffold linearly functionalized with both isocyanide and thiol termini. **M.K. Okeowo**, C.L. Berrie, M.V. Barybin

INOR **277.** Chiral amplification by metal-ligand conjugation in chiral magnetic nanoparticles. **J. Yeom**, N. Kotov

INOR **278.** Structure and properties of sodium enneaborate. **D. Neiner**, Y. Sevryugina, D.M. Schubert

INOR **279.** Wet-spinning of graphene fibers from giant graphene oxide sheets by adopting a series of amine alcohol solution as coagulation solution. **C. Zhao**, W. Zeng, S. Tong, S. Mo, J. Wang, T. Fan, W. Tang, C. Yuan, Y. Liu, Y. Min

INOR **280.** Water based PAN conductive coatings for antistatic application. **Y. Feng**, X. Liu, C. Ma, J. Shen, Z. Xiao, T. Fan, S. Tong, Y. Liu, Y. Min

INOR **281.** Facile method to fabricate transparent, flexible conducing graphene thin films via liquid phase deposition. **C. Yuan**, W. Tang, J. Wang, S. Mo, C. Zhao, T. Fan, S. Tong, Y. Liu, Y. Min

INOR **282.** Supercritical CO_2 method of graphene preparation. **J. Shen**, Y. Feng, C. Ma, X. Liu, Z. Xiao, T. Fan, S. Tong, Y. Liu, Y. Min

INOR **283.** Production of graphene by dry ice ball milling method. **Z. Xiao**, J. Shen, Y. Feng, C. Ma, X. Liu, T. Fan, S. Tong, Y. Liu, Y. Min

INOR **284.** Preparation and properties of different phase of hydrothermal synthesis of 3D graphene. **S. Mo**, S. Tong, C. Yuan, W. Tang, J. Wang, C. Zhao, T. Fan, J. Shen, Y. Liu, Y. Min

INOR **285.** Synthesis and instability of cuprous nitride nanocrystals. **M. Reichert**, J. Vela

INOR **286.** Categorizing defects in nanowires produced through electrodepostion. **K.J. Kysor**, D. Vu, C. Myers, B.D. Smith

INOR **287.** Rapid synthesis of carbon nitride materials and composites for use in photocatalysis. **A. Montoya**, E.G. Gillan

INOR **288.** Thermal and electronic effects on the solvothermal formation of nanocrystalline WSe_2 in aromatic solvents. M.P. Hanrahan, **J.S. Edgar**, S.A. Darveau, C.L. Exstrom

INOR **289.** Formation of WSe_2 thin films via annealing of a solvothermally prepared nanocrystalline precursor. **J.S. Edgar**, M.P. Hanrahan, C.L. Exstrom, S.A. Darveau

INOR **290.** Metal-sulfur-arene semiconducting frameworks. **H. Hu**, T.P. Vaid

INOR **291.** Sulfonium derivatives of the [*closo*-1-$CB_{11}H_{12}$]$^-$ anion as polar liquid crystals. **P. Zagorski**, J.G. Pecyna, P. Kaszynski

INOR **292.** Liquid crystalline derivatives of the [*closo*-$B_{12}H_{12}$]$^{2-}$ anion. **P. Tokarz**, P. Zagorski, P. Kaszynski

INOR **293.** New network of Mn_{12} molecules. **A.E. Thuijs**, G. Christou, K.A. Abboud

INOR **294.** Functionalization of GaP substrates for use in photoelectrochemical cells. **O. Williams**, A.H. Cowley, M.J. Rose

INOR **295.** Thermodynamic stability of aqueous metal clusters: A dynamic approach. **T.J. Mustard**, L.A. Wills, I. Chang, D.A. Keszler, P.H. Cheong

INOR **296.** Computational study of polyoxometalate formation mechanisms. L.A. Wills, **D.B. Fast**, M. Dolgos, P.H. Cheong

INOR **297.** Carbon nanofoams as porous scaffolds for iron-air battery electrodes. **M.F. Mayther**, S.D. Murphy, J.C. Lytle

INOR **298.** Doping Cu_2ZnSnS_4 nanorods with tetrahedral, high spin metals: Co^{2+}, Mn^{2+}, and Ni^{2+}. **M. Thompson**, M. Reichert, J. Vela-Becerra

INOR **299.** Efficient dye degradation via non-photocatalytic route by perovskite type $LaNiO_{3-\delta}$ materials. **W. Zhong**, C. Kuo, S. Chen, S.L. Suib

INOR **300.** Functionalization of metal oxide surfaces for photoelectrocatalysis of CO_2 reduction. **S.K. Heiskanen**, J.M. Ziegler, D.A. Rider, J.D. Gilbertson

INOR **301.** Control of the crystalline phase and morphology of CdS deposited on microstructured surfaces by chemical bath deposition. **D. Fernando**, M. Khan, Y. Vasquez

INOR **302.** Colloidal synthesis of silicon and germanium nanorods and nanowires. **X. Lu**, B. Korgel

INOR **303.** Graphene oxide assisted hydrothermal carbonization of carbon hydrates. **D. Krishnan**, K. Raidongia, J. Shao, J. Huang

Section L

Colorado Convention Center
Hall C

Inorganic Spectroscopy

S. A. Koch, *Organizer*

6:00 - 8:00

INOR **304.** New multifunctional Schiff base as fluorescence sensor for Al^{3+} and colorimetric sensor for CN^- in aqueous media: an application to bioimaging. **G. You**, Y. Na, S. Lee, K. Ryu, C. Kim

INOR **305.** Colorimetric organic chemo-sensor for Co^{2+} in a fully aqueous environment. H. Jo, **S. Lee**, J. Lee, Y. Kim, C. Kim

INOR **306.** Water-soluble chemosensor for detecting Al^{3+} in aqueous media and living cells. **J. Lee**, P. Kim, C. Kim

INOR **307.** Withdrawn.

INOR **308.** Measurement of NMR relaxation rates in a series of cobalt (II) β-diketonates. **R.R. Baum**, D.L. Tierney

INOR **309.** Monitoring the ring opening polymerization of hexachlorocyclotriphosphazene through NMR spectroscopy. **J.A. Stiel**, C. Tessier, Z. Tun

INOR **310.** Scalar and spin-orbit relativistic calculations of $^1J_{WH}$ in Cp_2WH_2 complexes. **T.A. Mobley**

INOR **311.** Investigating the stereoelectronic consequences of diphosphine ligands on M-P and M-Cl covalency in late transition metal complexes. **C. Donahue**, B.J. Bellott, A. Blake, C.M. Forrest, J.M. Keith, S. McCollom, S.R. Daly

INOR **312.** Photoinduced properties of bimetallic polypyridyl complexes. **T.J. Whittemore**

INOR **313.** Colorimetric "naked-eye" Cu(II) chemosensor and pH indicator in an 100% aqueous solution. **Y. Choi**, M. Lee, G. Park, K. Bok, T. Jo, C. Kim

INOR **314.** Chiral conducting polymers as efficient spin filters. **P.C. Mondal**, C. Fontanesi, R. Naaman

Section L

Colorado Convention Center
Hall C

Lanthanide and Actinide Chemistry

A. De Bettencourt Dias, *Organizer*

6:00 - 8:00

INOR **315.** Synthesis of "rare earths – magnesium" master alloys by high temperature exchange reactions. **A.V. Krylosov**, K.V. Maksimtsev, I.B. Polovov, V.A. Volkovich, O.I. Rebrin

INOR **316.** Synthesis, structural characterization, and magnetic properties of dinuclear, tetranuclear, and polynuclear lanthanide(III) complexes of a symmetric ditopic carbohydrazone based ligand (H_2L). **S.S. Tandon**, S.D. Bunge, S.K. Adas, L.K. Thompson, C. Lucas

INOR **317.** Speciation studies between a novel pincerlLigand with lanthanum (III) salts. **D. Kremer**, M. Guino-o, A. De Bettencourt Dias

INOR **318.** Chiral light emitting ionic liquids. **B. Zercher**, T. Hopkins

INOR **319.** New calix[4]arene based precursors for stationary phases useful in separation of rare earth metals. **S. Menon**, J.A. Schmidt

INOR **320.** Magnetic properties of mononuclear uranium-acetylide complexes. **R. Higgins**, B. Newell, A.K. Rappe, M.P. Shores

INOR **321.** Optimization of rare earth element chromatography. **H. Knutson**, A. Holmqvist, B. Nilsson

INOR **322.** Stability and cation exchange dynamics of γ-irradiated actinyl peroxide nanocapsules. **T.A. Olds**, B.J. Moeller, P.C. Burns

INOR **323.** Methylcyclopentadienide as a supporting ligand for a reduced dinitrogen complex of yttrium. **D.H. Woen**, J.W. Ziller, W.J. Evans

INOR **324.** Synthesis and *f*-element coordination of phosphine oxide decorated polypyridine ligand. **J. Dehaudt**, D.A. Dickie, B.P. Hay, R.T. Paine

INOR **325.** Dinitrogen reduction and isoprene polymerization via photochemical activation of bis(cyclopentadienyl) rare earth allyl complexes. **C.W. Johnson**, M. Fieser, J.W. Ziller, W.J. Evans

INOR **326.** Tuning of structural dimensionality in lanthanide cyanometallates. **R. Sykora**, F.D. White, L. Pham, K. Xaing, A.T. Thames, J. Hendrich, J.D. Taylor

INOR **327.** Dicyanoaurate and tetracyanoplatinate compounds as potential chemical sensors for volatile organic compounds. **F.D. White**, R. Sykora, J. Hendrich

INOR **328.** Emissive electropolymerizable lanthanide complexes. **M.V. Tran**, D.J. Strohecker, M.T. Raiford, B.J. Holliday

INOR **329.** Lanthanide-organic frameworks as asymmetric heterogeneous catalysts. **D.T. de Lill**

INOR **330.** Synthesis and structural characterization of Y^{2+} and Gd^{2+} in heteroleptic tris(cyclopentadienyl) rare earth complexes. **C.T. Palumbo**, J.W. Ziller, W.J. Evans

Section L

Colorado Convention Center

Hall C

Nanoscience

Cosponsored by PRES

R. M. Richards, *Organizer*

6:00 - 8:00

INOR **331.** Pt-Au and Pd-Au bimetallic heterostructures using mask assisted seeded growth. **C. Crane**, J. Chen

INOR **332.** Effective regulation of post-preparative cation exchange reactions in PbS quantum dots. **B.P. Mainali**, P.G. Van Patten

INOR **333.** Incorporation of transition metal cations into PbS QDs via cation exchange. **W. Tilluck**, A.D. Evans, J.K. Gurchiek, C.M. Mings, A.L. Morris, P.G. Van Patten

INOR **334.** Supersaturation-precipitation strategies to colloidal hybrid nanoparticles. **C.G. Read**, A.J. Biacchi, R.E. Schaak

INOR **335.** Synthesis of acetamide from acetonitrile hydrolysis using EEW catalyzed with metal nanoparticles. E. Abdelkader, **S.W. Buckner**, P.A. Jelliss

INOR **336.** Growth kinetics of zinc oxide quantum dots. **B. Colon**, **H. Egido-Betancourt**, **C.P. Mccord**, P.P. Vaughan, A.K. Schrock, K.S. Molek

INOR **337.** Effect of synthetic levers on phosphorus incorporation in nickel phosphide nanoparticles: Ni_5P_4 and NiP_2. **D. Li**, S. Brock

INOR **338.** Electrophoretic deposition of gold nanospheres for explosives detection. **K. Roberts**, Y.J. Han, T.Y. Olson

INOR **339.** Formation of Ag nanoclusters via the direct dissolution of bulk Ag. **J.R. Changstrom**, C.M. Sorensen

INOR **340.** Ion exchange and protection-deprotection chemistry in the total synthesis of colloidal hybrid nanoparticles. **J.M. Hodges**, A.J. Biacchi, R.E. Schaak

INOR **341.** Polyaniline/laponite/gold coordination polymer nanoassemblies for solar applications. **P. Quah**, M.E. Hagerman

INOR **342.** New routes to clean water: Laponite/copper oxide nanomaterials for bacterial remediation. **A.J. Cavert**, M.E. Hagerman

INOR **343.** Synthesis and characterization of titanium oxide nanopowders. **H. Chenoweth**, **L.F. Barnes**, **C.J. Van Leeuwen**, K.A. Reyes, C.K. Butterfield

INOR **656.** Ligand-induced fate of embryonic seeds in the shape-controlled synthesis of rhodium nanoparticles. **A.J. Biacchi**, R.E. Schaak

Section L

Colorado Convention Center

Hall C

Undergraduate Research at the Frontiers of Inorganic Chemistry

Main Group Chemistry

C. Nataro, *Organizer*

6:00 - 8:00

INOR **344.** Synthesis and characterization of spirocyclic monoalkylated organosilicon complexes of 1-hydroxy-2-pyridinone. **J.G. Koch**, W.W. Brennessel, B.M. Kraft

INOR **345.** Synthesis and characterization of five-coordinate aluminum complexes that polymerize ε-caprolactone. **A.M. Longo**, J.M. Fritsch

INOR **346.** Polymerization of ε-caprolactone by aluminum alkoxide complexes supported by tridentate ketoiminates bearing electron-withdrawing groups. **A.M. McCollum**, A.L. Rheingold, J.M. Fritsch

INOR **347.** L-Lactide and sym

-caprolactone ring opening polymerization by binary catalysts systems that include *bis*-ligated magnesium complexes. **R.M. Slattery**, A.L. Rheingold, J.M. Fritsch

INOR **348.** Polymerization of lactide by aluminum ion pairs studied with 27Al NMR. **L.A. Schmitz**, A.L. Rheingold, D.B. Green, J.M. Fritsch

INOR **349.** Si-H and Ge-H bond activation by a platinum dimer. **L. Matuszewski**, S.H. Schreiner

Section L

Colorado Convention Center

Hall C

Undergraduate Research at the Frontiers of Inorganic Chemistry

Solid State and Materials Chemistry

C. Nataro, *Organizer*

6:00 - 8:00

INOR **350.** Investigating the electronic coupling of quantum dots to crystal-bound thiols. **A.M. Fall**, S. Castillo, N.K. Brandon, M.J. Turo, A.D. La Croix, J.E. Macdonald

INOR **351.** Synthesis and photovoltaic performances of di-acetylide platinum complexes in dye-sensitized solar cells. **T. Schuyler**, S. Gauthier

INOR **352.** New phase discovered in the Cu-Ge-Te system by high-temperature solid state reaction. **B. Hogan**, J.A. Aitken

INOR **353.** Spectroelectrochemical determination of the Fe(III)/Fe(II) reduction potential in recombinant, cross-linked hemoglobins. **R. Bangle**, C.J. Parker Siburt, R. Kreulen, A.L. Crumbliss

INOR **354.** Green dechlorination via functional models of cyanocobalamin. **D. Marquis**, K.M. Van Heuvelen

INOR **355.** Optical and thermal properties of lithium-containing thiostannate with potential nonlinear optical applications. **A. Weiland**, J. Brant, J. Zhang, J.A. Aitken

INOR **356.** Surface chemistry of gold nanoparticles in natural environments. K. Roberts, **A.K. Bentley**

INOR **357.** Investigation of novel polymorphic $Li2_{-4}$-IV-S_4 diamond-like semiconductors utilizing synchrotron X-ray powder diffraction. **K.P. Devlin**, K. Daley, M.A. Moreau, J. Brant, J.A. Aitken

INOR **358.** Precursor approach to probing host-guest binding of synthetic supercontainers. **A. Hammerstrom**, F. Dai, Z. Wang

MONDAY MORNING

Section A

Colorado Convention Center

Bellco Theatre

ACS National Awards in Inorganic Chemistry: Plenary Session

S. A. Koch, N. S. Radu, *Organizers*

J. M. Boncella, *Organizer, Presiding*

8:30 INOR **359. Award Address** (F. Albert Cotton Award in Synthetic Inorganic Chemistry sponsored by the F. Albert Cotton Endowment Fund). Understanding and predicting the behavior of the actinides through organometallic chemistry. **J. L. Kiplinger**

9:00 INOR **360. Award Address** (ACS Award in Organometallic Chemistry sponsored by the Dow Chemical Co. Foundation). Importance of organometallic chemistry in the discovery of new oxidation states of the rare earth and actinide elements in molecular complexes. **W. J. Evans**

9:30 INOR **361. Award Address** (ACS Award in Inorganic Chemistry sponsored by Aldrich Chemical Co., LLC). Metalloporphyrins in chemical and biological catalysis. **J. T. Groves**

10:00 INOR **362. Award Address** (ACS Award for Creative Research and Applications of Iodine Chemistry sponsored by SQM S.A.). Fifty years of Iodine research. **K. O. Christe**

10:30 Intermission.

10:45 INOR **363. Award Address** (ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry sponsored by Strem Chemicals). Molecular magnetic and conducting materials inspired by coordination chemistry. **K. R. Dunbar**

11:15 INOR **364. Award Address** (Harry Gray Award for Creative Work in Inorganic Chemistry by a Young Investigator sponsored by the Harry Gray Award Endowment). Colloidal quantum dots: Where d10 ions go to glow. **E. A. Weiss**

11:45 INOR **365. Award Address** (ACS Award in the Chemistry of Materials sponsored by E. I. du Pont de Nemours & Co.). Use of organometallic complexes to squeeze every last photon out of an organic LED. **M. E. Thompson**

WCC Rising Stars Awards Symposium

Sponsored by WCC, Cosponsored by BIOT, COLL, GEOC, INOR, ORGN, PHYS, PMSE and PROF

MONDAY AFTERNOON

Section A

Colorado Convention Center

Room 105

Undergraduate Research at the Frontiers of Inorganic Chemistry

IONIc VIPEr on Mg

S. R. Smith, *Organizer*

C. Nataro, *Organizer, Presiding*

A. R. Johnson, *Presiding*

1:30 Introductory Remarks.

1:40 INOR **366.** Solvent loss and reuptake in $Na[BH(C_2H_3N_3)_3]$ frameworks. **B.A. Reisner**, W.T. Price, A.T. Muetterties

2:05 INOR **367.** Eggs in one basket: Is there a role for riboflavin binding protein in copper transport and storage? **S.R. Smith**, M. Benore, J.I. Matchynski

2:30 INOR **368.** Controlling electrochemistry in the synthesis of semiconductor nanoparticles. **A.L. Prieto**, E. Nock, P. Reining, G.P. Wheeler

2:55 INOR **369.** Asymmetric hydroamination with titanium and tantalum: experiment and theory. **A.R. Johnson**

3:20 INOR **370.** Reactivity of bis(phosphino) ferrocenediyl containing compounds. **C. Nataro**

3:45 Concluding Remarks.

Section B

Colorado Convention Center

Room 301

2015 Priestley Medalist: Symposium in Honor of Jacqueline K. Barton

E. Boon, S. Delaney, V. C. Pierre, *Organizers*

M. C. Buzzeo, *Organizer, Presiding*

1:30 INOR **371.** Allosteric and unexpected binding sites for small-molecule modulators. **M. Arkin**

2:00 INOR **372.** Aptamer technology for biosensing, therapeutics, and targeted release. **M.C. DeRosa**

2:30 INOR **373.** Electromechanical tissue reconstruction: A non-invasive surgical modality for reshaping cartilage of the head and neck. **M.G. Hill**, J. Kallick, M. Herzig, B. Hunter

3:00 Intermission.

3:10 INOR **374.** 19F MRI: Dream or reality. **V.C. Pierre**

3:40 INOR **375.** Real-time metabolic and molecular imaging In vivo by NMR hyperpolarization. P.**K. Bhattacharya**

4:10 INOR **376.** Structure and mechanism in the essential stereoinversion in carbapenem biosynthesis. **A.K. Boal**

Section C

Colorado Convention Center

Room 302

ACS Award in Organometallic Chemistry: Symposium in Honor of William J. Evans

J. R. Walensky, *Organizer*

J. C. Gordon, *Presiding*

1:30 INOR **377.** Preparation of isotopically labeled active site models for the [FeFe]- and [FeNi]-hydrogenases. **T.B. Rauchfuss**, R. Gilbert-Wilson, D. Schilter

1:50 INOR **378.** Studies of metal to ligand charge transfer states involving MM quadruply bonded complexes. **M. Chisholm**

2:10 INOR **379.** Bimetallic actinide complexes of constraining macrocycles for small molecule activation. **P.L. Arnold**, N. Potter, R. White, C. Stevens, M. Dutkiewicz, J. Farnaby, R. Caciuffo, C. Apostolidis, O. Walter, J.B. Love, N. Kaltsoyannis, M. Gardiner

2:30 INOR **380.** Rare earth doped alkali metal fluorides — promising new optical materials. **A.V. Mudring**

2:50 Intermission.

3:00 INOR **381.** Phosphorus- and arsenic-ligated lanthanide single-molecule magnets. **R.A. Layfield**, T. Pugh

3:20 INOR **382.** Catalytic conversion of biomass to fuels. **J.C. Gordon**, A.D. Sutton, A.E. King, L.A. Silks, R. Wu, M. Schlaf, F. Waldie

3:40 INOR **383.** Half-sandwich metallatricarbadecaboranyl complexes at the interface of main-group and organometallic chemistry. **L.G. Sneddon**, E.R. Berkeley, A. Perez-Gavilan, P.J. Carroll

4:00 INOR **384.** Spin-orbit coupling: Not just for *f* elements. **J. Telser**, S. Fortier, K. Holldack, T.A. Jackson, J. Krzystek, K. Meyer, D.J. Mindiola, J. Nehrkorn, A. Ozarowski, A. Schnegg

Section D

Colorado Convention Center

Room 303

Chemical Approaches to Spintronics Research

R. Beaulac, *Organizer*

J. K. McCusker, *Presiding*

1:30 INOR **385.** Bistability of magnetic molecules on surfaces: An overview. **R. Sessoli**, M. Mannini, L. Malavolti, V. Lanzilotto, L. Poggini, I. Cimatti, G. Poneti, S. Ninova, F. Totti, A. Cornia

2:00 INOR **386.** New single-molecule magnets with high blocking temperatures. K.R. Meihaus, J.M. Zadrozny, S. Demir, X. Feng, P.C. Bunting, J.D. Rinehart, M. Nippe, **J.R. Lon**g

‡ *Cooperative Cosponsorship*

2:30 INOR **387.** Molecular control of the magnetic exchange between self-assembled metal- complexes and ferromagnetic surfaces: towards molecular spintronics. **V.E. Campbell**

3:00 Intermission.

3:30 INOR **388.** Ligand-field engineering of atomic clock transitions in molecular spin qubits. **S. Hill**, M. Shiddiq, D. Komijani, Y. Duan, S. Cardona-Serra, A. Gaita-Ariño, E. Coronado

4:00 INOR **389.** Magnetic cyanide-based coordination nanoparticles and heterostructures. **L. Catala**, Y. Prado, M. López Jordà, S. Mazerat, T. Mallah

4:30 INOR **390.** Metal-molecule-metal junctions: A versatile platform to investigate molecular electronics/spintronics. R.C. Bruce, J.D. Yablonski, T.W. LaJoie, **W. You**

Section E

Colorado Convention Center
Room 201

ACS Award in Inorganic Chemistry: Symposium in Honor of John T. Groves

R. N. Austin, *Organizer*
P. J. Chirik, *Organizer, Presiding*

1:30 INOR **391.** Transition metal-catalyzed nucleophilic (radio)fluorination. **A.G. Doyle**

2:00 INOR **392.** Formation and reactivity of new primary copper(I)-dioxygen adducts. **K.D. Karlin**

2:30 INOR **393.** Effects of heme ruffling on vibrational dynamics, electronic structure, and electronic coupling. **K.L. Bren**, N. Lehnert, P.M. Champion, S.J. Elliott, M. Galinato

3:00 Intermission.

3:15 INOR **394.** Protein-like proton exchange in a synthetic host cavity. **K.N. Raymond**, R.G. Bergman, D. Toste

3:45 INOR **395.** Cytochrome P450 oxidations: A controlled burn of inert organic compounds. **M.T. Green**

Section F

Colorado Convention Center
Room 304

Interactions of Metal Complexes with Proteins or Nucleic Acids

J. R. Morrow, C. Turro, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 INOR **396.** Platinum and other third row transition metals for treating cancer. **S.J. Lippard**

2:05 INOR **397.** Coordination chemistry underlying the promise and pitfalls of Ti(IV) anticancer drugs. **A. Valentine**

2:35 INOR **398.** Covalent photo-adducts of Ru-TAP complexes with DNA guanine bases: Their applications and mechanisms of formation. **A. Kirsch-De Mesmaeker**, L. Marcelis

3:05 Intermission.

3:20 INOR **399.** Metalloglycomics approach to antimetastatic platinum. **N. Farrell**, E. Peterson, M. von Itzstein, C. Parish, A. Bezos, S.J. Berners-Price

3:50 INOR **400.** Transient spectroscopic studies of enantiomerically-resolved intercalating ruthenium dipyridophenazine (dppz) complexes bound to defined sequence DNA. **J.M. Kelly**, C. Cardin

4:20 INOR **401.** Selective binding of bifunctional Zn(II) complexes to G-quadruplex DNA. **M. Fountain**, J.R. Morrow, K.E. Siters, M. Shapovalova, M. Shively

4:50 INOR **402.** Multifunctional supramolecules for interactions with DNA and cancer cells exploiting photohemical activation. **R. Padilla**, J.A. Rodriguez Corrales, J. Zhu, J. Newman, R. Prussin, K.S. Brewer, **E.M. Naughton**

Section G

Colorado Convention Center
Room 401

ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry: Symposium in Honor of Kim R. Dunbar

Cosponsored by WCC

C. P. Berlinguette, D. J. Mindiola, E. J. Schelter, M. Shatruk, *Organizers, Presiding*

1:30 INOR **403.** Molecular spintronics: The role of chemistry. **E. Coronado**

1:50 INOR **404.** Strong magnetic exchange, slow magnetic relaxation, and spin crossover in iminobenzoquinonoid dinuclear complexes. I. Jeon, J. DeGayner, J.G. Park, A. Gaudette, **D. Harris**

2:10 INOR **405.** Multifunctionality in spin-crossover complexes: Toward "molecular multiferroics". H. Phan, J.J. Hrudka, J. Lengyel, S. Benjamin, E. Steven, N.S. Dalal, J. Brooks, **M. Shatruk**

2:30 INOR **406.** Recent fun in homo- and heterometallic manganese cluster chemistry. **G. Christou**, A.E. Thuijs, K. Mitchell, A.M. Mowson, A. Fournet, K.A. Abboud

2:50 Intermission.

3:05 INOR **407.** Adventures in spin crossover phenomena: (Giant) memory effect in magnetic and in hybrid conducting materials. **J. Galan-Mascaros**, C. Saenz de Pipaon, P. Maldonado-Illescas, Y. Koo, V. Gomez

3:25 INOR **408.** Magnetic metal-cyanide coordination clusters and chains. X. Feng, D. Freedman, T. Harris, H. Choi, B.M. Bartlett, D.M. Jenkins, H. Karunadasa, J. Zadrozny, M. Bennett, **J.R. Long**

3:45 INOR **556.** Halogen photoelimination from Ni(III) complexes: An energy storing transformation. S. Hwang, D.C. Powers, S. Zheng, Y. Chen, **D.G. Nocera**

4:05 INOR **410.** Multifunctionality at extreme conditions: spin cross-over photomagnetic behavior induced by pressure. **D. Pinkowicz**

Section H

Colorado Convention Center
Room 203

F. Albert Cotton Award in Synthetic Inorganic Chemistry: Symposium in Honor of Jaqueline L. Kiplinger

Cosponsored by WCC

D. E. Morris, *Organizer*
G. G. Stanley, *Organizer, Presiding*

1:30 INOR **411.** Spectroscopic and computational studies on a bimetallic hydroformylation catalyst system. **G.G. Stanley**, R. Fernando, M. Moulis

1:50 INOR **412.** Activation of C-F bonds: The next stage. **T.G. Richmond**

2:10 INOR **413.** Dehydrocoupling: Then and now. **J.Y. Corey**

2:30 INOR **414.** Interplay between theory and experiment in investigations of organo-actinide complexes: A retrospective. **P.J. Hay**

2:50 INOR **415.** Covalency in the actinides probed with ligand K-edge X-ray absoprtion spectroscopy. **R.L. Martin**

3:10 INOR **416.** Small molecule activation by complexes of low-valent f elements. **M. Mazzanti**, J. Pécaut, C. Camp, V. Mougel, J. Andrez

3:30 Intermission.

3:40 INOR **417.** Selective transformations of organic vompounds mediated by transition metal complexes. **R.G. Bergman**

4:10 INOR **418.** Supramolecular chemistry of anions: Organic, inorganic and biological studies. **K.R. Dunbar**

4:40 INOR **419.** Technetium halide chemistry. **A.P. Sattelberger**, F. Poineau, E.V. Johnstone, W.M. Kerlin, C. Malliakas, P.M. Forster, K. Czerwinski

5:00 INOR **420.** Computational actinide chemistry: Searching for understanding and holy grails. **B.E. Bursten**

Section I

Colorado Convention Center
Room 205

Division of Inorganic Chemistry Celebration of the Alfred Bader Award in Bioinorganic or Bioorganic Chemistry: Symposium in Honor of Michael A. Marletta

M. A. Marletta, *Organizer, Presiding*

1:30 INOR **421.** Reinventing natural product discovery. **D. Mitchell**

2:00 INOR **422.** Metals and Immunity. **E.M. Nolan**

2:30 INOR **423.** Synthetic cluster models of the biological oxygen evolving catalyst from photosystem II. **T. Agapie**

3:00 Intermission.

3:15 INOR **424.** Biosynthesis and tailoring of acyl peptidic siderophores. **A. Butler**, M.P. Kem, H. Naka, H.K. Zane, M.G. Haygood

3:45 INOR **425.** Glycocalyx engineering toward probing cancer glycome evolution. **C.R. Bertozzi**

Section J

Colorado Convention Center
Room 402

Bioinorganic Chemistry

S. A. Koch, *Organizer*
L. A. Finney, *Presiding*

1:30 INOR **426.** Second-sphere tuning of enzymatic activity in noncanonical heme oxygenase. **M.D. Liptak**, A.B. Graves, C.L. Lockhart

1:50 INOR **427.** Pif97 as a framework protein for association of organic-inorganic layers of nacre. **S. Bahn**, B. Jo, Y. Choi, H.J. Cha

2:10 INOR **428.** Model compounds of [NiFe]-hydrogenase in the Ni-SI_2 and Ni-L states. **G.M. Chambers**, T.B. Rauchfuss, E.J. Reijerse, K. Weber, W.W. Lubitz

2:30 INOR **429.** Evolution of thioether S-ligated primary Cu'/O_2 adducts: The 1st example of Cu^{II}-superoxo species with enhanced reactivity. **J.C. Lee**, S. Kim, R. Cowley, J.W. Ginsbach, M. Siegler, E.I. Solomon, K.D. Karlin

2:50 INOR **430.** Fundamental reactivity studies of hydrogen sulfide with metalloporphyrins. **D.J. Meininger**, H. Arman, Z.J. Tonzetich

3:10 INOR **431.** Dioxygen activation under ambient conditions using bio-inspired manganese(II) complexes to generate mid-valent oxidants for catalytic O–H bond oxidations. **G.B. Wijeratne**, A.D. Burr, B. Corzine, T.A. Jackson

3:30 INOR **432.** Short peptides self-assemble to produce catalytic amyloids. **C.M. Rufo**, Y.S. Moroz, O.V. Moroz, J. Stoehr, T.A. Smith, X. Hu, W.F. Degrado, I.V. Korendovych

3:50 INOR **433.** New insights in the chemistry of nickel in urease. L. Mazzei, S. Benini, **S. Ciurli**

4:10 INOR **434.** Understanding the reaction mechanism of the tungstoenzyme, acetylene hydratase. **M.A. Cranswick**, E. Vergunst, B. Trujillo

4:30 INOR **435.** Tethered C,N,S ligands containing an iron-carbamoyl motif as synthetic models of mono-iron hydrogenase. **M.J. Rose**, G. Durgaprasad

4:50 INOR **436.** Family of starch-active polysaccharide monooxygenases. **V.V. Vu**, W.T. Beeson, D. Suess, E.A. Span, E.R. Farquhar, R. Britt, M.A. Marletta

WCC Rising Stars Awards Symposium

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Undergraduate Research Posters

Inorganic Chemistry

Sponsored by CHED, Cosponsored by INOR and SOCED

MONDAY EVENING

Section A

Colorado Convention Center
Halls C/D

Sci-Mix

S. A. Koch, N. S. Radu, *Organizers*

8:00 - 10:00

4, 79, 161-162, 165, 167, 171, 180, 182, 184, 197, 204, 211, 213, 217-218, 224, 226, 228-229, 238-239, 241, 243-244, 248, 256, 260, 270-273, 287, 291, 295, 307, 310-311, 318, 320, 323, 329, 331-332, 336, 348, 356. See previous listings.

INOR **437.** Investigation of copper exchange between the avian egg proteins riboflavin binding protein, phosvitin and vitellogenin. **J.I. Matchynski**, A.W. Chamoun, M. Benore, S.R. Smith

509, 585, 590-591, 595, 598, 600-601, 604, 607, 610-611, 614, 623-624, 631-632, 634-635, 644-647, 649-650, 653, 659, 663, 666, 670, 672, 674-676, 688, 694, 697-698, 709, 713, 715, 719, 723, 725. See subsequent listings.

TUESDAY MORNING

Section A

Colorado Convention Center
Room 105

Undergraduate Research at the Frontiers of Inorganic Chemistry

Bioinorganic Chemistry

C. Nataro, S. R. Smith, *Organizers*
A. J. Reig, *Presiding*

9:00 Introductory Remarks.

9:05 INOR **438.** Biochemical and molecular modelling studies of the interaction of organometallic ruthenium complexes containing thiosemicarbazones or curcuminoids as ligands with DNA and proteins. **F.A. Beckford**, K.L. Hall, K.R. Webb

9:25 INOR **439.** Formation and characterization of Langmuir-Blodgett films of lipid rafts. **D.L. Calkins**, I. Kuznetsov, **E. Magallanes**, C. Menoni, D. Crick, D.C. Crans

9:45 INOR **440.** Functional model of the first and second coordination spheres of type 2 copper nitrite reductase. **G. Rowe**, S.L. Behnke, S. Weaver, E. Foerster, M. Bezpalko, B.M. Foxman

10:05 Intermission.

10:15 INOR **441.** Voltammetric studies of the Rieske protein. **K.R. Hoke**, R.J. Quarles

10:35 INOR **442.** X-ray crystallographic analysis of reduction potential mutants of the Rieske protein from *Thermus thermophilus*. **L.M. Hunsicker Wang**

10:55 INOR **443.** Understanding functional tuning in binuclear non-heme iron enzymes through systematic variation of the G4DFsc active site. **A.J. Reig**, S. Cimerol, J. Pellegrino, R. Polinski, K.A. Drost, C.L. Kanya, K. Biernat, K. O'Shea

11:15 INOR **444.** Homoleptic transition metal complexes of the 7-azaindolide ligand featuring κ1-N1 coordination. **M. Kiewit**, Z.J. Tonzetich

Section B

Colorado Convention Center
Room 301

2015 Priestley Medalist: Symposium in Honor of Jacqueline K. Barton

M. C. Buzzeo, S. Delaney, V. C. Pierre, *Organizers*
E. Boon, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 INOR **445.** Coupling oxygen consumption with substrate oxidation in bacterial multicomponent monooxygenases. **S.J. Lippard**

9:05 INOR **446.** Are metal-associated misfolded proteins involved in Alzheimer's disease? **M. Lim**

9:35 INOR **447.** Cephalopod-derived materials for photonic and protonic devices. **A.A. Gorodetsky**

10:05 Intermission.

10:15 INOR **448.** Exploring the physiological role of selenium redox chemistry. **M.C. Buzzeo**

10:45 INOR **449.** Nucleic acids in quadruplexes. **F. Shao**

11:15 INOR **450.** Photochemical dynamics of stacked perylenediimide assembly constructed on DNA. **T. Takada**

Section C

Colorado Convention Center
Room 302

ACS Award in Organometallic Chemistry: Symposium in Honor of William J. Evans

J. R. Walensky, *Organizer*
J. C. Gordon, *Presiding*

8:30 INOR **451.** Highly selective chemical processes for tailored electronic materials: Interfaces, depositions, and treatments. **R.D. Clark**

8:50 INOR **452.** Progress toward fluid materials for chemical hydrogen storage. **B.L. Davis**, A. Carre-Burritt, B.D. Rekken

9:10 INOR **453.** Effects of fast charging on lithium-ion cells. **I. Bloom**

9:30 INOR **454.** Peptido-mimetic sequence-defined polymers based on a new synthetic architecture. **J.W. Grate**, K. Mo, M. Daily, C. Chen

9:50 Intermission.

10:00 INOR **455.** Development of a 3D composite for NASA's Orion spacecraft compression pad. **J.D. Feldman**

10:20 INOR **456.** Optimizing the performance of polyolefins via stabilization chemistry and effects. **R.E. King**

10:40 INOR **457.** Natural gas to ethylene in one step: Siluria technologies OCM (oxidative coupling of methane). **G. Nyce**

11:00 INOR **458.** Cobalt complexes containing pendant amines in the second coordination sphere as electrocatalysts for energy storage. **M. Fang**, E.S. Wiedner, R. Bullock

Section D

Colorado Convention Center
Room 303

Chemical Approaches to Spintronics Research

R. Beaulac, *Organizer, Presiding*

8:30 INOR **459.** Zero-field spin polarization effects on Dexter transfer. J. Kouzelos, M. Soler, **J.K. McCusker**

9:00 INOR **460.** Theoretical characterization of conduction-band electrons and magnetic exchange interactions in photodoped and aluminum-doped diluted magnetic semiconductors. **X. Li**, J. Goings

9:30 INOR **461.** Near-infrared paramagnetic manganese-doped PbS nanocrystals. **L. Turyanska**

10:00 Intermission.

10:00 INOR **462.** Chirality induced spin selectivity (CISS) effect-chiral molecules for spintronics. **R. Naaman**

10:30 INOR **463.** Decoherence in crystals of quantum molecular magnet. **S. Takahashi**

11:00 INOR **464.** Effects of the addition of spin on donor-acceptor excited state electronic structure. B. Stein, C. Tichnell, D. Stasiw, D. Shultz, **M.L. Kirk**

11:30 INOR **465.** π-System superexchange in cross-conjugated donor-bridge-acceptor triads: Electronic structure contributions to quantum interference. **D. Shultz**, D. Stasiw, B. Stein, D. Habel-Rodriguez, M.L. Kirk

Section E

Colorado Convention Center
Room 201

Chemistry of the Energy Water Nexus: Focus on Fracking

C. McInnis, *Organizer, Presiding*

9:00 INOR **466.** Thinking constructively about hydraulic fracturing fluid design in the new resource landscape. **B.A. MacKay**

9:30 INOR **467.** Review of industrial biocides used for microbial control in hydraulic fracturing. **T.M. Williams**

10:00 Intermission.

10:10 INOR **468.** Electrochemically produced biocides: A greener disinfectant for waters used in hydraulic fracturing. **A.K. Boal**

10:40 INOR **469.** Reclaiming produced water: Using chemistry to convert a waste stream into a resource. **K. Sikkema**

Section F

Colorado Convention Center
Room 304

Interactions of Metal Complexes with Proteins or Nucleic Acids

J. R. Morrow, C. Turro, *Organizers*
P. C. Glazer, *Presiding*

8:30 INOR **470.** Noncovalent recognition of "unusual" but active DNA and RNA structures. **M.J. Hannon**

9:00 INOR **471.** Tuning *in cellulo* targeting and function of metal complex bioprobes. **J.A. Thomas**

9:30 INOR **472.** Platinum biomolecule target analysis using click chemistry. J.D. White, A.D. Moghaddam, R. Cunningham, K. Plakos, M.F. Osborn, M.M. Haley, **V. DeRose**

10:00 Intermission.

10:30 INOR **473.** Catalytic metallodrugs: Structure-function and activity studies of a broad therapeutic platform. **J.A. Cowan**

11:00 INOR **474.** Tuning the pharmacological properties of platinum-acridine anticancer agents using novel prodrug and subcellular targeting strategies. **U. Bierbach**

11:30 INOR **475.** Unusual synergism of serum transferrin titanium(IV) coordination brings insight into its potential transport and bioactivity in the human body. **A.D. Tinoco**

Section G

Colorado Convention Center
Room 401

ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry: Symposium in Honor of Kim R. Dunbar

Cosponsored by WCC

C. P. Berlinguette, E. J. Schelter, M. Shatruk, *Organizers*
D. J. Mindiola, *Organizer, Presiding*

8:30 INOR **476.** Drug membrane interactions and uptake as key aspects of drug action. **D.C. Crans**

8:50 INOR **477.** Understanding anion-π interactions: from substituted benzenes to N-heterocycles. **S.E. Wheeler**

9:10 INOR **478.** Role of inorganic chemistry in the activities of antimicrobial peptides. **A.M. Angeles Boza**

9:30 INOR **479.** Highly unsaturated cationic metal complexes supported by pincer ligands. **O. Ozerov**, J.C. DeMott, R. Huacuja

9:50 Intermission.

10:05 INOR **480.** Nonexistent compounds. **C.C. Cummins**, R. Field, M. Nava, B. Park, W. Transue, A. Velian

10:25 INOR **481.** New Carbon-Hydrogen Activation Reactions by Titanium Alkylidynes and Phosphino-Alkylidynes. **D.J. Mindiola**

10:45 INOR **482.** Ligand and reagent effects in C–H borylation. **M.R. Smith**

11:05 INOR **483.** Carbene-stabilized allotropes: Synthesis, structure, and reactivity. **G.H. Robinson**

11:25 INOR **484.** Mobile zinc signaling in the brain – learning, memory, hearing, olfaction, and vision. **S.J. Lippard**

Section H

Colorado Convention Center
Room 203

F. Albert Cotton Award in Synthetic Inorganic Chemistry: Symposium in Honor of Jaqueline L. Kiplinger

Cosponsored by WCC

G. G. Stanley, *Organizer*
D. E. Morris, *Organizer, Presiding*

8:30 INOR **485.** Covalency in lanthanides. **S.A. Kozimor**, J.M. Keith, A.B. Altman, E.R. Batista, D.L. Clark, R.L. Martin, S.G. Minasian, T. Tyliszczak, D.K. Shuh, M.P. Wilkerson

8:50 INOR **486.** Uranium-element multiple bond formation facilitated by redox-active pyridine(diimine) ligands: Synthesis, characterization, and reactivity of a unique class. **S.C. Bart**

9:10 INOR **487.** Reactions of oxygen with late transition Metal Complexes. **K.I. Goldberg**

9:30 INOR **488.** DFT studies of Cp2An(P)2 complexes as catalysts for pyridine and thophene ring opening. **E.R. Batista**, A.W. Pierpont, R.L. Martin, N.E. Travia, J.L. Kiplinger

9:50 INOR **489.** Pursuits of rare oxidation states in actinide chemistry. **M.R. Antonio**, L. Soderholm

10:10 INOR **490.** Perturbation of the electronic properties of non-innocent vanadium(V) complexes and the chemical properties of vanadium and copper coordination complexes in inhomogeneous environments. **D.C. Crans**, I. Sánchez Lombardo, J. Koehn, E. Magallanes

10:30 Intermission.

10:40 INOR **491.** Formation, characterization, and uses of metallacycles via coordination directed self-assembly. **P.J. Stang**

11:10 INOR **492.** Interplay of metal ions and oxidative damage in DNA G-quadruplexes. **C.J. Burrows**

11:40 INOR **493.** Reduction chemistry with group 3 metals supported by a ferrocene diamide ligand. **P. Diaconescu**

12:00 INOR **494.** Uranium imido complexes: A window into actinide-ligand bonding and reactivity. **J.M. Boncella**, N.C. Tomson, **E.R. Batista**, B. Scott

Section I

Colorado Convention Center
Room 205

Molecular Catalysts for Solar Fuels

Cosponsored by MPPG

A. M. Appel, M. Helm, J. Y. Yang, *Organizers, Presiding*

8:30 INOR **495.** Bimetallic hydrides inspired by the hydrogenase active sites. **T.B. Rauchfuss**, G.M. Chambers, U.C. Olbelina, W. Wenguang

9:00 INOR **496.** Enzyme-like behavior achieved with amino acids in the outer coordination sphere of H_2 oxidation catalysts. **W.J. Shaw**, A. Dutta, D. DuBois, J. Roberts

9:30 INOR **497.** Theoretical design of hydrogen-evolving molecular electrocatalysts. **S. Hammes-Schiffer**

10:00 INOR **498.** Molecular proton reduction catalysts in metal-organic frameworks. **S. Ott**

10:30 Intermission.

10:45 INOR **499.** Production of C1 sources via reduction of CO_2 on redox active iron ligand platforms. **J.D. Gilbertson**

11:15 INOR **500.** Harnessing heterobimetallic complexes for CO_2 activation and reduction. **J. Yang**, S. Poteet, J. Ritter

11:45 INOR **501.** Deep photoreduction of carbon dioxide to methanol and formate by ruthenium polypydridyl chromophores with pendant pyridyl sites. **F.M. MacDonnell**, M. West, D.J. Boston, N. de Tacconi

Section J

Colorado Convention Center
Room 402

Soluble Inorganic Semiconductors: Synthesis, Properties, and Applications

R. L. Brutchey, B. M. Cossairt, *Organizers, Presiding*

8:30 INOR **502.** Magic-size II-VI nanoclusters as semiconductor precursors. Y. Wang, Y. Zhou, F. Wang, **W.E. Buhro**

9:00 INOR **503.** High throughput investigations of colloidal metal chalcogenide nucleation and growth. **J.S. Owen**, M.P. Hendricks, M.P. Campos, S. Hong, G.T. Cleveland, E. Chan

9:30 INOR **504.** Photochemical reactions of semiconductor nanocrystals coupled with redox catalysts. **G. Dukovic**

10:00 Intermission.

10:15 INOR **505.** All-inorganic design of colloidal nanocrystals: New inorganic ligands and new atomistic insights into their surface binding. **M. Kovalenko**

10:45 INOR **506.** Novel fabrication strategies for heterostructured PbS and PbSe QDs via controllable cation exchange reactions. **M.C. Beard**, J. Zhang, J. Luther, E. Miller, J. Gao

11:15 INOR **507.** Near-infrared photoluminescence enhancement in Ge/CdS and Ge/ZnS core/shell nanocrystals: Utilizing IV/II–VI semiconductor epitaxy. **J. Vela-Becerra**

ACS Award for Creative Research and Applications of Iodine Chemistry: Symposium in Honor of Karl O. Christe

Sponsored by FLUO, Cosponsored by INOR

TUESDAY AFTERNOON

Section A

Colorado Convention Center
Room 105

Undergraduate Research at the Frontiers of Inorganic Chemistry

Solid State and Materials Chemistry

C. Nataro, S. R. Smith, *Organizers*
M. T. Whited, *Presiding*

1:30 Introductory Remarks.

1:35 INOR **508.** Infrared Spectroscopic tracking of Q-state particle formation in ionomers. **F.A. Meyer**, J.H. Doan, E. Kingston, K.P. Anderson, A.K. Vong, E.S. Smotkin

1:55 INOR **509.** Ultrasmall Cu nanoparticles: A greener synthesis and catalytic studies. **G.A. Ferko**, A.D. Brumbaugh, S.K. St Angelo

2:15 INOR **510.** Synthesis, characterization, and utility of trifluoroacetic acid and fluoroalkoxy lanthanide precursors for production of fluorinated lanthanide nanomaterials. **D. Yonemoto**, T.J. Boyle, M.L. Neville, R.F. Hess, S.P. Bingham

2:35 INOR **511.** Phenoxy-mercapto derivatives of group 4 alkoxides as core-shell precursors to group 4 ceramic-coinage metal nanomaterials. **M.L. Neville**, T.J. Boyle, P. Lu, M.V. Parkes

2:55 Intermission.

3:05 INOR **512.** Oxidizing aldehydes with water: Catalysts for the aldehyde-water shift. **J.C. Tran**, T. Brewster, D.M. Heinekey, K.I. Goldberg

3:25 INOR **513.** Multifunctional nanoclusters for biomedical applications. **S. Park**, S.K. Cho, W. Park

3:45 INOR **514.** Student explains international undergraduate research and cultural experiences. **A. Walker**, G. Royal, T.J. Hubin, R. Duran

4:05 INOR **515.** Computational and synthetic study of organic-inorganic conjugate dyes for solar energy harvesting. **R.E. Bachman**, A.E. Connor, S.A. Parks, M.R. Leidy, N.J. Deyonker

4:25 Concluding Remarks.

‡ *Cooperative Cosponsorship*

Section B

Colorado Convention Center
Room 301

2015 Priestley Medalist: Symposium in Honor of Jacqueline K. Barton

E. Boon, M. C. Buzzeo, S. Delaney, V. C. Pierre, *Organizers*
A. K. Boal, *Presiding*

1:30 INOR **516.** Targeting mitochondrial DNA. **S.O. Kelley**

2:00 INOR **517.** Novel development of electrolytes in lithium ion battery. **Y. Tanaka**

2:30 INOR **518.** Peptide nucleic acids (PNAs) as diagnostic and therapeutic molecules. **E. Yavin**

3:00 Intermission.

3:10 INOR **519.** Controlling molecular display and cell behavior with nanocrystals. **C.J. Murphy**

3:40 INOR **520.** Sensitive and selective real-time electrochemical monitoring of DNA repair. **J. Slinker**, M. McWilliams, F. Anka, K.J. Balkus

4:10 INOR **521.** Evolution of an idea born in my postdoc with Jackie Barton: From rhodium-peptide conjugates to Alzheimer's disease. **R.P. Houser**

Section C

Colorado Convention Center
Room 302

Solid-State Inorganic Chemistry

C. G. Lugmair, *Organizer*
V. Poltavets, *Organizer, Presiding*
M. Dolgos, *Presiding*

1:30 Introductory Remarks.

1:35 INOR **522.** Low temperature synthesis of (noncentrosymmetric) oxide-fluoride materials. **K.R. Poeppelmeier**, K.B. Chang, A. Vinokur, M. Marvel

2:15 INOR **523.** Low temperature synthesis of bimetallic carbide nanomaterials and their electrocatalytic activity. **S.M. Schmuecker**

2:35 INOR **524.** Single source precursor approach to metastable molybdate phases. **A.W. Apblett**, A.M. Moneeb, A. Alabdulrahman, A. Bagabas, C. Perkins

2:55 INOR **525.** Mechanistic studies in kinetically controlled solid state synthesis: The case of $[(SnSe)_{1.13}][VSe_2]$. **M. Esters**, M. Falmbigl, D.C. Johnson

3:15 INOR **526.** Following the journey from aqueous polyoxometalate to metal oxide. Y. Hou, D. Fast, L.B. Fullmer, M.D. Nyman, **M. Dolgos**

3:35 Intermission.

3:50 INOR **527.** Synthesis of metal sulfides in sulfur/iodine flux using furnace or microwave reactions. R. Groom, **S.E. Latturner**

4:10 INOR **528.** Extraction behavior of mesoporous silica SBA-15 for soluble uranyl peroxo clusters. **Y. Liu**, A. Czarnecki, J.E. Szymanowski, M. Dembowski, G. Sigmon, P.C. Burns

4:30 INOR **529.** Negative thermal expansion and other anomalous properties in rock salt ordered mixed metal fluorides $M^{III}ZrF_6$ with a ReO_3-type structure. J.C. Hancock, C.R. Morelock, L.C. Gallington, K.W. Chapman, G.J. Halder, B.S. Kaplan, A. Bongiorno, C. Han, S. Zhou, **A.P. Wilkinson**

4:50 INOR **530.** Dark reactions project: a machine learning approach to materials discovery. **A.J. Norquist**

5:10 INOR **531.** Ferromagnetic behavior in non-metal anionic element reagent complexes. **M.P. Rowe**, R. Desautels, E. Skoropata, J. van Lierop

Section D

Colorado Convention Center
Room 303

Inorganic Catalysts

S. A. Koch, *Organizer*
Y. Zhang, *Presiding*

1:30 INOR **532.** Novel CeO_2 yolk-shell structures loaded with tiny Au nanoparticles for highly catalytic reduction of *p*-nitrophenol. **C. Fan**, A. Xu

1:50 INOR **533.** Diphenyl ether based secondary phosphine oxide as preligand for nickel-catalyzed carbon-sulfur cross-coupling reactions. **N.P. Nambukara Wellala**, H. Guan

2:10 INOR **534.** Dehydration and dehydrogenation of ethanol over Au-exchanged ZSM-5 zeolite: A DFT study. **T. Maihom**, B. Boekfa, **J. Limtrakul**

2:30 INOR **535.** Withdrawn.

2:50 INOR **536.** Mesoporous Co_3O_4 catalyst for CO oxidation at -60C: Controlled porosity, reaction mechanism, and deactivation reason. **W. Song**, A. Poyraz, Y. Meng, Z. Ren, S. Chen

3:10 Intermission.

3:20 INOR **537.** Dinitrogen silylation facilitated by a dicobalt catalyst. **R.B. Siedschlag**, K.D. Vogiatzis, V. Bernales, N. Planas, L. Gagliardi, C.C. Lu

3:40 INOR **538.** Cyclic alkyl amino carbene (CAAC) ruthenium complexes as remarkably active catalysts for ethenolysis. **V.M. Marx**, A.H. Sullivan, M. Melaimi, S.C. Virgil, G. Bertrand, R.H. Grubbs

4:00 INOR **539.** Iron porphyrin carbenes as catalytic intermediates: Structures, Mössbauer and NMR spectroscopic properties, and bonding. R. Khade, **Y. Zhang**

4:20 INOR **540.** Electrochemical studies of cobalt (II) N_2P_2 complexes and a nickel (II) bis(diphosphine) complex toward catalytic proton reduction. **J.F. Khosrowabadi Kotyk**, J. Yang

Section E

Colorado Convention Center
Room 201

Chemistry of the Energy Water Nexus: Focus on Fracking

Cosponsored by MPPG‡

C. McInnis, *Organizer, Presiding*

1:30 INOR **541.** Development of advanced polymers for hydraulic fracturing applications. **C.R. Hilliard**, C. Meza, R. Schlemmer, J. Donovan

2:00 INOR **542.** Shale gas and oil flowback and produced water modeling and treatment. **M.B. Tomson**, Z. Zhang, Z. Dai, V. Bolanos, A.T. Kan, F. Yan, R. Tomson

2:30 INOR **543.** Dynamic microbial communities in hydraulic fracturing water: Implications for vhemistry and water management. **K.B. Gregory**

3:00 INOR **544.** Characterizing oil and gas exploration and production waste streams: Collaborative inter-laboratory comparison. **T.Y. Cath**

3:30 Panel Discussion.

Section F

Colorado Convention Center
Room 304

Interactions of Metal Complexes with Proteins or Nucleic Acids

J. R. Morrow, C. Turro, *Organizers*
U. Bierbach, *Presiding*

1:30 INOR **545.** In vitro selection and characterization of metallo-DNAzymes and their delivery into cells for sensing and imaging applications. **Y. Lu**, K. Hwang, P. Wu, S. Torabi

2:00 INOR **546.** Is the geometry of Vanadium in active site of phosphatases important for inhibitor design and antidiabetic properties of vanadium compounds. **D.C. Crans**, B.J. Peters, M.L. Tarlton, G.R. Willsky, C.C. McLauchlan

2:30 INOR **547.** Metal ion incorporation in peptide nucleic acid triplexes. **C. Achim**, D. Jayarathna, Y. Bae, H. Stout

3:00 Intermission.

3:15 INOR **548.** Development of redox-active ruthenium polypyridyl complexes as an anticancer agents for the treatment of platinum resistant tumors. **F.M. MacDonnell**, N. Alatrash, E. Narh, C. Griffith

3:45 INOR **549.** Cobalt Schiff base complexes as targeted inhibitors of transcription factors. M.C. Heffern, **T.J. Meade**

4:15 INOR **550.** Inhibition of cysteine proteases with ruthenium-caged compounds. **J.J. Kodanko**

4:45 INOR **551.** Strategies for the photochemical uncaging of bioactive small molecules. **P.C. Ford**, J.V. Garcia, A. Pierri, M. Crisalli, A.W. DeMartino, P. Huang

Section G

Colorado Convention Center
Room 401

ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry: Symposium in Honor of Kim R. Dunbar

Cosponsored by WCC

C. P. Berlinguette, D. J. Mindiola, M. Shatruk, *Organizers*
E. J. Schelter, *Organizer, Presiding*

1:30 INOR **552.** Lewis acidic properties of organoantimony compounds: From bidentate distiboranes to perfluorinated stibonium cations. **F.P. Gabbai**

1:50 INOR **553.** Platinum diimine dithiolate chromophores and dyads for the light-driven generation of hydrogen. **R. Eisenberg**

2:10 INOR **554.** Manipulation of the electronic structures of cerium complexes toward the development of a new class of photosensitizers. **E.J. Schelter**, H. Yin, P. Carroll

2:30 INOR **555.** Control of excited states of transition metal complexes: Optimizing multiple excited state pathways. **C. Turro**, K.R. Dunbar

2:50 Intermission.

3:05 INOR **409.** How to get what you want: A control freak's guide to inorganic nanoparticle synthesis. **R.E. Schaak**

3:25 INOR **557.** How nickel/iron films catalyze the oxygen evolution reaction. **C.P. Berlinguette**, R.D. Smith

3:45 INOR **558.** Inorganic chemistry, solution processed solar cells, and the era of perovskites. **M.G. Kanatzidis**

4:05 INOR **559.** Cyanide-bridged iron complexes as analogues of tri-iron arrangements in hydrogenase active site precursors. A.M. Lunsford, C. Beto, **M.Y. Darensbourg**

Section H

Colorado Convention Center
Room 203

F. Albert Cotton Award in Synthetic Inorganic Chemistry: Symposium in Honor of Jaqueline L. Kiplinger

Cosponsored by WCC

D. E. Morris, *Organizer*
G. G. Stanley, *Organizer, Presiding*

1:30 INOR **560.** Microfluidic separations for actinide processing and analysis. **R.M. Chamberlin**, S.L. Yarbro, N. Xu

1:50 INOR **561.** Production of Mo-99 for nuclear medicine. A. Anderson, L. Bitteker, M. Connors, R. Copping, M. Cover, W. Crooks, G. Dale, D. Dalmas, M. Gallegos, E. Garcia, J. Gioia, R. Gonzales, D. Graves, W.K. Hollis, M. Janicke, C. Kelsey, I. May, M. Mocko, M. Pieck, M. Rawool-Sullivan, S.D. Reilly, D. Rios, T. Romero, F. Stephens, **F. Taw**, D. Thorn, K. Woloshun

2:10 INOR **562.** CO_2 conversion using organometallic and organic molecular catalysts. **T. Cantat**

2:30 INOR **563.** Organometallic thorium azide complexes. **M.J. Monreal**, J.L. Kiplinger, B. Scott

2:50 INOR **564.** Pursuit of high-oxidation state phosphinidene complexes of the group 6 metals for metathesis reactivity. **R.K. Thomson**

3:10 INOR **565.** Aluminum chemistry featuring nitrogen-based ligands for stabilization of cations and radicals. **J.D. Masuda**, W.L. McClennan, N.A. Giffin

3:30 Intermission.

3:40 INOR **566.** Actinide speciation in aqueous chloride and pseudochloride solutions. **L. Soderholm**, S. Skanthakumar

4:00 INOR **567.** Synthesis and combustion of nitrogen-rich f-element complexes. **J.M. Veauthier**, J.L. Kiplinger, B.C. Tappan, N.E. Travia, K. Browne, B.L. Scott, N.J. Henson, A.H. Mueller, D.E. Chavez, A.T. Nelson

4:20 INOR **568.** Actinide-arene interactions and their use in carbon-element bond forming reactions. **P.L. Arnold**, J. McKinven, J. Hlina, R. Lord, R. Batrice, N. Kaltsoyannis, M. Eisen, M. Gardiner, J.B. Love

4:50 INOR **569.** Covalency and the relative roles of 5f and 6d orbitals in actinide metal-ligand bonds. **D.L. Clark**

5:20 INOR **570.** Enabling the exploration of metal-ligand bonding in light actinides: One of Jackie Kiplinger's many synthetic legacies. **D.E. Morris**

Section I

Colorado Convention Center
Room 205

Molecular Catalysts for Solar Fuels

Cosponsored by MPPG

A. M. Appel, M. Helm, J. Y. Yang, *Organizers, Presiding*

1:30 INOR **571.** Selective heterogeneous electrocatalytic reduction of CO_2 to CO or $HCOO^-$ using iron porphyrin complexes. **A. Dey**

2:00 INOR **572.** Navigating structure-activity relationships in molecular electrocatalysts for CO_2 reduction. **R.J. Nielsen**, S.I. Johnson, Y. Lam, W.A. Goddard

2:30 INOR **573.** Ir–H species as key intermediates in CO_2 hydrogenation, formic acid dehydrogenation and photochemical CO_2 reduction. **E. Fujita**, J.T. Muckerman, Y. Himeda

3:00 INOR **574.** Reduction of CO_2 to methanol by an organic hydride via hydride transfer/proton transfer steps. **J.T. Hynes**, C. Musgrave, C. Lim, A. Holder

3:30 Intermission.

3:45 INOR **575.** Homogeneous reduction of CO_2 by $[Ni(cyclam)]^+$, poisoning by CO, detoxification by CO sponge, and useful conversion of CO by tandem catalysis. **C.P. Kubiak**, J. Froehlich, J. Tillman

4:15 INOR **576.** What theory can reveal about carbon dioxide reduction and the role of molecular catalysts. **E.A. Carter**

4:45 INOR **577.** Molecular catalysis of water oxidation and CO_2 reduction in dye sensitized photoelectrosynthesis cells (DSPEC). **T.J. Meyer**, J. Concepcion, Z. Chen, M. Norris, M. Zhang, M. Coggins, R. Binstead, N. Song, D.L. Ashford, M. Sheridan, P. Kang, S. Zhang, N.Y. Iha, M. Brookhart, J.L. Templeton

Section J

Colorado Convention Center
Room 402

Soluble Inorganic Semiconductors: Synthesis, Properties, and Applications

R. L. Brutchey, B. M. Cossairt, *Organizers*
G. Dukovic, J. S. Owen, *Presiding*

1:30 INOR **578.** Single junction CZTSSe and tandem CZTSSe/hybrid perovskite solar cells from molecular-inks: Mapping the effects of composition on material quality and device performance. **H.W. Hillhouse**

2:00 INOR **579.** Solution-processed electrochromic and photovoltaic thin films from nanocrystal building blocks. **D.J. Milliron**, A. Llordes, A. Singh

2:30 INOR **580.** Synthesis of transition metal chalcogenide and pnictide nanoparticles for applications in photovoltaics. **A.L. Prieto**, D. Agocs, M.B. Braun, S. Fredrick, L. Korala, R.C. Miller

3:00 Intermission.

3:15 INOR **581.** Photophysics in metal enriched and stoichiometric quantum dots. **M. Sfeir**, E. Busby, N.C. Anderson, J.S. Owen

3:45 INOR **582.** New matrix engineering strategies for efficient charge transport in quantum dot solids. **M. Law**

4:15 INOR **583.** Designer semiconductor nanocrystal electronic and optoelectronic materials and devices. **C.R. Kagan**, S. Oh, J. Choi, Y. Lai, D. Kim, E.D. Goodwin, A.T. Fafarman, B. Diroll, C.B. Murray

ACS Award for Creative Research and Applications of Iodine Chemistry: Symposium in Honor of Karl O. Christe

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TUESDAY EVENING

Section A

Colorado Convention Center
Hall C

Bioinorganic Chemistry

DNA, RNA and Inorganic Drugs

S. A. Koch, *Organizer*

6:00 - 8:00

INOR **584.** Luminescent ruthenium probe for DNA mismatches. **A.N. Boynton**, A.J. McConnell, J.K. Barton

INOR **585.** 1H- and 19F-NMR spectroscopic studies of 4-fluorophenylbiguanide with the interface of reverse micelles. J. Sripradite, N. Samart, A. Tongraar, **D.C. Crans**

INOR **586.** N-hydroxysulfonamides RSO_2NHOH as nitroxyl (HNO) donors: Improved preparation and kinetics of nitroxyl generation. **S.K. Adas**, N.E. Brasch, P. Sampson

INOR **587.** Exploring the cellular activity of polyazine bridged Ru(II)-Rh(III) supramolecules in rat malignant glioma F98 cells. **J. Zhu**, K.S. Brewer

INOR **588.** Cytotoxic and DNA binding properties of Mn(I) and Re(I) carbonyl perrhenato complexes. **J. Taylor,** S.K. Pramanik, J.A. Krause, S.K. Mandal

INOR **589.** Photosensitization of singlet oxygen by ruthenium(II) polypyridyl complexes for DNA photocleavage. **S. Yang**, **K. Wang**, B.R. Williams, S.J. Nieter Burgmayer

INOR **590.** Evaluation of heme peripheral groups interactions in low-dielectric constant media. **A. Stockhausen**, J. Cerda

Section B

Colorado Convention Center
Hall C

Bioinorganic Chemistry

Proteins and Enzymes and Model Systems

S. A. Koch, *Organizer*

6:00 - 8:00

INOR **591.** Spectroscopic methods to characterize non-heme iron enzymes (monooxygenase and dioxygenase). **B. Subedi**, B.S. Pierce

INOR **592.** Formation, characterization, and O-O bond activation of a bio-inspired peroxomanganese(III) complex. **H.E. Colmer**, T.A. Jackson

Technical program information known at press time.
The official technical program for the 249th ACS National Meeting is available at:
www.acs.org/denver2015

INOR **593.** Binuclear complexes: Analogs for superoxide dismutase enzyme substrate binding studies. **J.W. Kreft**, E. Sinn

INOR **594.** Crystallization of protein models of non-coupled dinuclear copper proteins. **A. Sauer**, M. Ladd, S. Pedersen, S.M. Berry

INOR **595.** Modeling oxidoreductase enzymes in the protein azurin. **T. Roach**, G. Stoddard, S.M. Berry

INOR **596.** Role of halogen substituents and substrate pK_a in defining the substrate specificity of 2,6-dichlorohydroquinone 1,2-dioxygenase (PcpA). **J.E. Burrows**, M.Q. Paulson, T.E. Machonkin

INOR **597.** Nitrite reduction activity of azurin variants. **B. Khatiwada,** J. Strange, S.M. Berry

INOR **598.** Synthetic models for nickel superoxide dismutase. **S.K. Senaratne**, D.M. Eichhorn

INOR **599.** Job's method and high resolution NMR studies of trinuclear bis(bis(O-ethyl-L-cysteinato)$_2$Ni)$_2$Ni^{2+}. **R.J. Dougherty**, K.V. Krishnan, M.L. Golden

Section C

Colorado Convention Center
Hall C

Interactions of Metal Complexes with Proteins or Nucleic Acids

J. R. Morrow, C. Turro, *Organizers*

6:00 - 8:00

INOR **600.** Tuning mechanisms of action of Ru(II) polypyridyl complexes as anticancer targets by changing charge states. **Y. Sun**, M. Dickerson, B. Howerton, D. Heidary, E. Glazer

INOR **601.** Selective recognition of G-quadruplex and thymine bulge DNA using bifunctional Zn(II) complexes. **K.E. Siters**, S.A. Sander, J. Devlin, J.R. Morrow

INOR **602.** Evaluation of the binding of Zn(II) complexes to G-quadruplexes using a PCR-stop assay. **M. Shively**, **M. Shapovalova**, M. Fountain, J.R. Morrow, K.E. Siters

INOR **603.** Determining titanium (IV) transport for its potential use by humans. **T.M. Planas-Fontanez**, S. Conklin Lopez, A. Lopez-Cubero, A.D. Tinoco

INOR **604.** Non-covalent interactions of a Ru-Rh supramolecular complex with DNA and their effect on covalent modification of the biomolecule. **J.A. Rodriguez Corrales**, K.S. Brewer

INOR **605.** Light-activated drug release using heterobimetallic ruthenium and cobalt complexes. **R. Whitman**, C. Turro

Section D

Colorado Convention Center
Hall C

Coordination Chemistry

Synthesis and Characterization

D. C. Crans, *Organizer*

6:00 - 8:00

INOR **606.** Synthesis, characterization, and reactivity of pyridazine-oxime metal complexes. **S.O. Elsiddieg**, F.R. Fronczek, A.W. Maverick

INOR **607.** "Super Bulky" guanidinates for the support of low-coordinate metal complexes. **L. Griego**, A.K. Maity, S. Fortier, A.J. Metta-Magana

INOR **608.** Synthesis and characterization of a new guanidinate-guanidinate ligand featuring an imidazolin-2-iminate backbone. **B. Barraza**, J. Lu, R. Aguilar, A. Maity, S. Fortier, A.J. Metta-Magana

INOR **609.** Reactivity of group 11 formamidinate complexes. **A. Lane**, J.R. Walensky, W.E. Antholine

INOR **610.** Vanadium(V) catecholates: Correlating redox potential with 51V NMR chemical shifts. **J. Koehn**, P. Chatterjee, A. Waterhouse, T. Lucia, T.E. Polenova, M.D. Johnson, D.C. Crans

INOR **611.** Octahedral to trigonal prismatic distortion in Ruthenium and Osmium bis-homoleptic complexes of a noninnocent ligand. **J. Cipressi**, S.N. Brown

INOR **612.** Recent developments in cyano-substituted polypyrazolylborates chemistry. **L. Kadel**, D.M. Eichhorn

INOR **613.** Synthesis, structural and spectroscopic studies of six-coordinate iron and cobalt phosphasalen complexes. J.M. Fritsch, **C.M. Bakewell**, A.J. White, C.K. Williams

INOR **614.** Electron transfer between metal and ligand in chromium complexes with tetrazine-containing pincer ligand. **A.V. Polezhaev**, C. Chen, N.A. Maciulis, K.G. Caulton

INOR **615.** Pyrazolate and polypyrazoleborate complexes of platinum and palladium. **A. Oberley**, D.M. Eichhorn

INOR **616.** Chemistry of copper and nickel pyridyltriazole complexes. **T.M. Wheat**, U.R. Pokharel, F.R. Fronczek, A.W. Maverick

INOR **617.** Synthesis and characterization of bis-bipyridyl ruthenium(II) complexes with high nitrogen content tetrazole aromatic ligands. **R.R. Ruminski**, M.A. Hiskey, R. Malkan, B. Powell

INOR **618.** Novel synthesis of a dinuclear ruthenium(II) polypyridyl complex based on a polymeric carbonyl complex. **L.M. Puckett**, B. Durham

INOR **619.** Synthesis and crystallographic study of zinc and mercury complexes with a three-N-donor asymmetric pyridine–amine ligand 2,9-di(pyridin-2-yl)-1,3,6-triazabicyclo[4.2.1]nonane. **M. Hakimi**

INOR **620.** Synthesis and characterization of [M(tacn)(dppz)(solvent)]n+ complexes of Ru, Rh, and Ir: New DNA metallointercalators possessing modifiable groups. H.L. Hancock, M. Pham, G. Culcu, **S.C. Haefner**

INOR **621.** Combined experimental and theoretical investigation of electronic structures and anion sensing aspects of $Os^{II}(bpy)_2(HL^{2-})$ AND $[\{Os^{II}(bpy)_2\}_2(\mu\text{-}HL^{2-})]^{2+}$. **A. Das**

Section E

Colorado Convention Center
Hall C

Coordination Chemistry

Synthesis and Characterization

D. C. Crans, *Organizer*

6:00 - 8:00

INOR **622.** Dehydrohalogenation as an effective route to unsaturated bimetallic and monometallic systems featuring a proton-responsive pincer ligand. **B. Cook**, C. Chen, M. Pink, R.L. Lord, K.G. Caulton

INOR **623.** Low-valent organometallics incorporating the 2,2'-biazulenyl motif. **M.D. Hart**, D.M. McGinnis, B.M. Neal, M.V. Barybin

INOR **624.** Six-coordinate 16-electron complexes of tungsten (II): Synthesis, electrochemistry, and density functional theory. **A.F. Greene**, S. Dahlhauser, J.T. Mague, J.P. Donahue

INOR **625.** Structural trends for triple-decker organometallic sandwiches formed by highly charged π-bowls with mixed alkali metal cores: Li/K vs. Li/Rb. S.N. Spisak, A.S. Filatov, A. Zabula, A.Y. Rogachev, **M.A. Petrukhina**

INOR **626.** Novel, multizonal, crystalline composite based upon self-assembled, helical coordination polymers and exhibiting seven primary zones in the solid state. **S.R. Seidel**, R. Wilkens

INOR **627.** Synthesis of new dithiolene-type ligands. **E. Haas**, J.P. Donahue, J.T. Mague

INOR **628.** Cd(II) complexation with 1,1-dithiolate and nitrogen donors: Synthesis, luminescence, crystal structure and antifungal activity. **A. Das**

INOR **629.** Reversible addition of alcohols across C=N bonds of a N_4 Schiff base ligand coordinated to copper (II). **W. Zhang**, H. Nie, M.S. Mashuta, C.A. Grapperhaus, R.M. Buchanan

INOR **630.** Design and synthesis of lightweight MOFs for gas storage. **M. Shimazu**, X. Bu, X. Zhao

INOR **631.** First row transition metal complexes of tetrazine based ligands as a new class of energetic materials. **T.W. Myers**, S.K. Hanson, J. Veauthier, D.E. Chavez

INOR **632.** Role of ligand modifications in structural outcomes of dinucleating, criss-crossed cobalt peroxo (μ-OH,μ-O_2) complexes. **Y. Cho**, M. Ward, M.J. Rose

INOR **633.** Investigations of the reaction of PMe_2Ph with a Pt-Ru heterometallic complex. **Z.J. Manning**, N.C. Dopke

INOR **634.** Chemo-induced spin-state switching using tunable iminopyridine ligands. **T. Ozumerzifon**, J. Kolanowski, M.P. Shores

INOR **635.** Iron(II) complexes of the dimethylated tris(pyrazolyl)ethane ligands. **M.S. Goodman**, M.A. Goodman, A.Y. Nazarenko

INOR **636.** Atropisomerism of iron 5,10,15,20-tetrakis(2-chloro-6-fluorophenyl) porphyrinates. **D.J. Meininger**, N. Muzquiz, Z.J. Tonzetich

INOR **637.** Electrochemical analysis of iron nitrilotriacetate complexes. P.**A. Defnet**, L.N. Ball, U.J. Williams

Section F

Colorado Convention Center
Hall C

Main Group Chemistry

T. W. Hudnall, *Organizer*

6:00 - 8:00

INOR **638.** Exploring the impact of ligand variation on arsenic-sulfur bonding using X-ray Absorption Spectroscopy (XAS). **A.V. Blake**, C.M. Donahue, S.R. Daly

INOR **639.** Cytoselectivity of organotin and transition metal-substituted organotin compounds on cancer cells. **J.S. Enriquez**, J.A. Muniz, A. Varela, K.H. Pannell, R. Aguilera

INOR **640.** Synthesis of novel bismuth complexes for small molecule activation. **M. Castillo**, O. Barreda, R. Aguilar, S. Fortier, A.J. Metta-Magana

INOR **641.** Synthesis and reactivity of a novel doubly base stabilized five-coordinate "silene" derivative, $[k^3\text{-}C(SiMe_2benzimid^{i\text{-}Pr})_2]SiMe_2$: Addition of a Zn–Me bond of Me_2Zn to afford $[k^3\text{-}C(SiMe_3)(SiMe_2benzimid^{i\text{-}Pr})_2]ZnMe$. **S. Ruccolo**, G.F. Parkin

Section G

Colorado Convention Center
Hall C

Organometallic Chemistry

Applications to Materials and Polymer Science

N. S. Radu, *Organizer*

6:00 - 8:00

INOR **642.** Multistep synthesis of the biocompatible lactone 3,6-dihydro-2H-pyran-2-one. **B.S. Cundiff**

INOR **643.** Coupling of cyclohexadiene oxide and CO_2 via metal catalysts. **C.J. Arp**, W. Chung, F. Tsai, S.J. Kyran, D.J. Darensbourg

INOR **644.** Synthesis and characterization of aluminum β-diketiminate complexes and their application in ring opening polymerization of lactides and synthesis of cyclic carbonates. **S. Bian**, G. Du

INOR **645.** Synthesis, characterization, and polymerization of thienyl phosphine palladium(II) complexes. **J.L. Shott**, B.J. Reeves, B.M. Boardman

INOR **646.** Extending π-conjugation for metallo-organic photon harvesting. M.H. Chisholm, **J. Leizerman**

INOR **647.** Theoretical study of the sodium mediated coupling of organchlorosilanes: Stable α-chloro-ω-sodium cyclosilane intermediates in the Wurtz synthesis of polysilanes? **S.J. Holder**

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Section H

Colorado Convention Center
Hall C

Nanoscience

R. M. Richards, *Organizer*

6:00 - 8:00

INOR **648.** Synthesis of aluminum nanoparticles capped with *o*-carborane. A. Benziger, P.A. Jelliss, S.W. Buckner

INOR **649.** Stability of gold nanoparticle-based films deposited on plasma-etched borosilicate glass *via* a layer-by-layer physisorption technique. **R.L. Svatora**, S.A. Darveau, C.L. Exstrom

INOR **650.** Stabilization of anisotropic gold nanoparticle shapes by Protein A. **B.A. Lueck**, S.A. Darveau, C.L. Exstrom

INOR **651.** Heat-mediated drug release from inorganic nanoparticles. **N.D. Klein**, K.R. Hurley, H.L. Ring, J.T. Buchman, C.L. Haynes

INOR **652.** Soft inorganic oxide nanofibrous membranes and their applications. **X. Mao**, B. Ding

INOR **653.** Design and synthesis of precursors for surface plasmon mediated chemical solution deposition of metal nanoparticles. **N. Richey**, Y. Wu, J. Qiu, W.D. Wei, L. McElwee-White

INOR **654.** Role of oxygen vacancy in nanocrystalline perovskite oxides for electrochemical reactions. **J. Kim**, X. Yin, K. Tsao, S. Fang, H. Yang

INOR **655.** Direct assembly of zeolite beta into mesoporous nanoparticles. **T. Chen**, Y. Liu, C. Mou

INOR **657.** Binding and static quenching behavior of iridium (I) dyes on monodispersed zinc oxide nanocrystals. **T.J. Morin**, D.A. Blank, W.L. Gladfelter, K.R. Mann

INOR **658.** Digestive ripening of gold nanorods in aqueous solution: Effect of CTAB and Au concentration. **P. Guimera Coll**, C.M. Sorensen

INOR **659.** Design and controllable synthesis of Au@MOF Core@Shell Nanotructures. **C. Tian**, S.G. Boyes, A. Worcester

INOR **660.** Studies of CdSe and CdSe/CdS core-shell quantum belts. **Y. Zhou**, F. Wang, Y. Wang, L. Mu, W.E. Buhro

Section I

Colorado Convention Center
Hall C

Inorganic Catalysts

S. A. Koch, *Organizer*

6:00 - 8:00

INOR **661.** Synthesis of palladium diphosphine complexes for XAS analysis. **C.M. Forrest**, C.M. Donahue, A. Blake, S.R. Daly, **B.J. Bellott**

INOR **662.** Transition metal carbides as noble metal fuel cell support materials. **J.M. Thode**

INOR **663.** Synthesis and analysis of heterobimetallic cobalt-zirconium complex for artificial photosynthesis. **S. Chapp**, N. Celia, A. Hill

INOR **664.** Nonheme iron complex-catalyzed efficient alcohol oxidation by *t*-BuOOH with *N*-hydroxyphthalimide as a cocatalyst. **S. Lee**, P. Kim, C. Kim

INOR **665.** Versatile syntheses of optically pure ECE' pincer complexes. **X. Yang**, W. Tay, Y. Li, P.A. Sumod, P. Leung

INOR **666.** Toward inner-sphere photoactivation of carbonyl and imine groups using Earth-abundant Schiff-base photocatalysts. **D.J. Boston**, F.J. Sarabia, M.P. Nguyen, C. Midkiff, E.M. Ferreira, A.K. Rappe, M.P. Shores

INOR **667.** Synthesis, electrochemistry, and catalytic properties of hexacoordinate bis-bipyridylsilicon(IV) complexes. **C. Maguylo**, S. Garofalo, T. Le, T. Huynh, T.A. Schmedake

INOR **668.** Investigation of substituted bidentate polypyridyl vanadium chromophores for photocatalysis. **M.P. Nguyen**, A.K. Rappe, M.P. Shores

Section J

Colorado Convention Center
Hall C

Organometallic Chemistry

New Ligand Platforms

N. S. Radu, *Organizer*

6:00 - 8:00

INOR **669.** Synthesis of dual gunction *ansa*-metallocene ligands via hydrocarbon radical anion coupling of 1,3-diphenyl-6-(alkyl/aryl)fulvenes. M.M. Lai, **G.J. Balaich**, S.T. Iacono

INOR **670.** Novel binuclear pincer ligands for applications in catalysis and energy. **C. Palit**, O. Ozerov

INOR **671.** Probing molecular and electronic structures of conjugated molecular linkers based on linear polyazulenic motifs. **N. Erickson**, A.D. Spaeth, M.V. Barybin

INOR **672.** Efficient synthesis and heterobimetallic complexation of the first aromatic π-linker featuring mercapto and isocyano junctions within the same molecule. **J. Applegate**, N. Gerasimchuk, M.V. Barybin

INOR **673.** Synthesis of ambiphilic nickel-silyl complexes for cooperative small molecule activation. **C.A. Olivares**, M.T. Whited

INOR **674.** E-H bond activation and hydrofunctionalization via bifunctional bis(pyridylimino)isoindolate complexes. **J.B. Geri**, N.K. Szymczak

INOR **675.** Synthesis of ligand platforms for metalloenzyme mimics. **O.M. Crandell**, J.A. Dopke

INOR **676.** Withdrawn.

Section K

Colorado Convention Center
Hall C

Organometallic Chemistry

Synthesis and Characterization

N. S. Radu, *Organizer*

6:00 - 8:00

INOR **677.** Organometallic complexes of 1,6-methano[10]annulene: DFT investigation of dtructure and dynamic behavior. **D.A. Kissounko**, Y.F. Oprunenko, I.P. Gloriozov

INOR **678.** Room temperature carbon-sulfur bond activation by a reactive (dippe) Pd fragment. **L. Munjanja**, W. Brennessel, W.D. Jones

INOR **679.** Synthesis and characterization of ruthenium(II) complexes with hydrosilyl pincer-type ligands. **B.D. Nguyen**, M.T. Whited

INOR **680.** Scope, limitations, and mechanistic aspects of a regioselective acylation of cycloplatinated complexes. **J.S. Carroll**, **H.G. Woolard**, R. Mroz, C.A. Nason, **S. Huo**

INOR **681.** Organosilver scaffolds for small-molecule activation and catalysis. B. Tate, C.M. Wyss, J.P. Sadighi, J.T. Nguyen, J. Bacsa, L. Gelbaum

INOR **682.** Synthesis, structure, and cross-coupling of 2,3,5-tris(4-ferrocenylethynylphenyl)boroxine. **D.A. Kissounko**, V.P. Dyadchenko, V.N. Okulov, M.A. Dyadchenko, A.V. Churakov, L. Wang, D.A. Lemenovskii

INOR **683.** Complexation studies of bipyridine aza-crown macrocycles. **B. Carpenter**, M. Harris

INOR **684.** Synthesis of bis(diorganodithiocarbamato)iron(II) by the thermal decomposition of *cis*-dicarbonylbis(diorganodithiocarbamato)iron(II). **J.E. Coffield**, N.V. Duffy

INOR **685.** Computed structures of cyclic platinum-metal-directed self-assembled complexes. **E.A. Buchanan**, J. Michl

INOR **686.** Dual-metal NHC phenanthroline complexes. **A.J. Landis**, J.O. Hoberg

INOR **687.** Fused siloles for electronic applications. **D.A. Lee**, T.A. Schmedake

INOR **688.** Actinide high-nitrogen chemistry. **K.P. Browne**, D.E. Morris, B.L. Scott, D.E. Chavez, A.T. Nelson, B.C. Tappan, J.L. Kiplinger, J. Veauthier

INOR **689.** New synthetic pathways to $(C_5Me_5)_2ThS_3$. **J.M. Dorhout**, A. Lichtscheidl, N.E. Travia, P.K. Dorhout, B. Scott, K. Czerwinski, J.L. Kiplinger

INOR **690.** Actinide metal fluorides: Synthesis, characterization, and chemistry. **A.G. Lichtscheidl**, M.J. Monreal, K. Browne, D.E. Morris, B. Scott, A. Nelson, J.L. Kiplinger

INOR **691.** Molecular chemistry of thiophene with actinide complexes. **N.E. Travia**, A.W. Pierpont, B.J. Barker, K. Browne, M.J. Monreal, E.R. Batista, J.M. Berg, R.L. Martin, R. Michalczyk, D.E. Morris, B. Scott, M.P. Wilkerson, J.L. Kiplinger

Section K

Colorado Convention Center
Hall C

Soluble Inorganic Semiconductors: Synthesis, Properties, and Applications

R. L. Brutchey, B. M. Cossairt, *Organizers*

6:00 - 8:00

INOR **692.** Low-temperature solution processing of stibnite thin films. **C.L. McCarthy**, R.L. Brutchey

INOR **693.** Synthesis and characterization of metal chalcogenide nanomaterials for potential application in nanoelectronic devices. **A.J. Biacchi**, A.R. Hight Walker

INOR **694.** Colloidal cinnamic acid capped PbSe quantum dots: Solution phase ligand exchange, thin film formation, and electrical conductivity for photovoltaic applications. **D.M. Kroupa**, A. Sellinger, M.C. Beard

INOR **695.** Probing structure-property relationships at the nanoscale: Combined X-ray and spectroscopic methods for the study of colloidal cadmium selenide. **A. Beecher**, P. Chen, Z. Norman, J.S. Owen

INOR **696.** Effect of precursor reactivity on nickel phosphide nanocrystal synthesis. **H. Andaraarachchi**, J. Vela-Becerra

INOR **697.** Rational control over electron-transfer using inorganic cluster-anions directly coordinated to anatase-TiO_2 cores in water. **M. Raula**, I. Weinstock

Section L

Colorado Convention Center
Hall C

Earth-Abundant Materials for Sustainable Hydrogen Production and Storage

Cosponsored by MPPG

C. Ban, A. L. Prieto, Y. Yang, *Organizers*

6:00 - 8:00

INOR **698.** Electrocatalytic and photocatalytic hydrogen evolution using iron phosphide nanoparticles. **J.F. Callejas**, J.M. McEnaney, C.G. Read, R.E. Schaak

INOR **699.** Amorphous MoP and WP nanoparticles as electrocatalysts for the hydrogen evolution reaction. **J. McEnaney**, R.E. Schaak

INOR **700.** Fast kinetics of Ni-doped nanomagnesium for hydrogen storage and the difficulty of effectively comparing material performance in literature. **D.J. Shissler**, M.B. Braun, S.J. Fredrick, A.L. Prieto

INOR **701.** Solution synthesized magnesium nanoparticles: The role of synthesis, particle size, structure, and dopant incorporation on hydrogenation kinetics. **M.B. Braun**, D. Shissler, A.L. Prieto

INOR **702.** Efficient method of cleaning hydrogen sulfide at ambient temperature and pressure for hydrogen storage. X. Li, R. Morrish, C.A. Wolden, **Y. Yang**

Section L

Colorado Convention Center
Hall C

Electrochemistry

B. L. Lucht, *Organizer*

6:00 - 8:00

INOR **703.** Electrochemistry of neodymium in chloride-fluoride melts. D.A. Shuklin, **I.B. Polovov**, M.V. Chernyshov, V.A. Volkovich, O.I. Rebrin

INOR **704.** Functionalization of Si(111) photocathodes: Interplay between steric spacing of molecular linkers and ALD-deposited metal oxide films. **R. Pekarek**, M.J. Rose

INOR **705.** Stable 4 volt electrolytes for high energy electrochemical capacitors. C. Sun, **R.E. Ruther**, F.M. Delnick, J. Nanda

INOR **706.** Patterned electrodeposition of cobalt selenide nanostructure arrays as effective ORR catalysts. **J. Masud**, A. Swesi, M. Nath

Section L

Colorado Convention Center
Hall C

Environmental and Energy-Related Inorganic Chemistry

S. A. Koch, *Organizer*

6:00 - 8:00

INOR **707.** Humidity effects on the methylamine lead iodide perovskite solar cells with TiO_2 mesoporous structure. **F. Zheng**, Y. Ding, Z. Zhu

INOR **708.** Photoelectrochemical characterization of natural semiconducting minerals. **B.K. Durant**, B.A. Parkinson

INOR **709.** Synthesis and characterization of rhenium and manganese electrocatalysts containing diaminophenyl ligands for CO_2 reduction. **B.A. Corbin**, B. Dhakal, D.A. Kurtz, G.S. Nichol, G.A. Felton

INOR **710.** Bioaccumulation of arsenic in the bryophyte *Hygrohypnum ochraceum* in Fountain Creek watershed, Colorado. **J.S. Carsella**, **D.C. Crans**, S.J. Bonetti, D.R. Nimmo, S.J. Herrmann, D. Lehmpuhl

INOR **711.** Protein folding thermodynamics of cytochrome c_{552} from mesophilic and psychrophilic microbes. **N.K. Asous**, **E.A. Benzik**, **J. Chou**, **N. Dalchand**, **G.E. Gallagher**, **G.J. Salerno**, **J.S. Magyar**

INOR **712.** Improved lithium ion transference numbers in electrolytes for lithium-ion batteries with organosilyl and fluorosilyl solvents. **J. Gnirke**, **M.I. Bakhira**, L.J. Lyons

INOR **713.** Ionic conductivity studies of lithium electrolytes with organosilyl and carbonate solvent blends. **V. McGraw**, **N. George**, L.J. Lyons

INOR **714.** Ruthenium incorporated platinum copper nanotubes for electro-oxidation of methanol. **L.E. Mathurin**, J. Chen

INOR **715.** Oxidative cleavage of pyrolytic lignin using transition metal catalysts. **A. Lai**, M.S. Fortin, M.D. Mohadjer Beromi, C. Mullen, A.A. Boateng, N.M. West

INOR **716.** Preparation and applications of carbon interdigitated array electrodes (IDA). **F. Liu**, G. Kolesov, B.A. Parkinson

Section L

Colorado Convention Center
Hall C

Molecular Catalysts for Solar Fuels

Cosponsored by MPPG

A. M. Appel, M. Helm, J. Y. Yang, *Organizers*

6:00 - 8:00

INOR **717.** Withdrawn.

INOR **718.** Developing dirhodium(II,II) complexes that function as single-component photocatalysts for proton reduction to hydrogen. **T.A. White**, S. Witt, L. Zhanyong, K.R. Dunbar, C. Turro

INOR **719.** Pendant base groups in the secondary coordination sphere of pyridinediimine compounds for syngas conversion. **Y. Kwon**, J. Adams, J.D. Gilbertson

INOR **720.** Photocatalytic and photoelectrochemical generation of hydrogen from water Using CdSe quantum dots and CdSe quantum dot-sensitized photocathodes. **P. Ruberu**, A. Das, Y. Dong, R. Eisenberg

INOR **721.** FTIR studies of interactions between carbon dioxide and surface molecular photocatalysts. **M.E. Louis**, T. Fenton, G. Li

INOR **722.** Formamidinate bridged dirhodium complexes as a single component photocatalytic hydrogen evolution system. **S. Witt**, T.A. White, Z. Li, K.R. Dunbar, C. Turro

INOR **723.** Reactivity of pyridinediimine iron (II) complexes. **A. Breuhaus-Alvarez**

INOR **724.** Chemisorption of polycyclic molecules to GaP(111)A functionalized with single layer graphene probed with X-ray photoelectron, Raman, and grazing-angle attenuated total reflectance infrared spectroscopies. **E. Brown**, S. Eady, N. Lehnert, S. Maldonado

INOR **725.** Water oxidation by ruthenium complexes incorporating phosphonate-derivatized polypyridyl ligands. **Y. Xie**, D.J. Szalda, J.J. Concepcion

Section L

Colorado Convention Center
Hall C

Solid-State Inorganic Chemistry

C. G. Lugmair, V. Poltavets, *Organizers*

6:00 - 8:00

INOR **726.** Synthesis of $FeCu_2Sn_2Se_{10}$ via solid state flux methods. Z.T. Gossage, **B.J. Bellott**

INOR **727.** Synthesis, crystal structure and physical properties of $La_3Al_{1-x}Si_xCuQ_7$ (Q = S, Se; $0 < x < 1$). **C. Sturm**, X. Zhao, X. Bu, J. Gu, S. Derakhshan

INOR **728.** Synthesis and characterization of borates. **L.S. Harrower**, **G. Braiotta**, **D. Neiner**, D.M. Schubert

INOR **729.** Synthesis and characterization of rare-earth free phosphors with application to PC-LED lighting. **C. Quilty**, E.C. Sullivan

INOR **730.** Phosphazene superbase-Lewis acids adducts and their frustrated Lewis pair capabilities. **N.A. Johnson**, B.S. Thome, P.O. Wagers, M.J. Panzner, W.J. Youngs, C. Tessier

INOR **731.** Oxygen/chlorine transfer reactions of cyclic chlorophosphazenes using Lewis basic small molecules. **B.S. Thome**, S.R. Snyder, C.A. Tessier

INOR **732.** Chemical delithiation with acid of spinel lithium transition-metal oxides. **S. Therese**, J. Knight, A. Manthiram

INOR **733.** Labile hydrogen: the reactivity of oxyhydrides. **N. Masuda**, O. Hernandez, Y. Tang, S. Hosokawa, C. Tassel, T. Yamamoto, Y. Kobayashi, H. Kageyama

INOR **734.** Energetics of CO_2 adsorption on Mg-Al layered double hydroxides and related mixed metal oxides. **R. Shivaramaiah**, A. Navrotsky

INOR **735.** Anion and mole ratio effects on the coordination modes of an NO_2S_3donor macrocycle. **H. Lee**, I. Park, S. Lee

INOR **736.** Electronic properties of halide perovskites with organic cations. **J.F. Khoury**, P. Woodward

INOR **737.** Synthesis, structure and properties of low-dimensional materials, $PrCu_xTe_2$. **J. Evans**, R.N. McDougald, J. Chan, R.T. Macaluso

INOR **738.** Bulk nanostructured thermoelectric materials with quantum confinement. **V.V. Poltavets**, S.K. Kraemer

WEDNESDAY MORNING

Section A

Colorado Convention Center
Room 105

Coordination Chemistry

Synthesis and Characterization

D. C. Crans, *Organizer*
L. A. Berben, R. G. Hicks, *Presiding*

8:00 INOR **739.** Aluminum complexes of α-diimine ligands: Redox-active aluminum systems. **B.E. Cole**, C.R. Graves

8:20 INOR **740.** Ligand cooperation in the chemistry of small molecules mediated by aluminum complexes. **L.A. Berben**, E.J. Thompson, T.J. Sherbow, K.A. Erickson, C.R. Carr

8:40 INOR **741.** Heterobimetallic cobalt complexes with early transition metals (Ti, V, Cr) and their activation of dinitrogen. **L.J. Clouston**, V. Bernales, L. Gagliardi, C.C. Lu

9:00 INOR **742.** Synthesis, characterization, and catalysis assay of Cr(III) complexes bearing carbene-based NCN pincer ligands. **I. Kobrsi**, M. McDermott

9:20 INOR **743.** Rational design of ligands and synthetic methodologies toward novel oxorhenium(V) complexes with controlled structures and tunable catalytic properties for perchlorate reduction. **J. Liu**, D. Wu, J.R. Shapley, M.M. Abu-Omar, C.J. Werth, T.J. Strathmann

9:40 Intermission.

9:50 INOR **744.** Characterization of molecular cobalt complexes relevant to electrocatalytic CO_2 & H^+ reduction. **D.C. Lacy**, J.C. Peters

10:10 INOR **745.** Synthesis of heteroleptic ruthenium (II) dyes based on novel dibenzo[b,i][1,10]phenanthroline ligands and their characterization for use in dye-sensitized solar cells. **N. Johnson**, M. Nozari, D. Swearer, H. Ji

10:30 INOR **746.** Iron complexes with redox-active and proton responsive ligand for activation of small molecules. **A.V. Polezhaev**, C. Chen, N.S. Labrum, K.G. Caulton

10:50 INOR **747.** Effects of cationic charge and charge proximity in Lewis acid enhanced axial ligation of $[Mo_2]^{4+}$ compounds. B.S. Dolinar, J.F. Berry

11:10 INOR **748.** Highly oxidized graphene nanosheets from the oxidization of detonation carbon. **A. Nepal**, C.M. Sorensen

11:30 INOR **749.** Activation of white phosphorus by low-valent group 5 complexes: Formation and reactivity of *cyclo*-P_4 inverted sandwich compounds. **C. Camp**, L. Maron, R.G. Bergman, J. Arnold

11:50 INOR **750.** Redox chemistry of palladium complexes containing redox-active ligands. Driving on the wrong side of the road? **R.G. Hicks**

Section B

Colorado Convention Center
Room 301

Nanoscience

Cosponsored by PRES

R. M. Richards, *Organizer*
J. R. O'Brien, *Presiding*

8:30 INOR **751.** Jahn-Teller-like distortions in $Au_{25}(SR)_{18}$. **M.A. Tofanelli**, T. Ni, B. Phillips, B. Newell, C.J. Ackerson

8:50 INOR **752.** Effect of surface treatment on nanowire optical and electronic properties. **P. Paudel**, B.G. Barker, P. Kittikhunnatham, A.B. Greytak

9:10 INOR **753.** Surface plasmon interaction studies on hybrid nanoparticles with two plasmonic domains. **S.L. Arrowood**

9:30 INOR **754.** Photofunctional Bis(dipyrrinato) zinc(II) complex nanosheet. R. Sakamoto, **T. Nagayama**, K. Hoshiko, T. Yagi, H. Nishihara

9:50 INOR **755.** Effect of doping on the magnetostructural transition in MnAs nanoparticles: Optimizing properties for magnetic refrigeration. **S.R. Pimmachcharige**, S. Brock

10:10 INOR **756.** Formation and coarsening of Ni metal nanoparticles in 10YSZ measured by SQUID based AC susceptibility. **J.R. O'Brien**, I.E. Reimanis, A. Morrissey

10:30 Intermission.

10:40 INOR **757.** Organized arrays of functional molecules supported by gallium-porphyrin monolayers on HOPG. **W. Lau**, M.D. Hopkins

11:00 INOR **758.** Templated assembly of fullerenes on graphite by gallium–porphyrin monolayers. **J. Kamm**, M.D. Hopkins

11:20 INOR **759.** Multiple energy "exciton-shelves" in quantum-dot-DNA nanobioelectronic materials. **S.M. Goodman**, A. Siu, V. Singh, J.C. Ribot, A. Chatterjee, P. Nagpal

11:40 INOR **760.** Multifunctional magnetic nanomaterials for biomedical applications. **M. Nath**, A. Pariti

12:00 INOR **761.** Sequence-dependent structure/function elucidation of peptide-enabled nanoparticles using a combined experimental/computational approach. **N. Bedford**, R. Naik, M.R. Knecht, H. Heinz, T. Walsh

Section C

Colorado Convention Center
Room 302

Solid-State Inorganic Chemistry

C. G. Lugmair, V. Poltavets, *Organizers*
A. J. Lehner, A. V. Shevelkov, *Presiding*

8:00 INOR **762.** Intricacies of structure and the connection to property: Examples of some functional inorganic materials. **R. Seshadri**

8:40 INOR **763.** Inherent inhomogeneity of superconducting and non-superconducting $A_{1-x}Fe_{2-y}Se_2$ compounds. **A.V. Shevelkov**, M. Roslova, O.I. Lebedev, A.I. Boltalin, I.V. Morozov

9:00 INOR **764.** Synthesis of chromium magnetic semiconductors. **S.L. Stoll**, H. Dalafu

9:20 INOR **765.** First-principles investigation on the magnetic and magnetocaloric properties of MnRhAs. **Y. Zhang**, G.J. Miller

9:40 INOR **766.** Low temperature hydrothermal routes to transition metal phyllosilicates for grid level energy storage. S. Zhou, D. Smith, K. Nolan, **B.C. Melot**

10:00 Intermission.

10:15 INOR **767.** Pressure-induced Eu mixed valence and interplay between localized (4f) and itinerant (3d) ferromagnetism in $EuCo_2As_2$. X. Tan, D. Haskel, G. Fabbris, A. Yaroslavtsev, H. Cao, **M. Shatruk**

10:35 INOR **768.** Preparation of zirconium phosphate based hexagonal prisms. **J. Yu**, L. Sun

10:55 INOR **769.** Conflict management: Lessons from intermetallic chemistry. **S. Ponou**, G.J. Miller

11:15 INOR **770.** Preparation, crystal chemistry, optical properties, and electronic structure of complex metal halides related to perovskite. **A.J. Lehner,** E.E. Perry, C.A. Hebert, H. Wang, M.L. Chabinyc, R. Seshadri

11:35 INOR **771.** Antimony based copper sulfide ternaries as candidate thin film photovoltaic absorber materials. **A. Welch**, P. Zawadzki, S. Lany, C.A. Wolden, A. Zakutayev

11:55 Concluding Remarks.

Section D

Colorado Convention Center
Room 303

Organometallic Chemistry

Catalysis

N. S. Radu, *Organizer*
A. Poater, J. T. York, *Presiding*

9:00 INOR **772.** Metal-organic frameworks enabling base metal catalysis. **T. Zhang**, W. Lin, K. Manna, C.W. Abney, M. Carboni

9:20 INOR **773.** Postsynthetic metalation of bipyridylic containing metal–organic frameworks for highly efficient catalytic organic transformations. **K. Manna**, W. Lin, T. Zhang

9:40 INOR **774.** Comparing Ru and first row transition metal-catalyzed olefin metathesis. **A. Poater**

10:00 INOR **775.** Structure and activity in cyclometallated Ru-based *Z*-selective metathesis catalysts. **B. Quigley**, D.J. OLeary, R.H. Grubbs

10:20 INOR **776.** Theory-assisted design of Z-selective olefin metathesis catalysts. G. Occhipinti, V. Koudriavtsev, K.W. Törnroos, **V.R. Jensen**

10:40 INOR **777.** Efficient olefin epoxidation with an iron-NHC-carbene complex. **J.W. Kuck**, M.R. Anneser, S. Haslinger, A. Pothig, M. Cokoja, F.E. Kuehn

11:00 INOR **778.** Electronic fine tuning of an iron(II) N-heterocyclic carbene complex. **S. Haslinger**, J.W. Kuck, E.M. Hahn, D.T. Weiss, A. Pothig, M. Cokoja, J. Basset, F.E. Kuehn

11:20 INOR **779.** Gold(I)-alkene bonding interactions in complexes with N-heterocyclic carbene ligands: Insight gained from computational investigations. **J.T. York**

11:40 INOR **780.** Synthesis and reactivity of a Cp*Co(NHC) complex. J. Andjaba, **C.A. Bradley**

Section E

Colorado Convention Center
Room 201

Organometallic Chemistry

Synthesis and Characterization

N. S. Radu, *Organizer*
B. Boardman, L. P. Spencer, *Presiding*

8:30 INOR **781.** Transition metal carbonyl complexes with new pyridine/thione ligands for the reduction of CO_2. C. Oian, D. Rabinovich

8:50 INOR **782.** Comparative reactivity of CO_2 with transition metal alkyls. **K. Lau**, B.J. Petro, R.F. Jordan

9:10 INOR **783.** Osmium(II) σ-methane complex: Isotopic analysis reveals the methane binding mode. **P.J. Sempsrott**, C.E. Flener-Lovitt, **G.S. Girolami**

9:30 INOR **784.** Homogeneous energy transfer between Ruthenium(II) bis-(2,2'-bipyridyl) (5,5'-dicarboxy-2,2'-bipyridyl) metal centers doped into a zirconium(IV)-based metal-organic framework and its application as a DSSC. **W.A. Maza**, A.J. Haring, S.R. Ahrenholtz, C.C. Epley, C.S. Day, A.J. Morris

9:50 INOR **785.** Synthesis of organometallic C0-releasing molecules (CORMs) in the absence of a bulk organic solvent. J. Wong, N. Macdonald, C. Mottillo, I. Hiskic, **I.S. Butler**, T. Friscic

10:10 INOR **786.** Structural and reactivity trends of heterobimetallic complexes featuring direct Cu-M bonds (M=Cr, Mn, Co, Mo, Ru, W, Re). **M.K. Karunananda**, S. Banerjee, S. Bagherzadeh, U. Jayarathne, S.R. Parmelee, G.W. Waldhart, N.P. Mankad

10:30 INOR **787.** Withdrawn.

10:50 INOR **788.** Synthesis and photophysical properties of novel Platinum(II) acetylide complexes. **R. Winkel**, K.S. Schanze

11:10 INOR **789.** Synthesis and characterization of phosphorescent complexes containing corannulene. **J.W. Facendola**, M. Seifrid, P.I. Djurovich, J.S. Siegel, M. Thompson

Section F

Colorado Convention Center
Room 304

Interactions of Metal Complexes with Proteins or Nucleic Acids

J. R. Morrow, C. Turro, *Organizers*
J. J. Kodanko, *Presiding*

8:30 INOR **790.** Tunable dirhodium complexes for photochemotherapy: Enhanced production of singlet oxygen and oxygen-independent activity toward cancer cells. **K.R. Dunbar**, C. Turro

9:00 INOR **791.** Unusual modifications of protein and DNA targets by precious metal photoactivated and organometallic anticancer agents. C. Wootton, P.B. O'Connor, **P.J. Sadler**

9:30 INOR **792.** Exploring the nucleic acid and protein interactions of cytotoxic ruthenium complexes. **P.C. Glazer**

10:00 Intermission.

10:15 INOR **793.** Development of rhodium metalloinsertors as chemotherapeutic agents. **A. Komor**, J.K. Barton

10:45 INOR **794.** Photoinduced dual-binding by dirhodium (II,II) complexes with DNA. **A.M. Palmer**, J.D. Knoll, C. Turro

11:15 INOR **795.** Self-assembly of multimetallic complexes featuring coordination of hexacoordinate Fe^{2+} or Co^{2+} to aminoethylglycine derivatized $Ru(bpy)_3^{2+}$ with pendant bipyridines. **S. Sun**, C.P. Myers, M. Williams

‡ *Cooperative Cosponsorship*

Section G

Colorado Convention Center
Room 401

ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry: Symposium in Honor of Kim R. Dunbar

Cosponsored by WCC

C. P. Berlinguette, D. J. Mindiola, E. J. Schelter, *Organizers*
M. Shatruk, *Organizer, Presiding*

8:30 INOR **796.** Further adventures with heterometallic rings. **R.E. Winpenny**

8:50 INOR **797.** Looking for photomagnetic single molecule magnets. **C. Mathoniere**, R. Clerac

9:10 INOR **798.** Power of the coordination cluster in modern inorganic chemistry. **A.K. Powell**

9:30 INOR **799.** Indigo coordination and color chemistry: New ligands, new complexes, and new materials from a very, very old dog. **R.G. Hicks**

9:50 Intermission.

10:05 INOR **800.** Functional MOFs toward the synergistic control of electrons, spins, structures, and chemical interactions. **H. Miyasaka**

10:25 INOR **801.** Optical and magnetic molecular switches. **R. Clerac**, C. Mathoniere, I. Jeon, E. Koumousi, D. Li, P. Dechambenoit

10:45 INOR **802.** Frontier of quantum molecular spintronics based on single-molecule magnets. **M. Yamashita**

11:05 INOR **803.** Developing rational design principles for the synthesis of qubits. J. Zadrozny, M. Graham, M. Fataftah, S. Coste, **D.E. Freedman**

11:25 INOR **804.** High-field electron paramagnetic resonance determination of the magnetic anisotropy in pseudo-octahedral mononuclear VIII complexes. K. Thirunavukkuarasu, M.R. Saber, M. Atanasov, F. Neese, **S. Hill**, K.R. Dunbar

Section H

Colorado Convention Center
Room 203

Coordination Chemistry

Characterization and Applications

D. C. Crans, *Organizer*
S. S. Massoud, E. Norkus, *Presiding*

8:30 INOR **805.** Hexacoordinate silicon complexes as cathodic colorants. **D.M. Peloquin**, D. Dewitt, T. Lamb, S. Patel, T.A. Schmedake

8:50 INOR **806.** Trojan horse and Achilles heel: Can coordination complexes of Ga3+ and Cu2+ fight bacterial resistance, or is it Greek mythology? **K.D. Mjos**, C. Orvig

9:10 INOR **807.** Cobalt(II) complexes as efficient artificial nucleases for hydrolytic cleavage of DNA. **S.S. Massoud**, F. Louka, R. Perkins, F.A. Mautner, H. Terenzi

9:30 INOR **808.** Redox properties of hemoglobins, engineered hemoglobins and hemoglobin-protein assemblies: A spectroelectrochemistry study. **R. Kreulen**, S. Bannerjee, R. Bangle, C.J. Parker Siburt, A.L. Crumbliss

9:50 INOR **809.** Design and synthesis of novel octacarboxy porphyrin based metal-organic frameworks and photocatalytic applications. **J. Johnson**, X. Zhang, J. Zhang

10:10 INOR **810.** Giant magnetic anisotropy in mononuclear cobalt(II) complexes with trigonal antiprism geometry. **Y. Zhang**, A. Brown, K.R. Dunbar

10:30 INOR **811.** Controlling magnetic properties of bistable spin-crossover and valence tautomeric metal complexes at room temperature. **M.M. Khusniyarov**, A. Witt, M. Milek

10:50 INOR **812.** Guest modulated magnetic ordering in TCNQ-based metal-organic frameworks. **X. Zhang**, M.R. Saber, A. Prosvirin, L. Sun, J. Reibenspies, K.R. Dunbar

11:10 INOR **813.** Fluorescence of a gold(I) complex with a stable fluorescent organic radical ligand. **Y. Hattori**, T. Kusamoto, H. Nishihara

11:30 INOR **814.** Equilibria in alkaline formaldehyde-containing electroless copper plating solutions. **E. Norkus**

Section I

Colorado Convention Center
Room 205

Molecular Catalysts for Solar Fuels

Cosponsored by MPPG

A. M. Appel, M. Helm, J. Y. Yang, *Organizers, Presiding*

8:30 INOR **815.** Electrocatalytic oxygen reduction with soluble mediators. **S.S. Stahl**, J.B. Gerken, C. Anson, Y. Wang

9:00 INOR **816.** Studies of electrocatalytic dioxygen reduction. **J.M. Mayer,** M.L. Pegis, B.A. McKeown, D.J. Wasylenko, C. Rodriguez, M. Rigsby, S. Raugei, E.A. Mader, C.T. Carver, B.D. Matson

9:30 INOR **817.** Perfluoropinacolate complexes in water and their electrochemistry. S.F. Hannigan, J.L. Steele, **L.H. Doerrer**

10:00 INOR **818.** Metal-oxo and metal-hydroxo species in biology. **A. Borovik**

10:30 Intermission.

10:45 INOR **819.** Water-oxidation catalysis for solar fuel production. **G.W. Brudvig**, V.S. Batista, R.H. Crabtree, C.A. Schmuttenmaer

11:15 INOR **820.** Molecular catalysts for homogeneous and heterogeneous water oxidation catalysis. **J.J. Concepcion**, D.W. Shaffer, Y. Xie, D.J. Szalda, J.T. Muckerman, E. Fujita

11:45 INOR **821.** Integrated catalyst-electrodes for the production of solar fuels. **J.D. Blakemore**, A. Gupta, B.S. Brunschwig, **H.B. Gray**

Section J

Colorado Convention Center
Room 402

Nanoscience

Semiconductors

Cosponsored by PRES

R. M. Richards, *Organizer*
R. Beaulac, E. Miller, *Presiding*

9:00 INOR **822.** Dye-sensitized solar cells using nanostructured p-type cuprous oxide. **K. Haynes**, W. Youngblood

9:20 INOR **823.** Thiols in nanocrystal synthesis: Capping ligands that are more than skin deep. **M.J. Turo**, J.E. Macdonald

9:40 INOR **824.** Transport properties of sulfide-capped $CZTS_xSe^{(1-x)}$ nanoparticle films made from a one pot solution based synthesis. **M.B. Braun**, L. Korala, A.L. Prieto

10:00 Intermission.

10:15 INOR **825.** Effect of ligand binding group on excited state electron transfer to ZnO nanocrystals. **A.N. Oehrlein**, A. Sánchez-Díaz, T.M. Pappenfus, K.R. Mann, D.A. Blank, W.L. Gladfelter

10:35 INOR **826.** Photoelectron and inverse photoelectron spectroscopy of PbS quantum dots. **E. Miller**, D. Kroupa, R. Crisp, A. Marshall, J. Zhang, P. Schulz, A. Kahn, J. Luther, M.C. Beard, c. perkins, j. van de Lagemaat

10:55 INOR **827.** New approach to the synthesis of quantum confined indium nitride colloidal nanoparticles. **R. Beaulac**, B. Chakraborty, Z. Liu

WEDNESDAY AFTERNOON

Section A

Colorado Convention Center
Room 105

Chemistry of Materials

Materials Synthesis and Properties

C. G. Lugmair, *Organizer*
E. G. Gillan, C. Lampropoulos, *Presiding*

1:30 INOR **828.** Conductivity tuning of the ITO sol-gel materials by thermal program modification and adjusting the tin oxide concentration. **R. Baghi**

1:50 INOR **829.** Synthesis and characterization of energetic cations based on 1,1-diamino-2,2-dinitroethene (FOX-7) and 1-amino-1-hydrazino-2,2-dinitroethene (HFOX). **T.T. Vo**, J.M. Shreeve

2:10 INOR **830.** Recent developments in the facile synthesis of phosphorus-rich metal phosphides and metal thiophosphates via PCl_3 elimination. E.**G. Gillan**, N. Coleman, Jr.

2:30 INOR **831.** One-minute synthesis of crystalline microporous aluminophosphate $AlPO_4$-5. **Z. Liu**, T. Wakihara, D. Nishioka, K. Oshima, T. Takewaki, T. Okubo

2:50 INOR **832.** Synthesis, characterization, and application of mixed metal vanadium oxyhydroxides. **A.A. Alothman**, A.W. Apblett

3:10 INOR **833.** Synthesis and reactivity of only Lewis base stabilized pnictogenylboranes. **C. Marquardt**, M. Scheer

3:30 INOR **834.** Introducing dimensionality in single-molecule magnets. **C. Lampropoulos**, J.M. Cain, S. Corrales, N. Mhesn, A.M. Mowson, C. Papatriantafyllopoulou, A. Ozarowski, J.S. Kinyon, N. Dalal, G. Christou, A. Tasiopoulos

3:50 INOR **835.** Ternary synthesis of colloidal Zn_3P_2 quantum dots. **B.A. Glassy**, B.M. Cossairt

4:10 INOR **836.** Origin and tuning of chirality in quantum dots. **M. Balaz**, U.N. Tohgha, L. Pap, J. Choi, J. Kubelka, K. Varga

4:30 INOR **837.** Structural origins of optoelectronic properties in quantum dots: Studies of atomically precise cadmium selenide. **A. Beecher**, J.S. Owen

Section B

Colorado Convention Center
Room 301

Nanoscience

Metals

Cosponsored by PRES

R. M. Richards, *Organizer*
S. M. Humphrey, M. A. Mahmoud, *Presiding*

1:30 INOR **838.** Facile technique to break the symmetry of the growth of silver nanocrystals into silver nanoplates. **M.A. Mahmoud**

1:50 INOR **839.** Extended surface staple motifs in thiolate-protected Au_{23} and Au_{24} nanoclusters: Implications for nano-gold catalysis. **A. Das**, R. Jin

2:10 INOR **840.** Robust organometallic gold nanoparticles. A.A. Mohamed, S. Orefuwa, **J.B. King**

2:30 INOR **841.** Dynamic assemblies of gold nanoclusters enabled by surface modifications. **W.S. Compel**, O. Wong, X. Chen, C. Yi, H. Hakkinen, K.L. Knappenberger, C.J. Ackerson

2:50 INOR **842.** Microwave synthesis of unusual noble metal nanoparticle catalysts: Immiscible alloys and core-shell structures. **S.M. Humphrey**, G. Henkelman, S. Garcia, L. Zhang, P. Kunal, G.W. Piburn, L. Polanco

3:10 Intermission.

3:20 INOR **843.** Nanoparticle synthesis using switchable ionic liquids. **D. Lao**, B. Liu, X. Hua, M. Olszta, R. Kukkadapu, X. Yu, D.J. Heldebrant, S.K. Nune

3:40 INOR **844.** Synthesis and analysis of PdPt nanoalloys via alloying individual bulk Pd and Pt metals in molten lithium for methanol electro-oxidation applications. **H. Barkholtz**, T. Xu

4:00 INOR **845.** Anionic element reagent complexes: A generic reagent platform for nanoparticle synthesis. **M.P. Rowe**, R. Desautels, E. Skoropata, N. Singh, Y. Wroczynskyj, J. van Lierop

4:20 INOR **846.** Single-source molecular precursor route to metal phosphide nanoparticles and their evaluation as deoxygenation catalysts. **F.G. Baddour,** S.E. Habas, D.A. Ruddy, M. Pan, C.P. Nash, J. Wang, J.E. Hensley, J.A. Schaidle

4:40 INOR **847.** Physical and chemical synthesis of metal nitride catalysts. **S. Gage**, G. Leong, S. Agarwal, R.M. Richards

5:00 INOR **848.** Metal and metal carbide nanoparticles' synthesis using EEW. **E. Abdelkader**, S.W. Buckner, P.A. Jelliss

Section C

Colorado Convention Center
Room 302

Lanthanide and Actinide Chemistry

A. De Bettencourt Dias, *Organizer*
D. T. de Lill, D. A. Penchoff, *Presiding*

1:30 INOR **849.** Recycling of the nationally critical element erbium: Electrochemical reduction of erbium coordination compounds in ionic liquids. **R.F. Hess**, T.J. Boyle, T.N. Lambert, S. Limmer, D. Kammler, L.J. Small, J. Sears, A. Cook, M. Brumbach

1:50 INOR **850.** Theoretical studies of binding preferences in separations of lanthanides and actinides. **D.A. Penchoff**, G.K. Schweitzer, R.J. Harrison

2:10 INOR **851.** Plasmon-enhanced energy transfer and other photophysical effects in doped-lanthanide nanocrystals. **Q. Sun**, Y. Ding, V. Singh, P. Nagpal

2:30 INOR **852.** Sensitization of lanthanide luminescence via ligand-capped zinc sulfide quantum dots. **R.A. Tigaa**, G. Lucas, A. De Bettencourt Dias

2:50 Intermission.

3:00 INOR **853.** Physical properties of rare-earth complexes in the +2 oxidation state. M. Fieser, **J.W. Ziller**, W.J. Evans

3:20 INOR **854.** Coordination chemistry of lanthanide and actinide complexes with mixed O- and N-donor ligand scaffolds. **J.L. Brown-McDonald**, A. Gaunt

3:40 INOR **855.** Implications for strong inverse trans influence stabilization in the chemistry of uranium nitrogen multiple bonds. **K.C. Mullane**, A. Lewis, E.J. Schelter

4:00 Intermission.

4:10 INOR **856.** Investigating sensitized luminescence in lanthanide coordination polymers. **D.T. de Lill**

Section D

Colorado Convention Center
Room 303

Organometallic Chemistry

Catalysis

N. S. Radu, *Organizer*
P. J. Walsh, X. Wang, *Presiding*

1:30 INOR **857.** Arylation of weakly acidic C–H's with heterobimetallic catalysts. **P.J. Walsh**

1:50 INOR **858.** Addressing high barriers in base metal CH functionalization: Impact of non-innocent ancillary ligands. **A.J. Nett**, P.M. Zimmerman, J. Montgomery

2:10 INOR **859.** Mechanism of a ligand-promoted C(sp3)–H activation and arylation reaction via palladium catalysis: Theoretical demonstration of a Pd(II)/Pd(IV) redox manifold. **X. Wang**, Y. Dang, J.W. Nelson, H.D. Pham, Z. Wang

2:30 INOR **860.** Withdrawn.

2:50 INOR **861.** C-H activation and subsequent chemistry of alkyl tungsten and heteroatom-containing alkyl tungsten complexes initiated by $Cp^*W(NO)(CH_2CMe_3)(\eta^3\text{-}CH_2CHCHPh)$. **R.J. Wakeham**, P. Legzdins

3:10 INOR **862.** C-H functionalization of hydrocarbons and formation of new C-C bonds initiated by Cp*W(NO)(alkyl)(η3-allyl) and Cp*W(NO)(H)(η3-allyl) complexes. **R.A. Baillie**, P. Legzdins

3:30 INOR **863.** Direct *Csp2-Csp3* cross-coupling of diarylzinc reagents with 1°, 2° and 3° alkylhalides. **J.J. Dunsford**, M. Ingleson

3:50 INOR **864.** Chelating σ-aryl post-metallocenes: Unusual reaction pathways and synthetic models of weak attractive ligand–polymer interactions. **M. Chan**, C. Liu

4:10 INOR **865.** Well-defined boralumoxanes as convenient MAO modelling compounds. **H. Zijlstra**, S. Harder

4:30 INOR **866.** Exploring titanium biphenylphenol catalysts for ethylene-octene polymerization processes. **L.P. Spencer**, N. Aboelella, J. Klosin, P. Fontaine

TECHNICAL PROGRAM

Section E

Colorado Convention Center
Room 201

Inorganic Catalysts

S. A. Koch, *Organizer*
A. K. Vannucci, *Presiding*

1:30 INOR **867.** "Innocent" role of Sc^{3+} on a non-heme Fe catalyst in an O_2 environment. **A. Poater**, S. Chaitanya Vummaleti, L. Cavallo

1:50 INOR **868.** Electrocatalytic reductive carbon-carbon cross coupling using well defined Ni catalysts. **A.K. Vannucci**

2:10 INOR **869.** Characterization of BiOX compounds as photocatalysts for the degradation of pharmaceuticals in water. **J.C. Ahern**, R. Fairchild, J. Thomas, J. Carr, H.H. Patterson

2:30 INOR **870.** Molybdenum complexes for effecting organophosphate hydrolysis. **L.Y. Kuo**, Y. Shari'ati

2:50 INOR **871.** Chiral pincer complexes: A study on the influence of catalyst design in an asymmetric P-H bond addition reaction. **W. Tay**, X. Yang, Y. Li, P.A. Sumod, P. Leung

3:10 Intermission.

3:20 INOR **872.** Incorporation of Lewis acidic or Lewis basic group in the secondary coordination sphere of metal complexes for the modulation of C-H bond formation and cleavage. **Z. Thammavongsy**

3:40 INOR **873.** Electronic tuning of H2 production catalyzed by Co complexes with pentadentate ligands. **X. Zhao**, M. Vennampalli, G. liang, L. Katta, C.E. Webster

4:00 INOR **874.** Rigid tetraphenylelement linker scaffolds for immobilizing catalysts on oxide supports. **E.M. Steffensmeier**, J.H. Baker, B. Beele, J. Bluemel

4:20 INOR **875.** Active catalysts for oxygen containing substrates: Actinide coordination complexes. **I. Karmel**, N. Fridman, T. Bannenberg, M. Tamm, M. Eisen

Section F

Colorado Convention Center
Room 304

Organometallic Chemistry

New Ligand Platforms

N. S. Radu, *Organizer*
M. V. Barybin, D. V. Peryshkov, *Presiding*

1:30 INOR **876.** New developments in the chemistry of low-valent organometallics featuring linear azulenic π-linkers. **M.V. Barybin**

1:50 INOR **877.** Flexible coordination of PC=CP ligands to late transition metals. **B. Barrett**, V.M. Iluc

2:10 INOR **878.** Proton-switchable nitrile hydroboration by a rationally designed bifunctional ruthenium complex. **J.B. Geri**, N.K. Szymczak

2:30 INOR **879.** New pyrrole-based PNP pincer complexes with late transition metals. **J.A. Kessler**, V.M. Iluc

2:50 INOR **880.** Carborane clusters in metal-ligand cooperative substrate activation. **D.V. Peryshkov**, B.J. Eleazer

3:10 INOR **881.** Synthesis, reactivity, and catalystic behavior of heterobimetallic cooperative complexes based on a β-oxo-δ-diiminate ligand. **H. Chiu**, I.A. Tonks

3:30 INOR **882.** Flexible, open chain tetracarbene ligands: Diversity in structural motifs depending on ligand structure and metal center. **D.T. Weiss**, S. Haslinger, C. Jandl, A. Pothig, M. Cokoja, J.M. Basset, F.E. Kuehn

3:50 INOR **883.** Withdrawn.

4:10 INOR **884.** Synthesis, structure, and reactivity of bis(oxazoline)-substituted cyclopentadienyl and fluorenyl rhodium and iridium complexes. **B. Schmidt**, A.D. Sadow

4:30 INOR **885.** Development of new ligands for $[M'(CO)_3]^+$ (M= Re, ^{99m}Tc) complexes with enhanced chemical properties and stability. **T.R. Hayes**, P.A. Lyon, C.L. Barnes, S.L. Trabue, P.D. Benny

4:50 INOR **886.** Hydrogen bonding behavior of amide-functionalized α-diimine palladium complexes. **F. Zhai**, R.F. Jordan

Section G

Colorado Convention Center
Room 401

Environmental and Energy-Related Inorganic Chemistry

S. A. Koch, *Organizer*
M. Emmert, *Presiding*

1:30 INOR **887.** Photocatalytic CO_2 reduction from organic/inorganic hybrid system. S.O. Kang, H. Son, D. Won

1:50 INOR **888.** Water splitting with Prussian blue-type catalysts. **J. Galan-Mascaros**, B. Rodríguez-García

2:10 INOR **889.** Fixation of carbon dioxide to oxalate and carbonate by copper complexes. **U.R. Pokharel**, F.R. Fronczek, A.W. Maverick

2:30 INOR **890.** Mechanism of the doped hercynite cycle for solar thermal water splitting. **C. Muhich**, K. Weston, D. Arifin, A.H. McDaniel, E.N. Coker, B. Ehrhart, V. Witte, A.W. Weimer, C. Musgrave

2:50 Intermission.

3:00 INOR **891.** Peroxo-based oxygen-rich compounds for potential use as new high energy-dense oxidizers. **N.H. Gamage**, B. Stiasny, J. Stierstorfer, P.D. Martin, T.M. Klapötke, C.H. Winter

3:20 INOR **892.** Plasmonic behavior of copper iron sulfide nanoparticles. **K. Plass**, N.J. Freymeyer, C. Kim, C.J. Wisdo, Z. Georgieva

3:40 INOR **893.** Combining separation science and synchrotron X-ray fluorescence for fuels. **L.A. Finney**, S. Vogt, R.E. Winans

4:00 INOR **894.** A *p*-$GaInP_2$ photoelectrode for water reduction stabilized with TiO_2 and a molecular cobalt catalyst. **J. Gu**, Y. Yan, J. Young, N.R. Neale, J.A. Turner

4:20 INOR **895.** Sustainable methods for rare earth recycling: Chemical perspectives on critical materials. **M. Emmert**

4:40 INOR **1058.** Consequences of chloromethane (R40) mixed in with tetrafluoroethane (R134a); production of trimethylaluminum, reactivity of TMA and various refrigerant oils and methods to deactivate trimethylaluminum. **R.L. Luck**, Z. Chen, J.M. Marciniok, A.W. Schultz

Section H

Colorado Convention Center
Room 203

Electrochemistry

B. L. Lucht, *Organizer*
N. Bedford, *Presiding*

1:30 INOR **896.** Perfluoroalkyl-fluorophosphate anions for high voltage electrolytes in lithium cells: A DFT study. **S. Brutti**, **R. Spezia**, M. Carboni

1:50 INOR **897.** Bromine-free quinone flow battery chemistries. **M.P. Marshak**, M.J. Aziz, R.G. Gordon

2:10 INOR **898.** Non-platinum group metal bimetallic electrocatalyst for alternative fuel oxidation and ammonia production. **N. Bedford**, L.F. Greenlee, A.M. Herring

2:30 INOR **899.** Hemi-cage 5,5' substituted cobalt bipyridine complexes for use as dye sensitized solar cell mediators. **J.D. Thomas**, C.M. Elliott, A.L. Prieto

2:50 INOR **900.** Photoelectrochemical properties of p-type GaP(111)A after deliberate surface chemisorption. **E. Brown**, S. Maldonado

3:10 INOR **901.** Hybrid molecular/materials passivation of *p*-silicon(111) photocathodes: Band-edge modulation with organic surface linkers and thin film $Al2O_3$ or TiO_2. **M.J. Rose**, H. Kim, J. Seo, L. Le

Section I

Colorado Convention Center
Room 205

Organometallic Chemistry

Applications to Materials and Polymer Science

N. S. Radu, *Organizer*
B. Boardman, R. Wright, *Presiding*

1:30 INOR **902.** Influence of π-π Stacking, π-cation interactions and axial steric blockage on the ethylene polymerization behavior of asymmetric hosphine-sulfonate palladium methyl complexes. **G. Feng**, J.J. Defoe, R.F. Jordan

1:50 INOR **903.** Cobalamin-fluorophore based photoinitiators for hydrogel curing with tissue penetrating light. **Z. Rodgers**, R.M. Hughes, L. Doherty, J.R. Shell, B. Molesky, A. Brugh, A.M. Moran, M.D. Forbes, D.S. Lawrence

2:10 INOR **904.** Synthesis and characterization of chiral C_2-symmetric bimetallic zinc complexes of amido-oxazolinates: Active initiators for asymmetric copolymerization of CO_2 and cyclohexene Ooide. S. Abbina, **V.K. Chidara**, S. Bian, G. Du

2:30 INOR **905.** Hydrophilic polycarbonates derived from coupling of cyclohexadiene and CO_2 utilizing metal salen catalysts. **W. Chung**, D.J. Darensbourg

2:50 INOR **906.** Withdrawn.

3:10 INOR **907.** In situ tacticity control in lactide polymerization reactions. **J. Byers**, C.M. Manna, L. Yablon

3:30 INOR **908.** Synthesis, characterization, and the applications of novel zinc alkyl complexes for polylactide synthesis. **O. Falola**, J.S. Matthews

3:50 INOR **909.** Synthesis, characterization, and investigation of cobalt chalcogenide clusters with thienyl phosphine ligands as new acceptor materials for P3HT. **B.M. Boardman**, B.J. Reeves, D.M. Shircliff, J.L. Shott

4:10 INOR **910.** Formation of stoichiometric GaAs from thin films of $[t$Bu(H)$AsGaEt_2]_2$: Mechanistic studies and isolation of the novel cluster $\{[t$Bu(H)$AsGaEt_2]_3[t$BuAsGaEt$]_2\}$. **R. Wright**, A. Sokolov, G. Athens, A. Krasovskiy, R. Froese, L. Spencer, B. Gerhart, P.N. Nickias, J.C. Stevens

4:30 INOR **911.** Synthesis of unprecedented solution-stable metal organic oligomers via iClick and Au-Au bond formation. **X. Yang**, A. Powers, I. Ghiviriga, K.A. Abboud, A.S. Veige

4:50 INOR **912.** Solvent control of surface plasmon mediated chemical deposition of Au nanoparticles from phosphorus based organo-gold precursors. **C. Muhich**, J. Qiu, A. Holder, W. Wei, L. McElwee-White, C. Musgrave

Section J

Colorado Convention Center
Room 402

Inorganic Spectroscopy

S. A. Koch, *Organizer*
S. R. Daly, *Presiding*

1:30 INOR **913.** Photoluminescence decay dynamics of white light emitting ultrasmall cadmium selenide nanocrystals: Mechanistic insights to foster the development of an energy-efficient solid state sunlight-mimicking device. **N. Orfield**, J. Keene, T. Frecker, L.M. Davis, S.J. Rosenthal

1:50 INOR **914.** Impact of structure on metal-ligand covalency in late transition metal complexes: Do variations in diphosphine bite angle matter? **S.R. Daly**, C. Donahue, A. Blake, B.J. Bellott, C.M. Forrest, J.M. Keith, S. McCollom

2:10 INOR **915.** Fluorescent d10 metal complexes for the presumptive identification of substances of abuse and the implementation of a cell phone fluorimeter for field identification. **D.J. Nash**, R.G. Blair

2:30 INOR **916.** High temperature X-ray absorption spectroscopic investigation of $Sr_2Fe_{1.5}Mo_{0.5}O_{6-\delta}$ solid oxide fuel cell electrodes. B.C. Eigenbrodt, T. Sultana, A. D'Orazio, T. Marshall, J. Gerardi, C.U. Segre

2:50 INOR **917.** Measurement of the activation energies of exciton migration in ruthenium(II) and rhodium(III) polypyridyl and phenanthroline complexes via luminescence at cryogenic temperatures. **J.W. Kenney**, J. Macwillie, p. weaver, R. Ramos, N. Nunez, G.A. Crosby

3:10 INOR **918.** Variable-temperature multinuclear NMR spectra of the $[Mn_{12}O1_2(O_2CR)_{16}(H_2O)_4]$ family of single-molecule magnets in solution. **A. Fournet**, K.A. Abboud, G. Christou

3:30 Intermission.

3:40 INOR **919.** Iron(II) and cobalt (II) paraCEST MRI contrast agents responsive to pH and redox environment. **P.B. Tsitovich**, J.R. Morrow

4:00 INOR **920.** Optical properties of Ag nanocrystals self-assembled in thin 3D crystalline superlattices. J. Wei, N. Schaeffer, **M. Pileni**

4:20 INOR **921.** Investigation of valence tautomerism in cobalt-dioxolene vomplexes using K X-ray emission spectroscopy. **W. Liang**, D. Nordlund, T. Weng, D. Sokaras, C.G. Pierpont, K. Gaffney

4:40 INOR **922.** Bromine atom formation by visible light driven bromide oxidation with a Ru polypyridyl compound. **G. Li**, G.J. Meyer

5:00 INOR **923.** *d*- and *f*-Orbital mixing in open-shell systems. **S.E. Stieber**, E.R. Batista, D.L. Clark, M.W. Löble, R.L. Martin, S.G. Minasian, J.A. Trujillo, S.A. Kozimor

5:20 INOR **924.** Surface and bulk characteristics of Zn/Ni substituted cobalt oxide spinel p-type semiconductors. **C.C. Mercado**, C.L. Donley, C. Flynn, A. Zakutayev, K. Zhu, J. Cahoon, A.J. Nozik

THURSDAY MORNING

Section A

Colorado Convention Center
Room 105

Bioinorganic Chemistry

S. A. Koch, *Organizer*
K. E. Splan, *Presiding*

8:00 INOR **925.** Interaction of amino-acids with ferredoxin-like centers in a designed metallopeptid. **J. Schmitt**, J.M. Shearer

8:20 INOR **926.** DNA-mediated signaling by the *E. coli* helicase, DinG. **M.A. Grodick**, T.J. Zwang, J.K. Barton

8:40 INOR **927.** Ferromagnetically coupled (S = 1) peroxodicopper(II) complex. N. Kindermann, S. Dechert, S. Demeshko, E.J. Reijerse, E. Bill, **F. Meyer**

9:00 INOR **928.** Spectroscopic characterization of Cu(I) binding at the BIR2 domain of the X-linked Inhibitor of apoptosis protein. **K.E. Splan**, Y. Liang

9:20 INOR **929.** Label-free electrochemical detection of human methyltransferase from tumors. **A.L. Furst**, N. Muren, M.G. Hill, J.K. Barton

9:40 Intermission.

9:50 INOR **930.** Ru(II) complex-antibody conjugation for targeted photochemotherapy. **J.D. Knoll**, C. Turro

10:10 INOR **931.** Arming anticancer platinum(IV) complexes as prodrugs for targeted chemotherapy. **W. Ang**, D. Wong, J. Lim

Technical program information known at press time.
The official technical program for the 249th ACS National Meeting is available at: www.acs.org/denver2015

‡ *Cooperative Cosponsorship*

10:30 INOR **932.** Ruthenium anticancer agents with redox-active intercalating ligands (RAILs): Correlation of reduction potential with DNA cleavage activity. **E.S. Narh**, J. Nguyen, F.M. MacDonnell

10:50 INOR **933.** Characterization and reactivity of metallosalophen complexes with G-quadruplexes. **M.J. Ross**, J.A. Cowan

11:10 INOR **934.** New dirhodium (II,II) complex with potential dual-binding to DNA upon photoactivation. **R. Akhimie**, C. Turro

11:30 INOR **935.** Construction and application of a Rh-Pt DNA metalloinsertor conjugate. **A.G. Weidmann**, J.K. Barton

11:50 INOR **936.** *Mycobacterium tuberculosis* and cobalt: A new approach to the fight against *M. tb* resistance. **T.J. Greenfield**

Section B

Colorado Convention Center
Room 301

Chemistry of Materials

Nanomaterials

C. G. Lugmair, *Organizer*
L. V. Frolova, J. R. Soliz, *Presiding*

8:30 INOR **937.** Grain structure and transport in nanocrystalline cadmium selenide. **Z. Norman**, J.S. Owen

8:50 INOR **938.** Nanocrystals of lithium group 14 compounds: Synthesis, stability, and carbon encapsulation. **J.E. Cloud**, Y. Wang, X. Li, T. Yoder, L. Taylor, Y. Yang, Y. Yang

9:10 INOR **939.** How the crystalline structure of Co nanocrystals plays a role in the Kirkendall processes. Z. Yang, N. Yang, **M. Pileni**

9:30 INOR **940.** Graphene as the test material for chemical modifications of bulk graphite. **L.V. Frolova**

9:50 INOR **941.** Cation-vacancy and electron-hole relaxation in single-walled aluminosilicate nanotubes: A linear-scaling density functional theory study. **E. Poli**, G. Teobaldi

10:10 Intermission.

10:25 INOR **942.** Synthesis and characterization of magnetic nanoparticles for toxic gas adsorption. **J.R. Soliz**, A.J. Hauser, K.M. Bussmann, M.S. Osofsky, C.J. Karwacki

10:45 INOR **943.** First stoichiometric metal chalcogenide nanocrystal. **P. Chen**, N.C. Anderson, Z. Norman, J.S. Owen

11:05 INOR **944.** Chromium-based chalcospinel nanocrystals: Syntheses and magnetism. **K. Ramasamy**, A. Gupta

11:25 INOR **945.** Synthesis, functionalization, and surface modification of layered zirconium phosphate nanoplatelets. **Y. Kan**, A. Clearfield

11:45 INOR **946.** Effects of the spatial location of Ag in titania nanotube on its photocatalytic activity and toxicity. **S.A. Ferdousi**, Y. Li, K.L. Yeung, Y. Xu

Section C

Colorado Convention Center
Room 302

Coordination Chemistry

Synthesis and Characterization

D. C. Crans, *Organizer*
D. Harris, M. Harris, *Presiding*

8:00 INOR **947.** Closed-shell metal complexes of caffeine sulfide and selenide. **M. Styron**, D. Rabinovich

8:20 INOR **948.** 1DI coordination polymers of metallacrowns. **C.M. Zaleski**

8:40 INOR **949.** Multireceptor host-guest complexation studies of novel ruthenium(II) ethylene-oxide oligomers, poylamine macrocycles, and tripodal cage complexes. **M. Harris**, B. Carpenter, T. Carroll, W. Lewis, A. Thomas, M. McBride, A. Smale

9:00 INOR **950.** Synthesis and crystal structures of oxo-molybdenum(VI), oxo-vanadium(V) and alkaline earth cations-based clusters. **A. Moneeb**, A. Apblett, A. Alabdulrahman, A. Bagabas

9:20 INOR **951.** Polyoxometalate complexes of anatase-TiO_2 cores. M. Raula, G. Gan Or, M. Saganovich, Y. Wang, R. Gobetto, **I.A. Weinstock**

9:40 INOR **952.** Novel transition metal(II)-2,5-diamino-2(difluoromethyl)pentanoic acid hydrochloride-1- hydrate complexes: Syntheses, characterization, structural elucidation, and their biological potency. **J.A. Obaleye**, W.A. Osunniran, A.C. Tella, J.O. Adebayo, M.O. Bamigboye

10:00 Intermission.

10:10 INOR **953.** Coordination chemistry of a fluorescein-decorated phosphine ligand. **A. DeLaRosa**, F.P. Gabbai

10:30 INOR **954.** Updating Richman-Atkins for the 21st century: Simpler, faster, and greener azamacrocycle synthesis. M. Wasilewski, **M. Wetzler**

10:50 INOR **955.** Synthesis and characterization of tris-(2-aminoethyl)amine copper complexes ncorporating para-substituted electron withdrawing functional groups. **A.R. McGlone**

11:10 INOR **956.** Withdrawn.

11:30 INOR **957.** Tetrahedral Sn-silsesquioxane: Synthesis, characterization, and adsorption properties. **E.V. Beletskiy**, Z. Shen, M.V. Riofski, X. Hou, J.R. Gallagher, J.T. Miller, Y. Wu, M.C. Kung, H.H. Kung

11:50 INOR **958.** Generalization of the donor-acceptor charge transfer complexation of Pt(bipyridine)(dithiolate) donors and nitrofluorenone acceptors to exhibit "black-absorber" behavior in the solid state and solution. **C. Browning**

Section D

Colorado Convention Center
Room 303

Nanoscience

Applications

Cosponsored by PRES

R. M. Richards, *Organizer*
B. G. Trewyn, *Presiding*

8:30 INOR **959.** New and efficient surface modification of $NaYF_4$: Yb^{3+}, Er^{3+} upconversion phosphor nanoparticles (UCNP) for biomedical imaging and organic photovoltaic applications. **S.K. Cho**, S. Ahn, L. Su, T.W. Flaig, W. Park

8:50 INOR **960.** Cholera toxin subunit B-modified mesoporous silica nanoparticles as vehicles for the improved intracellular delivery of proteins. **W. Walker**, J.L. Vivero

9:10 INOR **961.** Incorporating enzyme and metal nanoparticle catalysts on mesoporous silica supports for tandem reactions. **M.M. Otting**, X. Sun, B.G. Trewyn

9:30 INOR **962.** Power of rust and sand at the nanoscale: Iron oxide and mesoporous silica nanoparticles for theranostic applications. **K. Hurley**, H. Ring, M. Etheridge, J. Zhang, N. Klein, V. Szlag, C. Chung, Q. Shao, T.M. Reineke, M. Garwood, J. Bischof, C.L. Haynes

9:50 Intermission.

10:00 INOR **963.** Withdrawn.

10:20 INOR **964.** Nanostructured organosilica hybrids as highly efficient and regenerable sorbents for rare earth extraction. **J. Florek**, A. Mushtaq, E. Juere, F.G. Fontaine, D. Lariviere, F. Kleitz

10:40 INOR **965.** Effects of bis[3-(triethoxysilyl) propyl]tetrasulfide on gold nano particle formation in gold intercalated in the wall of mesoporous silica. **Y. Ji**, R.M. Richards

11:00 INOR **966.** Tackling environment and energy challenges with mesoporous nanomaterial technology. **B.G. Trewyn**

11:20 INOR **967.** Selectively inner-surface methylated single-walled aluminosilicate nanotubes, toward integration of chemical separation and (photo-)catalysis in confined volumes? **J.D. Elliott**, G. Teobaldi

Section E

Colorado Convention Center
Room 201

Organometallic Chemistry

Catalysis

N. S. Radu, *Organizer*
S. C. Chmely, N. P. Mankad, *Presiding*

9:00 INOR **968.** Withdrawn.

9:20 INOR **969.** Deoxygenation of CO_2 and N_2O enabled by bimetallic cooperativity: Control of reactivity and selectivity using tunable bimetallic effects. **N.P. Mankad**, S. Bagherzadeh, S. Parmelee, U. Jayarathne

9:40 INOR **970.** Light-activated iron bifunctional catalysts for transfer hydrogenations of polar double bonds. **S.C. Chmely**, P. Das

10:00 INOR **971.** Studies on the reductive elimination of C-X (X = C, N, S) bonds from a Co(III) center and its applications in catalysis. **C. Palit**, S. Timpa, O. Ozerov

10:20 INOR **972.** Regulation of iron-catalyzed olefin hydroboration by ligand modifications at a remote site. **K.T. Tseng**, J. Kampf, N.K. Szymczak

10:40 INOR **973.** Understanding H_2 oxidation by [Fe-Fe] hydrogenase: From enzymatic function to functional mimics. **N. Kumar**, S. Raugei, B. Ginovska-Pangovska, M. Dupuis, M. Helm, M. Bullock

11:00 INOR **974.** Cooperative catalysts for the synthesis of polyesters. **R.J. Hue**, I.A. Tonks

11:20 INOR **975.** Rhodium-catalyzed reduction of secondary and tertiary amides to amines using phenylsilane. **Z. Weinstein**, A.D. Sadow

Section F

Colorado Convention Center
Room 304

Main Group Chemistry

T. W. Hudnall, *Organizer*
C. Martin, K. H. Pannell, *Presiding*

8:00 INOR **976.** Functionalization of nine-atom deltahedral germanium clusters. **F. Li**, S.C. Sevov

8:20 INOR **977.** Exploration of aluminum(I) chemistry: Reactions involving AlX (X= Cl or Br). **S.M. De Carlo**, B.W. Eichhorn

8:40 INOR **978.** Steric bulk as both inhibitor and promoter of reactivity: the case of group 15 $M[N(SiMe_3)_2]_3$ complexes. **N.C. Boyde**, T.P. Hanusa

9:00 INOR **979.** Inverse FLP and related acid-base chemistry of Verkade's superbase. **S. Mummadi**, C. Krempner

9:20 INOR **980.** Cationic carbon Lewis acids in frustrated Lewis pairs. **L. Curless**, M. Ingleson

9:40 INOR **981.** Hexacoordinate polypyridylsilicon(IV) chemistry for electronic and catalytic applications. **T.A. Schmedake**, B.T. Donovan-Merkert, C. Maguylo, D.M. Peloquin

10:00 Intermission.

10:10 INOR **982.** Stepwise anion-induced polarity reversal of an antimony-transition metal bond. **J. Jones**, F.P. Gabbai

10:30 INOR **983.** Synthesis, spectroscopic, and structural characterization of structurally unique trialkylboranes: Evidence of unusual geometries stabilized by dispersion effects. **M.A. Faust**, P.P. Power

10:50 INOR **984.** Investigating ring expansion reactions with pentaphenylborole. K. Huang, **C. Martin**

11:10 INOR **985.** Synthesis, spectroscopic properties, and structural characterization of new BODIPY fluorophores. **L.I. Saucedo**, E. William, Y. Li, L. Tan, P. Tu, R. Roacho, A.J. Metta-Magana, E. Pena-Cabrera, K.H. Pannell

11:30 INOR **986.** Stabilization of reactive main group species by coordination to carbonyl-decorated carbenes. **T.W. Hudnall**, C.L. Deardorff, R.E. Sikma, K.M. Melancon, M.B. Gildner

11:50 INOR **987.** Polyborates as coordination compounds. **D.M. Schubert**, D. Neiner, M.K. McCray

Section G

Colorado Convention Center
Room 401

Nanoscience

Metal Oxides

Cosponsored by PRES

R. M. Richards, *Organizer*
F. Kleitz, *Presiding*

9:00 INOR **988.** Fe-doped ZnO colloidal nanocrystals: Synthesis, characterization, and photodoping. D. Zhou, **K.R. Kittilstved**

9:20 INOR **989.** High-surface-area nanostructured mixed metal oxides for catalytic applications. H. Yen, **F. Kleitz**

9:40 INOR **990.** Preparation and characterization of magnesium oxide and nickel oxide nanostructures with polar surfaces. **S.M. Shulda**, F. Lin, D. Nordlund, T. Weng, R.M. Richards

10:00 INOR **991.** Cu- and Ni-doped α-MnO_2 electrocatalysts for reversible oxygen electrochemistry. **T.N. Lambert**, J.A. Vigil, S.E. White, B.S. Swartzentruber

10:20 Intermission.

10:30 INOR **992.** Growth and characterization of $LaNiO_3$ nanostructures using chemical vapor deposition. **J.S. Page**, A.L. Prieto

10:50 INOR **993.** Low-temperature synthesis of compositionally complex scheelite-structured nanocrystals. **S. Culver**, R.L. Brutchey

11:10 INOR **994.** Design of magnetically recoverable catalysts via controlled aggregation of iron oxide and catalytic nanoparticles. R. Easterday, Y. Losovyj, M. Pink, B. Stein, D. Morgan, V.Y. Doluda, L.Z. Nikoshvili, E.M. Sulman, W. Mahmoud, A.A. Al-Ghamdi, **L. Bronstein**

Section H

Colorado Convention Center
Room 203

Coordination Chemistry

Synthesis and Characterization

D. C. Crans, *Organizer*
D. Rabinovich, C. M. Zaleski, *Presiding*

8:00 INOR **995.** Synthesis, structure, and volatility of alkali and alkaline earth element hexafluoroacetylacetonate complexes. **D.B. Rego**, P.M. Forster, K. Czerwinski

8:20 INOR **996.** Effect of precursor ligand on particle size/morphology of zinc oxide nanomaterials. **E. Rukundo**, A. Apblett

8:40 INOR **997.** Unexpected facile access to dimetallic cryptates containing an elaborate hydrogen bonding network. **J.B. Gordon**, G. Guillet, K.A. Abboud, L.J. Murray

9:00 INOR **998.** Preparation and properties of a molecular analog of a perovskite-like structure. **A.E. Thuijs**, Y. Oh, S. Cheong, K.A. Abboud, G. Christou

9:20 INOR **999.** Supramolecular aggregates of single-molecule magnets. **A.M. Mowson**

9:40 INOR **1000.** Ligand field modification of cobalt-H_2bip complexes to control field induced magnetic relaxations. **I. Bhowmick**, A.K. Rappe, M.P. Shores

10:00 Intermission.

10:10 INOR **1001.** Dinuclear complexes as model systems to explore magnetic coupling through tetrazine-based radical ligands. **T.J. Woods**, M.F. Ballesteros-Rivas, K.R. Dunbar

10:30 INOR **1002.** Investigation of spin-crossover behavior in cobalt tetrazene complexes with chelating ligands. **A.C. Bowman**, H.J. Zecca, H. Kim

10:50 INOR **1003.** Electronic effects on dinuclear iron(II) spin crossover complexes bridged by diiminobenzoquinonoid. **J.G. Park**, I. Jeon, D. Harris

11:10 INOR **1004.** Employing hydrogen-bonding interactions to modulate magnetic relaxation in a Co(II) tripodal iminopyridine-based complex. **C.M. Klug**, I. Bhowmick, A.K. Rappe, M.P. Shores

11:30 INOR **1005.** Strong magnetic coupling in dinuclear transition metal complexes bridged by redox-active ligands. **I. Jeon**, D. Harris

11:50 INOR **1006.** Magnetic and spectroscopic properties of linear two-coordinate transition metal complexes. **C. Lin**, G.J. Long, P.P. Power

Section I

Colorado Convention Center

Room 205

Inorganic Catalysts

S. A. Koch, *Organizer*

T. J. Hubin, *Presiding*

8:30 INOR **1007.** Structure-function relationships for electrocatalytic water oxidation by molecular $[Mn_{12}O_{12}]$ clusters. **Y. Yan**, D.A. Ruddy

8:50 INOR **1008.** Functional ordered mesoporous metal carbides. **M. Xu**, M.R. Nimlos, B.G. Trewyn, R.M. Richards

9:10 INOR **1009.** Withdrawn.

9:30 INOR **1010.** Single-crystal to single-crystal structural and chemical transformation of a Fe-based mononuclear electrocatalyst for hydrogen production. **X. Wang**, T. Liu, M. Bullock

9:50 Intermission.

10:00 INOR **1011.** Two 4-step mechanisms for nanoparticle nucleation, growth, bimolecular agglomeration, and then autocatalytic agglomeration or secondary autocatalytic growth. **P. Kent**, R.G. Finke

10:20 INOR **1012.** Progress in developing an aerobic hydrocarbon oxidation catalyst. **C.C. Scarborough**, G.J. Karahalis, C.T. Buru, A. Thangavel

10:40 INOR **1013.** Measurement of aqueous hydricities of transition-metal hydrogen evolution catalysts. **C. Tsay**, B. Livesay, J. Yang

11:00 INOR **1014.** Activation of CO_2 utilizing Lewis acid/base cooperativity from a NiFe bimetallic Robson-type complex. **S. Poteet**, J. Yang

11:20 INOR **1015.** Synthesis, structural studies, and oxidation catalysis of the late first row transition metal complexes of a 2-pyridylmethyl pendant armed ethylene cross-bridged cyclam. **T.J. Hubin**, D.G. Jones, A.D. Shircliff, G. Yin, T.J. Prior

Section J

Colorado Convention Center

Room 402

Organometallic Chemistry

Synthesis and Characterization

N. S. Radu, *Organizer*

S. Fortier, V. M. Iluc, *Presiding*

8:30 INOR **1016.** Metal-ligand interactions: E-H activation and metal-element multiple bonding. **V.M. Iluc**

8:50 INOR **1017.** Synthesis, characterization, and coordination chemistry of a new guanidinate ligand class possessing ketimine backbones. **A. Maity**, S. Fortier, L. Griego, A.J. Metta-Magana

9:10 INOR **1018.** Identification and characterization of an η2 nitrogen-nitrogen complex between diazoalkanes and lithium dimethylcuprate. **J. Morse**, M.D. Murphy, S.H. Bertz, C. Ogle

9:30 INOR **1019.** U(bipy)$_4$: A mistaken case of U(0)? **S. Fortier**, J. Le Roy, K. Ghiassi, M.M. Olmstead, D. Villagran, M. Murugesu, A.J. Metta-Magana

9:50 INOR **1020.** Structural and chemical study of iron supported by "super bulky" guanidinates. **S. Fortier**, A. Maity, L. Griego, A.J. Metta-Magana

10:10 INOR **1021.** Mechanochemical vs. solution syntheses of group 15 bulky allyl metal complexes. **N.R. Rightmire**, D.L. Bruns, T.P. Hanusa

10:30 INOR **1022.** C–H bond activation by iridium (III) pincer dicarboxylate complexes. **A.M. Wright**, K.I. Goldberg

10:50 INOR **1023.** Synthesis, characterization, and reactivity study of a masked "Ti(II)" complex. **R. Aguilar**, S. Fortier, A. Metta-Magana

11:10 INOR **1024.** Size effect and odd-even alternation in the melting of single and stacked silver alkanethiolate layers: Experiment and phenomenological model. **Z. Ye**, L. de la Rama, L. Hu, M. Efremov, L. Allen

11:30 INOR **1025.** Molecular switches: Exploring the counter-ion problem. **J.A. Christie**, R. Forrest, S. Corcelli, N.A. Wasio, R. Quardokus, S.A. Kandel, Y. Lu, C.S. Lent, A.G. Oliver, K.W. Henderson

THURSDAY AFTERNOON

Section A

Colorado Convention Center

Room 105

Nanoscience

Semiconductors

Cosponsored by PRES

R. M. Richards, *Organizer*

N. R. Neale, M. Zamkov, *Presiding*

1:30 INOR **1026.** Progress towards complete photocatalytic water splitting utilizing hybrid nanoparticles. **A.D. LaCroix**, J. Macdonald

1:50 INOR **1027.** Phase dependent visible to near-infrared photoluminescence of $CuInS_2$ nanocrystals. **A. Leach**, J. Macdonald

2:10 INOR **1028.** Silicon monoxide: A convenient precursor for near infrared emitting silicon nanocrystals and switching-on quantum size effects. **W. Sun**, C. Qian, G.A. Ozin

2:30 INOR **1029.** Growth of $CuInS_2$ nanoplatelets by cation exchange and mechanism study. **L. Mu**, W.E. Buhro

2:50 Intermission.

3:00 INOR **1030.** Sub-diffraction imaging of exciton diffusion in semiconductor nanocrystal solids. **M. Zamkov**, N.N. Kholmicheva, P. Moroz

3:20 INOR **1031.** Surface passivation of group 14 nanocrystals. **N.R. Neale**

3:40 INOR **1032.** Cu_2ZnSnS_4/Cu_2Se core/shell nanocrystal thin films: Manipulation of charge carrier transport through surface modification. **L. Korala**, A.L. Prieto

Section B

Colorado Convention Center

Room 301

Lanthanide and Actinide Chemistry

A. De Bettencourt Dias, *Organizer*

P. C. Burns, N. E. Travia, *Presiding*

1:30 INOR **1033.** Withdrawn.

1:50 INOR **1034.** Coordination chemistry of the rare-earths in a tripodal nitroxide ligand framework: New chemistry for magnet recycling. **J.A. Bogart**, C.A. Lippincott, P.J. Carroll, E.J. Schelter*

2:10 INOR **1035.** Interactions of uranium and plutonium with phosphonate-functionalized mesoporous silica. **E.C. Uribe**, J. Shusterman, A. Bruchet, H. Mason, H. Nitsche

2:30 INOR **1036.** Exploring the chemistry of the f-elements with nitrogen-rich ligands. **N.E. Travia**, K. Browne, J.L. Kiplinger, D.E. Morris, A. Mueller, A. Nelson, A.J. Parkison, B. Scott, B.C. Tappan, J. Veauthier

2:50 Intermission.

3:00 INOR **1037.** Synthesis, characterization, and reactivity of U^{2+} in the $\{[C_5H_3(SiMe_3)_2]_3U\}^{1-}$ anion. **C.J. Windorff**, J.W. Ziller, W.J. Evans

3:20 INOR **1038.** Examining covalency in uranium-ligand multiple bonds through synthesis, spectroscopy, and theory. **N.C. Tomson**, L. Spencer, R.L. Shook, E.R. Batista, J.M. Boncella

3:40 INOR **1039.** Mechanistic insights into the early stages of crystallization of REE-carbonate. **J. Rodriguez Blanco**, K. Dideriksen, D. Tobler, K. Sand, B. Vallina, L. Benning, S.S. Stipp

4:00 Intermission.

4:10 INOR **1040.** Increasing the reactivity of actinide coordination compounds: Imidazolin-2-iminato actinide complexe. **I. Karmel**, N. Fridman, T. Bannenberg, M. Tamm, M. Eisen

Section C

Colorado Convention Center

Room 302

Chemistry of Materials

Metal-Organic Frameworks

C. G. Lugmair, *Organizer*

J. Jiang, J. V. Lockard, *Presiding*

1:30 INOR **1041.** Metal-organic frameworks for natural gas storage. **J.A. Mason**, M.K. Taylor, M.R. Hudson, Z. Hulvey, A. Guagliardi, C.M. Brown, N. Masciocchi, J.R. Long

1:50 INOR **1042.** Ultrastable piezofluorochromic metal-organic frameworks. **Q. Zhang**, H. Zhou

2:10 INOR **1043.** In situ spectroscopy studies of CO_2 adsorption in a dually functionalized microporous metal-organic framework. Y. Chen, H. Wang, J. Li, **J.V. Lockard**

2:30 INOR **1044.** Highly stable meso porous MOFs. **D. Feng**, K. Wang, T. Liu, J. Park, H. Zhou

2:50 INOR **1045.** Mechanistic insights into the gelation of cyanide-bridged coordination polymers. **I.C. Fortmeyer**, P.A. Hoijemberg, Y. Yan, I. Pelczer, A.B. Bocarsly

3:10 INOR **1046.** Alternative UiO-66 synthesis for HCl-sensitive nanoparticle encapsulation. **K.S. Walton**, K. Tulig

3:30 INOR **1047.** Prussian red: A carbon monoxide fused cyano bridging mixed valence FeII/III coordination polymer with unprecedented packing pattern and anisotropic negative thermal expansion. W. Lo, O. Ishal, D. Sultan, **J. Jiang**

3:50 INOR **1048.** Photochromic metal–organic frameworks toward control of singlet oxygen generation. **J. Park**, D. Feng, S. Yuan, H. Zhou

4:10 INOR **1049.** Solvothermally grown porphyrin metal-organic framework (MOF) thin films: Post metalation and electrocatalysis. C. Kung, **T. Chang**, L. Chou, J.T. Hupp, O.K. Farha, K. Ho

4:30 INOR **1050.** Novel phosphine coordination materials based on *bis*(phosphine) and methyl triarylphosphonium groups for applications in gas storage, separations, and sensing. **N. Waggoner**, A. Bohnsack, L. Cinninger, T. Kornfuehrer, B.J. Holliday, S.M. Humphrey

4:50 INOR **1051.** Pressure-induced switching in functional molecular materials. **G.J. Halder**, K.W. Chapman, A.A. Yakovenko, P.J. Chupas, A.M. dos Santos

Section D

Colorado Convention Center

Room 303

Coordination Chemistry

Characterization and Applications

D. C. Crans, *Organizer, Presiding*

A. C. Bowman, *Presiding*

1:30 INOR **1052.** Proton-responsive pincers: Enabling bifunctional Lewis acidic/Bronsted basic late metal complexes. **B. Cook**, C. Chen, M. Pink, R.L. Lord, K.G. Caulton

1:50 INOR **1053.** Synthesis and photocatalytic properties of a boron-centered ionic metal organic framework. **X. Zhang**, X. Zhang, Y. Chen, J. Zhang

2:10 INOR **1054.** Mechanism for ligand exchange processes in metal organic frameworks. **J. Byers**, C. Tsung, J.V. Morabito, L. Chou, Z. Li, R. Kyada

2:30 INOR **1055.** Highly dynamic coordination chemistry and redox chemistry of aromatic polyphosphorus complexes. **M. Fleischmann**, M. Scheer

2:50 INOR **1056.** $[Ru(bpy)_3]^{2+}$ linked with methyl viologen and phenothiazine substituted aminoethylglycines. **B. Biber**, M. Williams

3:10 INOR **1057.** Utilizing TREN-based copper complexes to calculate activation rate constant values in ideal atom transfer radical addition (ATRA) reactions. **K.A. Bussey**, K.D. Oshin

MEDI

Division of Medicinal Chemistry

W. B. Young, *Program Chair*

SUNDAY MORNING

Section A

Colorado Convention Center

Mile High Blrm 2A/2B

Applications of Positron Emission Tomography in Drug Discovery

D. Donnelly, C. D. Jesudason, *Organizers, Presiding*

9:00 MEDI **1.** Synthesis of radiopharmaceuticals and applications in functional positron emission tomography (PET) imaging. **P.J. Scott**

9:30 MEDI **2.** 18F-T807: A PET imaging compound for detecting tau in alzheimer's and non-alzheimer's neurodegenerative diseases. **G. Attardo**, A.T. Hoye, H. Xiong, X. Li, C.L. Horchler, K. Fan, N. Lim, F. Gomez, Y. Lin, Q. Liang, K. Conway, H. Kolb, D. Skovronsky, M. Mintun

10:00 MEDI **3.** Development of PET radioligands for imaging brain mGlu1 receptors. **P.W. Victor**

10:30 MEDI **4.** Preclinical peripheral enzyme occupancy and PK/PD modelling: A retrospective analysis of sildenafil. **C.D. Jesudason**, V.N. Barth, T.E. Eessalu, E. Yuen

11:00 MEDI **5.** Design, synthesis, and development of fluorine-18 and carbon-11 labeled lysophosphatidic acid receptor 1 (LPA1) PET radioligands for lung receptor occupancy imaging. **D. Donnelly**, S. Bonacorsi, S. Du, A. Pena, J. kim, W. Hayes, N. Nabulsi, J. Gallezot, Y. Huang, R. Carson

11:30 MEDI **6.** ImmunoPET imaging in the development of therapeutic antibodies. **J. Marik**

Section B

Colorado Convention Center

Mile High Blrm 1A/1B

Targeting the Microbiome

S. M. Firestine, *Organizer, Presiding*

9:00 MEDI **7.** Gut reactions: Understanding and manipulating chemistry from the human microbiota. **E.P. Balskus**

9:35 MEDI **8.** Chemical library in food presents the natural ligands for the gastrointestinal microbiome. **M.L. Heiman**

10:10 MEDI **9.** Discovery of small molecule therapeutics based on microbiome-host interaction analysis in inflammatory bowel disease. **T.Z. DeSantis**

10:45 MEDI **10.** Incorporation of therapeutic bacteria into the gut microbiome for treatment of obesity. **S.S. Davies**

11:20 MEDI **11.** Pharmaceutical control of the microbiome. **M. Redinbo**

Section C

Colorado Convention Center

Mile High Blrm 2C

General Oral Session

W. B. Young, *Organizer*

J. B. Schwarz, *Presiding*

8:30 MEDI **12.** γ-AApeptides as a new class of peptidomimetics. **H. Wu**, Y. Niu, J. Cai

8:50 MEDI **13.** Improved inhibitors of inducible nitric oxide synthase (iNOS) through fragment assisted lead generation and optimization. **F. Edfeldt**

‡ *Cooperative Cosponsorship*

9:10 MEDI **14.** SAR enablement of multifunctional BACE templates: Thioamidines. **B.T. O'Neill**, E. Beck, M.A. Brodney, M.W. Bundesmann, C. Butler, L. Buzon, L. Chenard, J. Davoren, J. Dutra, C.J. Helal, K.E. Henegar, J.M. Humphrey, E.A. LaChapelle, B. Li, R. Lira, L.A. Martinez-Alsina, J.C. Murray, K. Ogilvie, L. Price, T.P. Tran, S. Sakya, Y. Zhang, A. Yu

9:30 MEDI **15.** Development of novel NLRP3 inflammasome inhibitors and their potential application. **S. Zhang**, J. Chojnacki, C. Marchetti, S. Toldo, A. Abbate

9:50 MEDI **16.** Methionine aminopeptidases (MetAPs) as promising targets toward discovery of novel anti-infective agents. P. Wangtrakuldee, **C. Chen**, B. Staker, J.M. Wilk, J.R. Horn, T.J. Hagen

10:10 MEDI **17.** Development of pyridopyrimidine-based inhibitors of HIV-1 reverse transcriptase. **C. Lacbay**, J. Mancuso, Y. Lin, N. Bennett, M. Menni, M. Gotte, Y.S. Tsantrizos

10:30 MEDI **18.** Open source malaria: A new approach to drug discovery. **A.E. Williamson**, M.H. Todd, P. Willis, O. Consortium

10:50 MEDI **19.** Development of non-incorporating small molecule inhibitors of antibody fucosylation. **M.J. Frohn**, J.G. Allen, C.H. Fotsch, M. Mujacic, T. San Miguel, O.R. Thiel, J. McCarter, A.J. Pickrell, M. Lo, J.B. Jordan

11:10 MEDI **20.** Discovery and opioid receptor SAR of AT-076, the first small-molecule opioid pan antagonist with nanomolar affinity at mu, delta, kappa and nociceptin opioid receptors. **V.B. Journigan**, N.T. Zaveri, W.E. Polgar

11:30 MEDI **21.** Discovery of oral FSHR (follicle stimulating hormone receptor) allosteric modulators. **H.N. Yu**

11:50 MEDI **22.** Small molecule activators of Pro-apoptotic BAX for cancer therapy. **E. Gavathiotis**

Drug Discovery

Structural Informatics & Target Based: Structure-Based

Sponsored by COMP, Cosponsored by MEDI

SUNDAY AFTERNOON

Section A

Colorado Convention Center
Mile High Blrm 1A/1B

General Oral Session

W. B. Young, *Organizer, Presiding*

1:30 MEDI **23.** Discovery of TAK-063, a novel phosphodiesterase 10A (PDE10A) inhibitor. **M. Fushimi**, J. Kunitomo, M. Yoshikawa, A. Kawada, J.F. Quinn, H. Oki, H. Kokubo, M. Kondo, K. Nakashima, T. Taniguchi

1:55 MEDI **24.** Discovery of a novel and potent dual orexin 1/orexin 2 receptor antagonist, E2006, for the treatment of sleep disorders. **T. Terauchi**

2:20 MEDI **25.** Discovery of the clinical candidate BMS-816336, an adamantyl acetamide based 11β-hydroxysteroid dehydrogenase type-1 (11β-HSD1) inhibitor. **X. Ye**, S. Chen, S. Wu, D.S. Yoon, H. Wang, Z. Hong, S.P. Oconnor, J. Li, J. Li, S. Walker, L.J. Kennedy, A. Apedo, A. Nayeem, S. Sheriff, P. Morin, D. Camac, T. Harrity, R. Zebo, J. Taylor, N. Morgan, R. Ponticiello, R. Golla, R. Seethala, M. Wang, T. Harper, B. Sleczka, B. He, M. Kirby, J. DiMarco, R. Scaringe, R.L. Hanson, Z. Guo, J. Li, J. Sun, M.K. Wong, B. Chen, L. Haque, D.K. Leahy, C. Chan, Y. Li, T. Zvyaga, L. Hansen, C. Patel, D.A. Gordon, J.A. Robl

2:45 MEDI **26.** Discovery, optimization, and human microdosing study of a novel series of H3 antagonists. **M. Chytil**, S. Engel, K. Fang, K. Spear

3:10 MEDI **27.** Cholesteryl ester transfer protein inhibitor BMS-795311. **J.X. Qiao**, T.C. Wang, A. Chen, D.S. Taylor, R.Z. Yang, P.G. Sleph, J.P. Li, D. Li, M. Chang, X. Chen, C. Xu, J. Li, D. Smith, D. Wu, L. Leith, L.S. Harikrishnan, M. Kamau, R. Rampulla, M.M. Miller, D. Bilder, R. Lawrence, M.A. Poss, P. Levesque, C.S. Huang, L.P. Adam, R.R. Wexler, H.J. Finlay, M.S. Salvati

3:35 MEDI **28.** Discovery of potent and kinase-selective p21-activated kinase 1 (PAK1) inhibitors. **J. Rudolph**, I. Aliagas, E. Blackwood, T. O'Brien, J. Crawford, J. Drobnick, L. Gazzard, C. Heise, W. Lee, L. Murray, C. Ndubaku, W. Wang, X. Zhao, K.P. Hoeflich

4:00 MEDI **29.** Liver targeted HIF-PHD inhibitors for the treatment of anemia. **C. Sinz**, Y. Chen, V.J. Colandrea, Q. Dang, B. DuBois, P. Liu, P.T. Meinke, R. Liu, J. Tan, F. Ujjainwalla, L. Wang, J.J. Hale, J. Cai, D. Stickens, B. Bishwokarma, M. Zielstorff, D. Zaller, C. Chiu, M. Cheng, C. Alpert, J. Metzger, L. Yang, S. Vincent, K. Bleasby, M. Hafey, R. Houle

4:25 MEDI **30.** Discovery of BMS-852927, a potent LXR partial agonist possessing LXRbeta functional selectivity. **E.K. Kick**, B. Busch, R. Martin, Y. Xie, M. Nanao, T. Stout, A. Plonowski, I. Schulman, G. Yan, W. Stevens, M. Nyman, L. Nguyen, R. Narayanan, K. Behnia, G. Cantor, J. Lupisella, P. Sleph, D. Grimm, J. Ostrowski, T. Kirchgessner, R.R. Wexler, R. Mohan

4:50 MEDI **31.** Building ERK inhibitors. Mitigaing their clearance. **J.T. Bagdanoff**, D. Poon, W. Han, S. Zhu, R. Jain, M. Lindvall

Section B

Colorado Convention Center
Mile High Blrm 2A/2B

Biased Agonism: An Emerging Paradigm in GPCR Drug Discovery

J. Herr, Z. Rankovic, *Organizers, Presiding*

1:30 MEDI **32.** Harnessing ligand-directed signaling to improve pain therapeutics. **L.M. Bohn**, C.L. Schmid, K. Lovell, N.C. Ross, T.D. Bannister

2:10 MEDI **33.** Engineering enhanced, receptor-specific, and signaling-biased arrestins. **V. Gurevich**

2:50 MEDI **34.** Discovery of TRV130, a G protein biased agonist of the μ-opioid receptor, for the treatment of acute severe pain. **A.L. Crombie**, X. Chen, P.M. Pitis, G. Liu, C. Yuan, D. Gotchev, D.S. Yamashita, J.D. Violin

3:30 MEDI **35.** Discovery of functionally selective ligands of fopamine D_2receptors. K. Butler, J. McCorvy, X. Chen, M. Caron, W. Wetsel, B.L. Roth, **J. Jin**

4:00 MEDI **36.** Novel GPR40 agonists for the treatment of type-2 diabetes: The effect of b-arrestin signaling. **C. Hamdouchi**

4:30 MEDI **37.** Biased signaling with allosteric modulators of GPCRs. **C.W. Lindsley**

5:00 Concluding Remarks.

Section C

Colorado Convention Center
Mile High Blrm 2C

Young Investigator in Medicinal Chemistry

Cosponsored by YCC

T. E. Prisinzano, *Organizer, Presiding*

2:00 MEDI **38.** First structural disclosure, discovery, preclinical characterization, and FTIH pharmacokinetics for GSK2878175, a second generation boron-based inhibitor of the HCV RNA-dependent RNA polymerase. **J. Shotwell**

2:30 MEDI **39.** Hedgehog pathway modulators as therapeutic agents. **M.K. Hadden**

3:00 MEDI **40.** Discovery of halogenated phenazine and halogenated quinoline small molecules with antibacterial and antibiofilm activities against *staphylococcal* biofilms. **R. Huigens**

3:30 MEDI **41.** Novel small molecule immunomodulators that target toll-like receptors. **H.H. Yin**

4:00 MEDI **42.** Discovery and adverse safety findings of two new mGluR5 NAM chemotypes. **A.F. Stepan**

4:30 MEDI **43.** Efficient small molecule inhibitors of the HDM2-p53 protein-protein interaction. **M.R. Machacek**

Drug Discovery

Structural Informatics & Target Based: Structure-Based

Sponsored by COMP, Cosponsored by MEDI

SUNDAY EVENING

Section A

Colorado Convention Center
Hall C

General Poster Session

W. B. Young, *Organizer*

7:00 - 9:00

MEDI **44.** Design, synthesis, and biological evaluation of novel tubulysin analogs as payloads for antibody-drug conjugates for the targeted treatment of cancer. Y. Huang, H. Xie, J. Jia, H. Guo, S. Gai, X. Li, L. Qu, X. Zuo, X. Zhou, S. Sun, Q. Yang, W. Li, C. Lin, H. Ye, **R.Y. Zhao**

MEDI **45.** Withdrawn.

MEDI **46.** New flash purification capabilities decrease run times up to 67%. **J.R. Bickler**

MEDI **47.** New high-performance C18 flash cartridge significantly improves resolution and fraction purity. **J.R. Bickler**

MEDI **48.** Rapid cleanup of peptides with mass-directed flash chromatography and spherical C18 silica. **W.J. Hartsock**, **J.R. Bickler**, V. Vandell, F.A. Kero

MEDI **49.** Purification of peptides by flash chromatography. J.E. Silver, R. Lewis

MEDI **50.** Design, synthesis, and biological evaluation of *Rickettsia prowazekii* methionine aminopeptidase (MetAP) Inhibitors. **T.R. Helgren**, C. Chen, P. Wangtrakuldee, C. Long, M. Hathuc, R. Small, B. Curran, J.R. Horn, T.J. Hagen

MEDI **51.** Mutual solubilities of the antibiotic/β-lactamase inhibitor drug combinations vancomycin, piperacillin, and tazobactam in aqueous solution. **H.S. Gray**, **H.N. Gray**, S.C. Butler, R.N. Mason

MEDI **52.** Molecular mechanism and ligand design of a PLP/GABA-dependent bacterial transcription regulator GabR. **E. Cybulla**, R. Wu, C. Reidl, D. Gawron, D.P. Becker, D. Liu

MEDI **53.** Synthesis, conformational analysis, and pharmacokinetics of fluorinated antitubercular nucleosides. **S. Dawadi**, K. Viswanathan, H. Boshoff, C.E. Barry, C.C. Aldrich

MEDI **54.** Protein structure-based virtual screening led to identification of novel natural product-derived hits as cannabinoid receptor 1 modulators. **P. Pandey**, K.K. Roy, R.J. Doerksen

MEDI **55.** Building on the success of the first generation of N-alkylthiol beta-lactams yields a multimodal, multiaction prodrug therapy for MRSA. **J.L. Borja**

MEDI **56.** Investigating the conformational states and ligand binding of voltage gated sodium channels by multiple spectroscopic techniques. **M. Colledge**, B. Wallace

MEDI **57.** Incorporation of triazoles as disulfide mimics in chimeric AGRP-melanocortin peptide template. **S.R. Tala**, A. Singh, C. Haskell-Luevano

MEDI **58.** Drug discovery and large-scale synthesis for 7-azaindoline derivatives as potent, orally available, selective M1 and M4 muscarinic acetylcholine receptors agonists. **Y. Uruno**, Y. Inoue, Y. Konishi, A. Suwa, K. Takai, K. Hashimoto, H. Matsuda, T. Nakako, M. Sakai, G. Hashimoto, T. Enomoto, A. Kitamura, Y. Uematsu, A. Kiyoshi, T. Sumiyoshi

MEDI **59.** Design, synthesis, and structure-activity relationships of flupirtine derivatives for the treatment of neuronal ceroid lipofuscinosis. **N. Kinarivala**, J. Makoukji, F. Saadeh, R. Boustany, P.C. Trippier

MEDI **60.** Exploiting the Sigma-2 receptor as a therapeutic target for cancer and various CNS diseases. **J. Chan**, J. Sahn, S.F. Martin, L. Scott, J. Pierce-Shimomura

MEDI **61.** Optimization of synthetically novel agonists of the putative cannabinoid receptor, GPR55, using an activated state model. **M.A. Lingerfelt**, L. Alfakhori, D.P. Hurst, P. Zhao, M.P. Croatt, M.E. Abood, P.H. Reggio

MEDI **62.** Rational fesign of fual-site scetylcholinesterase inhibitors: Multifunctional lead for Alzheimer's disease therapy. W. Yang, S. Yang, G. Yang

MEDI **63.** Discovery of novel, potent γ-secretase inhibitors. Z. Zhao

MEDI **64.** Novel amyloid binding compounds: A search for PET imaging probes for neurofibrillary tangles. B. Hurtle, L. Cai, B. Qu, V.W. Pike

MEDI **65.** Crystallographic evaluation of chelidamic acid congeners. **A.L. Green**, K.M. Lincoln, R.E. Saunders, K.N. Green

MEDI **66.** Rational design and bioevaluation for novel acetylcholinesterase inhibitors for treating Alzheimer's disease. **Q. Sun**, G. Yang, . Yang

MEDI **67.** Structural insights into the mechanism of activation of the human cannabinoid type 2 (CB_2) receptor: Molecular dynamics study of an agonist-bound state. **K.K. Roy**, P. Pandey, R.J. Doerksen

MEDI **68.** Discovery, SAR, and biological evaluation of a novel series of piperazine-based inhibitors of glycine transporter-1 (GlyT-1). **C.L. Cioffi**, S. Liu, M.A. Wolf, P.R. Guzzo, K. Sadalapure, V. Parthasarathy, J. Maeng, E. Carulli, D.T. Loong, X. Fang, P. Gupta, S. Panduga, K.N. Kalesh, L. Matta, S. Choo, R.N. Buckle, R. Davis, S.A. Sakwa, M. Hu, D.H. Dethe, B.J. Sargent, N.A. Moore, M.M. Luche, Y.L. Khmelnitsky, J. Ismail, H. Decornez, D.B. Kitchen, P.L. Love, M.A. Watson, J. Adolphson, G. Padilla, K. Waikins, S. Tom, A. Ngo, M. Chung, M. Bai, N. Johal, S. Swaminathan, A.J. Mhyre

MEDI **69.** Arylguanidine NAMs for α7 nAChRs: Where do they bind and why? **O.I. Alwassil**, S. Khatri, M.K. Schulte, M. Dukat

MEDI **70.** Structure activity relationship of tetrahydroisoquinoline *N*-methyl-D-aspartate receptor positive allosteric modulators can be modified to target GluN2B-containing receptors. **K.L. Strong**, D.S. Menaldino, K.K. Ogden, S.F. Traynelis, D.C. Liotta

MEDI **71.** CPM: A potential moiety to reduce opioid dependence. **Z. Wu**, V.J. Hruby

MEDI **72.** Curcumin/melatonin hybrids as neuroprotective agents for Alzheimer's disease. **J. Saathoff**, K. Liu, J. Chojnacki, S. Zhang

MEDI **73.** Application of machine learning and regression techniques in developing novel homologous recombination inhibitors. **J. Zhu**

MEDI **74.** Simple and integrated approach to compound progress and work-request tracking. **J.W. Sager**, T.E. Mansley, P. Mounteney, C.P. Snyder

MEDI **75.** In silico modeling workflows in support of exploratory computational toxicology. **M.R. Goldsmith**, D. Chang, A. Deschenes, C. Williams, A. Ajamian

MEDI **76.** Importance of visualization in lead discovery: Supporting the medicinal chemist in designing compounds more efficiently. **C. Detering**

MEDI **77.** Chemoinformatics analysis of natural products databases: Toward the identification of tubulin polymerization inhibitors. **R. Aguayo-Ortiz**, R. Castillo-Bocanegra, A.M. Hernandez Campos, J.L. Medina-Franco

MEDI **78.** Discovery and synthesis of triphenylethanamine derivatives as highly potent cholesteryl ester transfer protein Inhibitors. **T. Wang**, J.X. Qiao, A. Chen, D.S. Taylor, R.Z. Yang, P.G. Sleph, J.P. Li, D. Li, M. Chang, X. Chen, C. Xu, J. Li, P. Levesque, C.S. Huang, L.P. Adam, M.S. Salvati, H.J. Finlay, R.R. Wexler

MEDI **79.** Identification of a novel class of covalent modifiers of hemoglobin as potential antisickling agents. **A.M. Omar**, M.A. Mahran, M. Ghatge, N. Chowdhury, F.H. Bamane, M.E. El-Araby, O. Abdulmalik, M. Safo

MEDI **80.** Process of blood coagulation investigated through the interactions of aspirin with bovine red blood cell lipid extract membrane monolayers. **K.A. Miller**, A. Sostarecz

MEDI **81.** Novel coumarin based monocarboxylate transport 1 & 4 inhibitors as anticancer agents. L. Solano, C. Ronayne, G.L. Nelson, S. Gurrapu, S.K. Jonnalagadda, V. Mereddy

MEDI **82.** Potent dual monocarboxylate transporter 1 & 4 inhibitors for triple negative breast cancer treatment. **L. Solano**, **G.L. Nelson**, **C. Ronayne**, V. Mereddy, S.K. Jonnalagadda, S. Gurrapu

MEDI **83.** Development of collagen films coated with synthetic photoreactive peptides that support cardiovascular repair and regeneration. **J. Malcor**, D. Bax, D. Bihan, S. Hamaia, R. Farndale

MEDI **84.** Withdrawn.

MEDI **85.** Total synthesis of clavatadine A analogs to produce a viable reversible inhibitor for factor XIa. **C.E. Malmberg**, S. Chamberland

MEDI **86.** Discovery of novel, potent, and highly selective factor xia inhibitors from HTS hit with X-ray crystallography-based rational design. T. Nishiyama, T. Kondo, K. Hisaichi, K. Ochi, A. Kinoshita, R. Miwa, **A. Imagawa**, S. Flanagan, C.J. Yarnold, S. Courtney, M. Gohda, K. Suzuki, T. Ono, S. Koyama, T. Hagio, M. Sakai, H. Habashita, K. Kawabata

MEDI **87.** Structure-based design, synthesis, and evaluation of novel peptide inhibitors of thrombin-induced activation of platelets aggregation. **C.C. Clement**, J. Gonzalez, A. Babinska, M. Philipp

MEDI **88.** Picomolar K_D ligands can be obtained by increasing the binding rate instead of decreasing the dissociation rate: Surprising structure-kinetic relationship among very similar thrombin inhibitors. **M.T. Khayat**, A.S. Murkin, M.M. Murphy, T.e. Ryan, B. Sathyamoorthy

MEDI **89.** Synthesis of resorufin derivatives as inhibitor indicators of cytochrome P450 enzymes. **L. Lovings**, J. Liu, M. Foroozesh

MEDI **90.** Radical-induced oxidation of tobacco-specific nitrosamines under physiological conditions. B.R. Daws, **S.P. Mezyk**, J.J. Kiddle

MEDI **91.** Pyrano- and furanochromones as specific inhibitors of human cytochrome P450 1A2. **J. Liu**, P. Pham, L. Lovings, N. Goyal, M. Foroozesh

MEDI **92.** Investigation of regulation of cytochrome P450 2J2 in adult human primary cardiomyoctyes. **R. Rowlands**, E. Evangelista, B. Raccor, R. Totah

MEDI **93.** Metabolic stability assessment of tumor-targeted drug delivery systems with fluorine-labeled taxoid probes by 19F NMR. **B. Lichtenthal**, J.D. Seitz, J.G. Vineberg, L. Wei, C. Lin, J. Kahn, I. Ojima

MEDI **94.** Drug release by remotely controlled magnetic anisotropy. **M. Shin**, B. Kang, S. Han, E. Jang, J. Suh, Y. Huh, S. Haam

MEDI **95.** Modular platform for the synthesis of a targeting and pH-responsive lipopeptide ligand in nanovectors. **M. Salinas**, G.R. Negrete

MEDI **96.** Fibrosis toolbox: Small molecules to investigate fibrosis pathways and mechanisms. **R. Hatley**

MEDI **97.** Novel Nrf2 activators from microbial transformation products suppress oxidant stress-induced cellular damage in ARPE-19 cells. **Y. Nakagami**, K. Masuda, E. Hatano, T. Inoue, S. Komoriya

MEDI **98.** Discovery of potent and selective S1P2 antagonists. **K. Kusumi**, A. Naganawa, H. Kurata, K. Shinozaki

MEDI **99.** Monster Mas agonist: Revealing the beauty in the beast. **J. Redmond**, S. Peace, G. Inglis, G. Vitulli, J. Barrett

MEDI **100.** Quatenary-ammonium salt derivatives as bifunctional muscarinic antagonist and beta2 agonist (MABA) for the treatment of COPD and asthma. **J. Igarashi**, E. Mitsuyama, T. Ida, H. Sugiyama, K. Segawa, J. Nomura

MEDI **101.** Novel strategy for the treatment of asthma by targeting $GABA_A$ receptors in the lung. **R. Jahan**, M.R. Stephen, G. Gallos, C.W. Emala, J.M. Cook

MEDI **102.** Design and synthesis of anti-inflammatory steroids with improved therapeutic index: Discovery of an inhaled dissociated steroid (selective glucocorticoid receptor modulator). **P.J. Biju**

MEDI **103.** Achieving desired levels of selectivity for a series of "acyclic-based" JAK inhibitors. **J. Kempson**, S.H. Spergel, S. Wrobleski, J. Das, L.M. Doweyko, J. Guo, J. Hynes, J. Duan, B. Jiang, Z. Lu, R.V. Moquin, S. Lin, H. Wu, B.V. Yang, S.M. Stachura, J.S. Tokarski, A. Gupta, J.C. Barrish, P.H. Carter, G.L. Schieven, W.J. Pitts

MEDI **104.** Determinants of activity at human toll-like receptors 7 and 8: Quantitative structure-activity relationship (QSAR) of diverse heterocyclic scaffolds. **E. Yoo**, D.B. Salunke, D. Sil, X. Guo, A.C. Salyer, A.R. Hermanson, M. Kumar, S.S. Malladi, R. Balakrishnan, W.H. Thompson, H. Tanji, U. Ohto, T. Shimizu, S.A. David

MEDI **105.** Enhancement of potency of the TLR7 ligand by conjugation to polysaccharide. **H. Shinchi**, T. Hayashi, M. Chan, A. Ahmadiiveli, S. Zhang, B. Crain, Y. Suda, H.B. Cottam, D. Carson

MEDI **106.** Design and synthesis of a dual-targeting liposomal spherical nucleic acid. **J. Ferrer**, N. Chernyak, J. Wertheim, C.A. Mirkin

MEDI **107.** Human toll-like receptor 8-selective agonistic activities in 1-alkyl-1*H*-benzimidazol-2-amines. **M. Beesu**, S.S. Malladi, L.M. Fox, C.D. Jones, A. Dixit, S.A. David

MEDI **108.** Design, synthesis, and testing of macrocyclic β-strand as protease inhibitors. **A.D. Pehere**, M. Pietsch, N.M. Paul, D.F. Callen, M. Gütschow, A.D. Abell

MEDI **109.** Single cell imaging and analysis for macrophage uptake of nanoparticles using fluorescent organosilica nanoparticles. **M. Nakano**, M. Nakamura, K. Hayashi, T. Kanadani, K. Miyamoto

MEDI **110.** Mitochondria targeted cardiolipin based high density lipoprotein mimicking nanoparticles for atherosclerosis. **R. Wen**, S. Dhar

MEDI **111.** Investigation on cellular uptake of functionalized gold nanoparticles and their biological effects. N. Ma, **C. Ma**, X. Mou, N. He

MEDI **112.** Molecular beacon-functionalized gold nanoparticle as miRNA detecting probe for cellular classification in gastric cancer. **K. Jisun**

MEDI **113.** Wire-framed gold nanoparticles for a multistep photothermic driven drug release system. **T. Lee**, D. Bang, J. Suh, Y. Huh, S. Haam

MEDI **114.** Virus-mimicking antimicrobial polymer brushes: The nanostructure and activity. **Y. Jiang**, W. Zheng, H. Liang

MEDI **115.** Targeting mitochondrial genome by cisplatin prodrug and its nanoparticle formulation to overcome chemoresistance. **R. Pathak**, S. Marrache, S. Dhar

MEDI **116.** Syntheses, characterization, and biomedical applications of novel organosilica nanoparticles. **M. Nakamura**

MEDI **117.** Activatable two-component photosentisizer: selective targeting and killing of cancer cells. **J. He**, Y. Wang, M.P. Bruchez

MEDI **118.** Withdrawn.

MEDI **119.** Silybin derivatives as antiprostate cancer agents: Synthesis and antiproliferative activity. **B. Vue**, S. Zhang, X. Zhang, K. Parisis, Q. Chen

MEDI **120.** Fluorescein hydrzones as novel nonintercalative topoisomerase catalytic inhibitors with low DNA toxicity. **A.M. Rahman**, S. Park, Y. Kwon, A.A. Kadi

MEDI **121.** Design and synthesis of a novel tri-branched asymmetric bowtie PAMAM dendrimer-based drug conjugate as a cancer theranostic agent. **L. Wei**, T. Wang, Y.G. Teng, I. Ojima

MEDI **122.** Synthesis and antitumor activity of *N,N'*-bisnaphthylated imidazole salts with lipophilic or hydrophilic substituents on the imidazole and benzimidazole rings. **K.L. Shelton**, P.O. Wagers, M.R. Southerland, M.A. DeBord, M.J. Panzner, N.K. Robishaw, C.A. Tessier, W.J. Youngs

MEDI **123.** Disrupting reactive oxygen species mediated pathways in human cancer models with ferrocenylated *N*-heterocyclic carbenes. **J.F. Arambula**, K. Arumugam, D.J. Magda, C. Bielawski, J.L. Sessler

MEDI **124.** Targeting the hypoxia-adenosinergic pathway via $A_{2A}R$ antagonists; Toward cancer immunotherapeutics. **G. Yuan**, S. Hatfield, M. Sitkovsky, M.J. Ondrechen, G. Jones

MEDI **125.** Triterpenoid derivatives and their biological activities. **M. Urban**, J. Sarek, M. Hajduch, J. Rehulka, P. Dzubak, L. Borkova

MEDI **126.** Development of a novel class of hydroxylated 2, 4-diphenyl indenopyridines as a selective non-intercalative topoisomerase IIα catalytic inhibitor. **T.M. Kadayat**, T. Thapa Magar, G. Bist, A. Shrestha, Y. Kwon, E. Lee

MEDI **127.** Preliminary structure-activity relationship studies of a fungal metabolite ophiobolin A – promising antiglioblastoma agent. **R. Dasari**, V. Mathieu, R. Kiss, A. Evidente, A.V. Kornienko

MEDI **128.** Identification of the first selective small molecule GRPR (BB2) antagonists. **N.D. Harriott**, S.B. Ravula, G. Beaton, N.J. Ashweek, J.P. Williams, S.R. Hoare, J. Fan

MEDI **129.** Withdrawn.

MEDI **130.** Bishomoisoprenoid triazoles as inhibitors of geranylgeranyl diphosphate synthase. **V.S. Wills**, J.I. Metzger, C. Allen, S.A. Holstein, D.F. Wiemer

MEDI **131.** Synthesis and structure-activity studies of drugs that affect a cancer causing mechanism and reduce cell growth. **A. Jelowicki**, K.E. Tan, E.H. Li, C. Wen, C.M. Ott, N.V. Patel, P. De Lijser, C.A. Martindale

MEDI **132.** Click chemistry approach to diversification of novel base-modified thymidine analogs that exhibit anticancer activity. **P.R. Wolfkiel**, K.M. Borland, E.J. Merino, M.C. Tranter, V.A. Litosh

MEDI **133.** Two-faced, biphenyl-based synthetic α-helix mimetics are effective inhibitors of the Mcl-1 oncoprotein. **M. Lanning**, P. Wilder, S. Fletcher

MEDI **135.** Structure-based design of functionalized salicylates as potent Mcl-1 inhibitors. **L. Chen**, J. Chauhan, J.L. Yap, P.T. Wilder, S. Fletcher

MEDI **136.** Design and synthesis of coumerin-aminoethylphenol hybrids as potential epigenetic modulators. **M. Branscum**, **T. Rowe**, J. Brider, M.A. Alam

MEDI **137.** Design and chemoproteomic functional characterization of a chemical probe targeted to bromodomains of BET family proteins. **B.A. Lefker**, K.F. Geoghegan, S.W. Wright, D.C. Limburg, J. Shin, C.M. Williams, P. Sahasrabudhe, P. Bonin, S. Ramsey

MEDI **138.** Identification and characterization of cellular histone deacetylase active site alterations Induced by deacetylase complex components. **T. Hanigan**, I. Kastrati, J. Frasor, P.A. Petukhov

MEDI **139.** Comparison of local and tropical plants used as herbal remedies and their chemical make-up. **M.D. Mann**

MEDI **140.** Transformations of allicin from garlic: The discovery of allylselenoalkylsulfonylpyridazines and Its antitumor activity. **M. Park**, **C. Kim**, **D. Shin**, M. **Choi**

MEDI **141.** Docking studies to develop GLI-associated oncogene inhibitors from natural products. **Y. Rifai**

MEDI **142.** Discovery of novel hit molecules for Sphingosine kinase -1 inhibitory activity by structure based virtual screening. C. Selvam, **B.C. Jordan**, S. Doshi

MEDI **143.** Novel method for targeting sphingosine kinase 2: Design, synthesis, and evaluation of bisubstrate inhibitors. **T.K. Dawson**, R. Dyer, Y. Kharel, K. Lynch, T.L. Macdonald

MEDI **144.** Serotonin-linked NSAIDs as inhibitors of FAAH, TRPV1, and COX 2. **T.M. Rose**, C.A. Reilly, C.E. Deering-Rice, C. Brewster, C. Brewster

MEDI **145.** Discovery of second generation P2X3 receptor antagonists for the treatment of chronic pain. **A. Ginnetti**, D. Paone, S. Stauffer, C. Potteiger, A. Shaw, J.Z. Deng, D.N. Nguyen, C. Segerdell, C.S. Burgey, S. Graham, J. Anquandah, A. Calamari, G. Cheng, S. Cook, S. Kane, M. Leitl, A. Liang, E. Moore, J. Panigel, C. Salvatore, M. Urban, J. Wang, K. Fillgrove, C. Tang

MEDI **146.** Design, synthesis, and in vitro evaluation of novel inhibitors of fatty acid amide hydrolase (FAAH). **S. Cramer**, J. Johnson, A. El-Alfy, J. Stec

MEDI **147.** Targeted far-red light activatable prodrugs: folate receptor-targeting, optical imaging, and a combination of photodynamic therapy and site-specific chemotherapy. G.N. Nkepang, **M. Bio**, P. Rajaputra, S.G. Awuah, Y. You

MEDI **148.** Synthesis of tripartite prodrugs via N → C amidative-installation of the Katzenellenbogen-spacer: Application of the *traceless* Staudinger ligation. **T. Kirby**, B.L. Barthel, T.H. Koch

MEDI **149.** Exploring CatSper channel openers and binding site interactions: Discovery of steroidal channel blockers. **E. Carlson**, J. Hawkinson, G.I. Georg

MEDI **150.** Enzyme sensitive conjugates as a macromolecular delivery platform for siRNA. **J.C. Carlson**, J. Benson, A. Sokoloff, D. Rozema, A.V. Blokhin

MEDI **151.** Development of a catalytic Mitsunobu reaction. **J.A. Buonomo**, C.C. Aldrich

MEDI **152.** Flow hydrogenation: A tool for creating 3D shaped molecules from flat precursors. **L. Kocsis**, S. Fekete, J. Gerencsér, G. Makara, F. Darvas

MEDI **153.** Discovery of potent α_{1L}-adrenoceptor agonists: Design and synthesis of bicyclic derivatives. **S. Suzuki**

MEDI **154.** Density functional calculations of the structural, thermodynamic, and spectroscopic properties of tautomers of avigan. F.L. Nesbitt

MEDI **155.** Novel 3-nitrotriazole-based amides and carbinols as bifunctional anti-chagasic agents. **M.V. Papadopoulou-Rosenzweig**, W.D. Bloomer, G.I. Lepesheva, H.S. Rosenzweig, M. Kaiser, E. Chatelain, J. Ioset

MEDI **156.** Syntheses and binding studies of novel benzimidazole compounds targeting the hepatitis C virus internal ribosome entry site. **A. Kanner**, A. Cholewczynski, D. Schmit, U. Milewicz, R. Wolkowicz, M.A. Boerneke, T. Hermann, M.B. Bergdahl

MEDI **157.** Discovery of MK-8325: A silyl proline containing HCV NS5A inhibitor with pan-genotype activity. **A.G. Nair**, Q. Zeng, S.B. Rosenblum, O. Selyutin, Y. Jiang, D. Yang, K. Keertikar, G. Zhou, M.P. Dwyer, S. Kim, S. Bandarpalle, W. Yu, L. Tong, R. Mazzola, J.P. Caldwell, H. Tang, R. Liu, E. Asante-Appiah, S. Agrawal, E. Xia, S. Curry, P. Ingravallo, J.A. Kozlowski

MEDI **158.** Discovery of silyl proline containing HCV NS5A inhibitors: SAR development. **J.A. Kozlowski**, N. Anilkumar, O. Selyutin, S.B. Rosenblum, Y. Jiang, D. Yang, K. Keertikar, G. Zhou, M.P. Dwyer, S. Kim, B. Shankar, W. Yu, L. Tong, R. Mazzola, J.P. Caldwell, H. Tang, S. Agrawal, E. Asante-Appiah, S. Curry, P. McMonagle, S. Black, A. Nomeir

MEDI **159.** Design and synthesis of dual-tropic HIV entry inhibitors that utilize a homologous CCR5/ CXCR4 binding site. **S. Gupta**, A.R. Prosser, B.D. Cox, L.J. Wilson, D. Liotta

‡ *Cooperative Cosponsorship*

MEDI **160.** Synthesis and biological evaluation of substituted pyrimidines. **B.S. Clark**, J. Kudrysch, S.Q. Smith, V.E. Zottig

MEDI **161.** Star-branched polymers with antioxidant activities. **U.G. Huynh**, C.Y. Lee, A. Sharma

MONDAY MORNING

Section A

Colorado Convention Center
Mile High Blrm 2A/2B

Innate Potential: Advances in Non-Biologic Modulation of Innate Immune Targets

A. J. Dyckman, J. Hynes, D. S. Weinstein, *Organizers, Presiding*

9:00 Introductory Remarks.

9:05 MEDI **162.** Structure-based design of small molecule modulators of TLR8. **S.A. David**

9:45 MEDI **163.** Development of novel IRAK4 inhibitors for the treatment of inflammation related disorders. **W.M. Seganish**, W.T. McElroy, S. Brumfield, G. Li, D. Tulshian, J. Tata, R. Herr, B.J. Lavey

10:15 MEDI **164.** Identification of highly potent and mono-selective RIP1 kinase inhibitors for the treatment of TNF-dependent diseases. **P.A. Harris**

10:45 MEDI **165.** Designing RIP2 kinase inhibitors for innate immunity-driven Indications. **L. Casillas**

11:15 MEDI **166.** Identification of selective TYK2 inhibitors and their role in IL12- and IL23-pathway signaling. **S. Magnuson**, J. Liang, V. Tsui, Y. Lai, B. Zhang, K. Williams, C. MacLeod, Y. Wenqian, S. Sohn, J. DeVoss, I. Peng, J. Lesch, M. Balazs, A. Van Abbema, K. Barrett, P. Bir Kohli, W. Blair, C. Chang, A. Johnson, L. Berezhkovskiy, J. Driscoll, P. Fan, A.N. Sambrone, P. Chiang, C. Eigenbrot, S. Shia, M. Ultsch, N. Ghilardi, L. Wu

11:45 MEDI **167.** Oligonucleotide inhibitors of endosomal toll-like receptors: Novel approach to treatment of autoimmune diseases. **S. Agrawal**

Section B

Colorado Convention Center
Mile High Blrm 1A/1B

Recent Advances in Targeting the Nav1.7 Sodium Channels

M. Chu-Moyer, *Organizer*
E. H. Harrington, *Organizer, Presiding*

9:00 MEDI **168.** Recent advances in therapeutic targeting of NaV channels. **D.C. Pryde**, B. Marron, N. Swain, C.W. West

9:30 MEDI **169.** Imaging pain generators in vivo using radiolabeled sodium channel toxin derivatives. **D. Behera**, A. Hoehne, W.H. Parsons, B. Shen, D.C. Yeomans, S. Biswal, F.T. Chin, J. Du Bois

10:00 MEDI **170.** Potent and selective Nav1.7 inhibitory peptides from tarantula venom. **K. Biswas**, J.K. Murray, B. Wu, J. Long, K. Sham, A. Zou, D. Liu, J.A. Ligutti, L. Poppe, J.B. Jordan, K.L. Andrews, S. McDonough, L.P. Miranda, B.D. Moyer

10:30 MEDI **171.** Identification of GNE-131: A potent and selective hNa$_v$1.7 inhibitor for the treatment of pain. **B.S. Safina**, G. Bankar, P. Bichler, C. Chabot, E. Chang, J. Chang, C. Chen, S. Chowdhury, C.J. Cohen, S. Decker, C.M. Dehnhardt, T. Focken, M.E. Grimwood, D. Hackos, I. Hemeon, K. Khakh, C. Koth, R. Kwan, S. Lin, K. Nelkenbrecher, D.F. Ortwine, J. Pang, J. Payandeh, L. Robinette, T. Sheng, S. Sun, M. Waldbrook, A. White, M. Wilson, C. Xie, C. Young, A. Zenova, Y. Zhang, D. Sutherlin

11:00 MEDI **172.** Design of subtype selective Na$_v$1.7 inhibitors for the treatment of pain. **N. Swain**

11:30 MEDI **173.** Development of oral Na$_v$1.7 inhibitors with excellent selectivity over Na$_v$1.5 for the treatment of pain. **M. Layton**, A.J. Roecker, J.E. Pero, M.S. Egbertson, B. Gomez, K. Jones, Z. Zhao, S. Wolkenberg, J. Mulhearn, M.J. Kelly, M.A. Rossi, H.D. Fiji, L. Zhao, P.J. De Leon, D. Li, K. Gilbert, A.K. Houghton, R. Kraus, B. Klein, M. Clements, C. Daley, J. Wang, T. Finger, J. Majercak, V. Santarelli, I. Gregan, M. Cato, T. Filzen, A. Jovanovska, Y. Wang, D. Wang, X. Peng, X. Wang

Section C

Colorado Convention Center
Mile High Blrm 2C

Approaches to Targeting RNA with Small Molecules

N. A. Meanwell, R. E. Olson, *Organizers, Presiding*

8:30 MEDI **174.** Rational design of small molecules to target the DNA/RNA of trinucleotide repeat (TNR) diseases. **S.C. Zimmerman**, L. Nguyen, L. Luu, J.Lee

9:05 MEDI **175.** New chemical and analytical tools for understanding RNA recognition. **B.L. Miller**

9:40 MEDI **176.** Identification of biologically active, RNA-binding small molecules using small molecule microarrays. **J. Schneekloth**

10:15 MEDI **177.** High-throughput platform assay technology for the discovery of pre-microRNA-selective small molecule probes. **A.L. Garner**

10:50 MEDI **178.** Giving SMN2 a push in the right direction: The discovery of small molecule splicing modulators. **M.G. Woll**, H. Qi, A. Turpoff, N. Zhang, X. Zhang, G. Chen, N.A. Naryshkin, A. Dakka, J. Narasimhan, V. Gabbeta, M. Weetall, X. Zhao, N. Risher, J. Sheedy, G.M. Karp

11:25 MEDI **179.** Progress on the development of rational methods to target RNA with small molecules. **M.D. Disney**

Medicinal & Aromatic Crops: Production, Phytochemistry, & Utilization

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Drug Discovery

Structural Informatics & Target Based: Structure-Based

Sponsored by COMP, Cosponsored by MEDI

MONDAY AFTERNOON

Section A

Colorado Convention Center
Mile High Blrm 1A/1B

New Models for Drug Discovery: Public, Private, and Non-Profit

J. Crawford, A. A. Estrada, B. Shotwell, *Organizers, Presiding*

2:00 MEDI **180.** Investigation of highly optimized LRRK2 kinase inhibitors in preclinical safety studies via a Michael J. Fox Foundation–Genentech collaboration. **A.A. Estrada**

2:30 MEDI **181.** New collaborative ways of discovering and developing anti-malarial therapies. **P. Willis**

3:00 MEDI **182.** ENABLE(ing) drug discovery: A public private partnership addressing antimicrobial resistance in serious gram negative infections. **A.T. Price**

3:30 MEDI **183.** Development of antiviral agents to treat poliovirus infections. **M. McKinlay**

4:00 MEDI **184.** Foundation-directed therapeutic development: Pfizer collaboration on PDE inhibitors. **C. Dominguez**

4:30 MEDI **185.** First small molecule clinical candidate discovered in Africa. **K. Chibale**

Section B

Colorado Convention Center
Mile High Blrm 2A/2B

Modulators of the Nuclear Receptor RORc

B. P. Fauber, S. J. Taylor, *Organizers, Presiding*

2:00 MEDI **186.** Development of RORalpha/beta/gamma subtype selective ligands. **T.P. Burris**

2:25 MEDI **187.** Small molecule inhibitors of RORgamma t: Their development to study the function of inflammatory immune cells. **J. Huh**

2:50 MEDI **188.** Structural basis for the inverse agonism of novel RORγt Inhibitors. **X. Li**

3:15 MEDI **189.** Optimization of quinoline tertiary alcohols as modulators of RORgt. **K. Leonard**, A. Fourie, X. Xue, M.J. Urbanski, H. Venkatesan, K. Barbay, D.A. Kummer, R. Nishimura, R.L. Wolin, K.D. Kreutter, C.R. Woods, V.M. Tanis, A. Wang, W. Jones, K. McClure, S.D. Goldberg, E. Fennema, C. Martin, J. Pierce, G. Bacani, J. Spurlino, C. Schalk-Hihi, C. Milligan, P. Wilkinson, T. Cao, M.C. Abad, R. Luna, K. Herman, A. De Leon, E. Nulton, M. Nelen, J. Yu, M.D. Cummings, B. Scott, K. Sepassi, S. Nguyen, M. Sablad, N. Rozenkrants, Y. Zhang, T. Rao, A. Ndifor, S. Branum, J. Spink, C.A. Teleha, D. Pippel, R. Russell, T. Schlueter, J.P. Edwards

3:40 MEDI **190.** Dealing with a highly lipophilic binding pocket: design and development of novel RORg inverse agonists with the consideration of ligand polarity and conformational diversity. **J. Chao**

4:05 MEDI **191.** Reversed sulfonamide series of selective RORc inverse agonists. **M.B. van Niel**, B.P. Fauber, M. Cartwright, S. Gaines, J.C. Killen, O. René, S.I. Ward, G.d. Boenig, Y. Deng, C. Eidenschenk, C. Everett, E. Gancia, A. Ganguli, A. Gobbi, J. Hawkins, A.R. Johnson, J.R. Kiefer, H. La, P. Lockey, M. Norman, W. Ouyang, A. Qin, N. Wakes, B. Waszkowycz, H. Wong

4:30 MEDI **192.** Discovery of novel RORγ antagonists. **M. Shiozaki**

Section C

Colorado Convention Center
Mile High Blrm 2C

Symposium in Honor of Richard Gibbs

B. Blagg, T. E. Prisinzano, *Organizers, Presiding*

2:00 MEDI **193.** Targeting indenoisoquinoline topoisomerase I inhibitors to cancer cells. D.E. Beck, T. Nguyen, W. Lv, P.N. Reddy, M. Abdelmalak, K. Agama, C. Marchand, Y. Pommier, J. Roy, A. Kanduluru, C. Venkatesh, P. Low, **M. Cushman**

2:35 MEDI **194.** Inhibition of geranylgeranyl diphosphate synthase by isoprenoid bisphosphonates. **D.F. Wiemer**

3:10 MEDI **195.** Small molecule epigenetic modulators for the treatment of cardiovascular disorders. C.J. Kutz, S.L. Holshouser, **P.M. Woster**

3:45 MEDI **196.** Protein prenylation: From enzymology to biotechnology and therapeutic application. **M.D. Distefano**, Y. Wang, C.C. Palsuledesai, J.K. Dozier

4:20 MEDI **197.** Biosynthesis of squalene: A new pathway in bacteria. J. Pan, **C.D. Poulter**

Medicinal & Aromatic Crops: Production, Phytochemistry, & Utilization

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Undergraduate Research Posters

Medicinal Chemistry

Sponsored by CHED, Cosponsored by MEDI and SOCED

Drug Discovery

ADME & Informatics

Sponsored by COMP, Cosponsored by CINF and MEDI

MONDAY EVENING

Section A

Colorado Convention Center
Halls C/D

Sci-Mix

W. B. Young, *Organizer*

8:00 - 10:00
44, 53, 56, 68, 70, 78, 84, 96, 99, 128, 137.
See previous listings.
278, 286, 294, 298, 323, 331, 333, 338, 343.
See subsequent listings.

TUESDAY MORNING

Section A

Colorado Convention Center
Mile High Blrm 2A/2B

E. B. Hershberg Award for Important Discoveries in Medicinally Active Substances: Symposium in Honor of Ruth R. Wexler

Cosponsored by WCC

W. B. Young, *Organizer*
J. E. Macor, *Presiding*

9:00 MEDI **198.** Lessons learned in the practice of medicinal chemistry. **P.S. Anderson**

9:35 MEDI **199.** In search of small molecule modulators for the treatment of autoimmune and inflammatory diseases. **J.C. Barrish**

10:10 MEDI **200.** Thrombin receptor antagonists for the prevention of arterial thrombosis: Discovery of vorapaxar (zontivityTM). **W.J. Greenlee**

10:45 MEDI **201.** Structure-based design of serine protease inhibitors: The quest for safer and efficacious anticoagulants. **M.L. Quan**

11:20 MEDI **202. Award Address**
(E. B. Hershberg Award for Important Discoveries in Medicinally Active Substances sponsored by Merck Research Laboratories). Adventures in cardiovascular drug discovery: New frontiers and lessons learned. **R.R. Wexler**

Section B

Colorado Convention Center
Mile High Blrm 1A/1B

Observations from Recent Drug Launches: The Rules of Today May Not Apply Tomorrow

J. B. Schwarz, *Organizer, Presiding*

9:00 MEDI **203.** Discovery of macitentan: Can we apply rules of yesterday tomorrow? **M.H. Bolli**

9:30 MEDI **204.** Discovery and development of covalent BTK inhibitors. **W. Chen**

10:00 MEDI **205.** Chiral, nonracemic hemi-aminals to the rescue: The discovery of the HIV-1 integrase inhibitors dolutegravir and cabotegravir. **B.A. Johns**

10:30 Intermission.

10:45 MEDI **206.** Discovery of thalidomide and amino substituted analogs as anticancer agents. **R. DAmato**

11:15 MEDI **207.** Ponatinib, a pan-Bcr-Abl kinase inhibitor approved for leukemia treatment, potently inhibits the T315I mutant and overcomes mutation-based resistance. **W. Huang**

11:45 MEDI **208.** Pirfenidone and optimized pirfenidone analogs for antifibrotic indications. J.Y. Ramphal, L. Pan, C. Schaefer, S.D. Seiwert, B.O. Buckman, **J.B. Schwarz**

Section C

Colorado Convention Center
Mile High Blrm 2C

Why You Should Have Paid Attention in P-Chem: Thermodynamics in Drug Discovery

A. J. Peat, B. Shotwell, *Organizers, Presiding*

9:00 MEDI **209.** Thermodynamic-based approach to the inhibition of HIV-1 cell infection. **E. Freire**

9:30 MEDI **210.** Thermodynamics guided lead discovery and optimization. **G.M. Keseru**

10:00 MEDI **211.** Ligand-protein binding thermodynamics from fragments to drugs. **G. Ferenczy**

10:30 Intermission.

10:45 MEDI **212.** Exploring applications and origins of binding kinetics in structure-based drug discovery. **D. Meinhold**

11:15 MEDI **213.** Accelerating drug discovery: the role of free energy calculations. **R. Abel**, R. Friesner, R. Farid, T. Lin, L. Frye, J. Knight, G. Krilov, L. Wang

11:45 MEDI **214.** Lipophilic efficiency as a tool for identifying and optimizing enthalpic interactions. **M.D. Shultz**

GSSPC: Designed by Nature, Developed by Science: Interdisciplinary Perspectives on Biocatalysis

Sponsored by CHED, Cosponsored by ANYL, BIOL, CATL, ENVR, I&EC, MEDI, ORGN and PRES

Phenolic & Polyphenolic Chemistry in Food Processing

Reactions/Properties

Sponsored by AGFD, Cosponsored by AGRO, BIOT, COMP and MEDI

Drug Discovery

Methodology

Sponsored by COMP, Cosponsored by CINF and MEDI

TUESDAY AFTERNOON

Section A

Colorado Convention Center

Mile High Blrm 1A/1B

Smissman Award: Symposium in Honor of Dennis Liotta

W. B. Young, *Organizer*

J. E. Macor, *Presiding*

2:00 MEDI **215.** Nucleoside analogs: Synthesis and medicinal chemistry. **Y. Guindon**, M. Prévost, S. Dostie, P. Mochirian, G. Tambutet

2:45 MEDI **216.** Therapeutic opportunities of chemical targeting of mitochondria. **P. Wipf**

3:30 MEDI **217.** Targeting protein-protein interactions for new cancer therapeutics. **S. Wang**

4:15 MEDI **218.** Discovery of novel therapeutics for treating various types of viral diseases, cancers, and inflammatory disorders. **D. Liotta**

Section B

Colorado Convention Center

Mile High Blrm 2A/2B

The Role of Rings in Drug Design

N. A. Meanwell, P. M. Scola, *Organizers, Presiding*

2:00 MEDI **219.** Rings in drugs. **R. Taylor**

2:35 MEDI **220.** Small, medium, and large ring systems: Observations and examples of their roles in molecular recognition and drug design. **D.L. Cheney**

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3:10 MEDI **221.** Development of novel transition metal-catalyzed approaches toward heterocycles. **V. Gevorgyan**

3:45 MEDI **222.** Rings in (candidate) drugs: Case stories. **J. Boström**

4:20 MEDI **223.** Sulfur-containing heterocycles in drug design. **M.D. Bartberger**

GSSPC: Designed by Nature, Developed by Science: Interdisciplinary Perspectives on Biocatalysis

Sponsored by CHED, Cosponsored by ANYL, BIOL, CATL, ENVR, I&EC, MEDI, ORGN and PRES

Phenolic & Polyphenolic Chemistry in Food Processing

Sources

Sponsored by AGFD, Cosponsored by AGRO, BIOT, COMP and MEDI

Drug Discovery

Methodology

Sponsored by COMP, Cosponsored by CINF and MEDI

WEDNESDAY MORNING

Section A

Colorado Convention Center

Mile High Blrm 2A/2B

General Oral Session

W. B. Young, *Organizer*

J. Rudolph, *Presiding*

8:30 MEDI **224.** Discovery and synthesis of first-generation single-drug "cocktails" to combat HIV. **A.R. Prosser**, B.D. Cox, S. Gupta, L.J. Wilson, D.C. Liotta

8:55 MEDI **225.** B-DNA structure-based removal of genotoxicity from a series of inhibitors of the IκB-kinase IKK2. **L. Borjesson**, **I. Shamovsky**, M. Andersson, T. Brimert, C. Ekström, A.K. Ray, P. Zlatoidsky, P. Åberg

9:20 MEDI **226.** Selective inhibition of group-II p-21-activated kinases (PAKs). **S.T. Staben**, J. Feng, W. Wang

9:45 MEDI **227.** Discovery of novel indole derived mineralocorticoid receptor antagonists. **A.K. Ogawa**

10:10 MEDI **228.** Discovery of phosphonic acid containing LpxC inhibitors as broad spectrum antibacterial agents. **Q. Dang**, P. McNicholas, D. Olsen, P.T. Meinke

10:35 MEDI **229.** Discovery of novel anti-chagas agents targeting *T. cruzi* CYP51. **J. Choi**, D. Vieira, C. Claudia, J. Siqueira-Neto, D. Kellar, J. Gut, J. Johnston, M. Cameron, J. McKerrow, L. Podust, W.R. Roush

11:00 MEDI **230.** Potent and selective pyridone BTK inhibitors with activity against mutant forms of BTK. **J. Crawford**

11:25 MEDI **231.** Understanding our love affair with *para*-chlorophenyl: Scientific rationale or unsubstantiated bias? **D.G. Brown**, M. Gagnon, J. Boström

11:50 MEDI **232.** Learning from experience: 15 years of protein-fragment X-ray crystal structures and the consequences for fragment library design. **D. Norton**

Section B

Colorado Convention Center

Mile High Blrm 1A/1B

Advances in the Treatment of Fibrotic Diseases

P. Devasthale, *Organizer*

W. B. Young, *Presiding*

8:30 MEDI **233.** Organ and tissue fibrosis: Principles and prospects for therapy. **S. Friedman**

9:00 MEDI **234.** Therapeutic targeting of Nox4 leads to reversal of age-associated persistent fibrosis. **L. Hecker,** N. Logsdon, L.H. Hurley, V. Thannickal, J. Garcia

9:30 MEDI **235.** Development of a small molecule inhibitor of integrin αvβ1. **W.F. Degrado**

10:00 MEDI **236.** Development of novel sGC activators that protect against the progression of diabetic nephropathy in ZSF-1 rats. **C.R. Sarko**, J. Brenneman, T. Bosanac, C. Boustany, H. Chen, H. Clifford, R. Fryer, J. Ginn, P.C. Harrison, J.I. Levin, K. Lincoln, H. Qian, S. Pullen, G. Reinhart, J. Richman, H. Wang, D. Wong, K. Gueneva-Boucheva

10:30 MEDI **237.** Galectin-3 antagonists with therapeutic implications in fibrosis. **U.J. Nilsson**, H. Leffler, H. Schambye, A. Mackinnon, T. Sethi

11:00 MEDI **238.** Needs and challenges in anti-fibrosis drug discovery: Experience from JNK inhibitors. **Y. Satoh**

11:30 Discussion.

Section C

Colorado Convention Center

Mile High Blrm 2C

Small Molecule Approaches to Autism Spectrum Disorder Therapy

K. A. Emmitte, *Organizer, Presiding*

9:00 Introductory Remarks.

9:05 MEDI **239.** Harnessing rodent models to develop new therapeutic targets in autism spectrum disorder. **J. Veenstra-VanderWeele**

9:40 MEDI **240.** Therapeutic strategies for restoring excitatory/inhibitory balance in Rett syndrome: Focus on BDNF/TrkB signaling. **D. Katz**

10:15 MEDI **241.** Utility of NMDA antagonists for the treatment of Rett syndrome. **R.J. Mather**

10:50 MEDI **242.** Development of a highly selective and CNS penetrant $mGlu_5$ NAM: An in vivo tool for further elucidating the role of group II mGlus in psychiatric disorders. J.L. Engers, L.C. Konkol, A.L. Rodriguez, R.D. Morrison, F.W. Byers, A.D. Thompson Gray, J.S. Daniels, C.M. Niswender, C.K. Jones, P.J. Conn, C.W. Lindsley, **K.A. Emmitte**

11:25 MEDI **243.** Approaches toward the identification of rodent models of autism spectrum disorder suitable for use in lead optimization efforts. **C.K. Jones**

Drug Discovery

Ligand-Based

Sponsored by COMP, Cosponsored by CINF and MEDI

WEDNESDAY AFTERNOON

Section A

Colorado Convention Center

Mile High Blrm 1A/1B

First Time Disclosures

L. A. Thompson, *Organizer, Presiding*

1:30 MEDI **244.** Discovery of JNJ-42847922, a selective orexin-2 antagonist for the treatment of insomnia disorder. **M.A. Letavic**, P. Bonaventure, K.S. Ly, Z. Aguilar, L. Aluisio, N.I. Carruthers, S. Chaplan, C. Dugovic, R. Halter, T. Koudriakova, B. Lord, T.W. Lovenberg, M. Kramer, K.L. Morton, A. Ndifor, M. Rizzolio, C. Shah, J. Shelton, J. Shoblock, S. Sutton

2:05 MEDI **245.** Discovery and optimization of the human histamine H4 antagonist Toreforant (JNJ38518168) for the treatment of inflammatory diseases. **J.D. Venable**, D.E. Kindrachuk, D.J. Buzard, P.J. Dunford, L. Karlsson, R.L. Thurmond, J.P. Edwards

2:40 MEDI **246.** Discovery of MK-8931: A BACE inhibitor in Phase 3 clinical development for Alzheimer's disease. **J.N. Cumming**, J.D. Scott, S.W. Li, M. Cartwright, X. Chen, K. Cox, M. Forman, E.J. Gilbert, R. Hodgson, L. Hyde, Y. Jin, I. Kazakevich, R. Kuvelkar, X. Liang, H. Mei, J. Misiaszek, P. Orth, J. Stone, C. Strickland, J.H. Voigt, H. Wang, B. Werner, J. Wong, E.M. Parker, W.J. Greenlee, M.E. Kennedy, A.W. Stamford

3:15 MEDI **247.** Discovery of GSK2881078A: A selective androgen receptor modulator (SARM) for the treatment of muscle wasting disorders. **P. Turnbull**, R. Cadilla, Y. Shen, C. Poole, E. Stewart, R. Gampe, R. Clark, B.R. Henke, A. Russell

3:50 MEDI **248.** Discovery of a next generation irreversible inhibitor targeting the resistance mutation T790M and activating mutations in NSCLC with a broad selectivity margin over EGFR wild type. **S. Planken**, B.W. Murray, J. Lafontaine, S. Weinrich, M. Hemkens, J.C. Kath, S.K. Nair, T.O. Johnson, H. Cheng, S.C. Sutton, M. Zientek, M. Yin, J. Solowiej, A. Nagata, K. Gajiwala

4:25 MEDI **249.** Discovery and early development of vibegron (MK-4618): A potent and selective β_3-AR agonist for the treatment of overactive bladder. **S. Edmondson**, C. Zhu, N.F. Kar, R. Berger, S.D. Goble, B. Harper, G. Morriello, C. Moyes, L. Wang, P.N. Brown, K.H. Dingley, J. DiSalvo, A. Fitzmaurice, T. Frenkl, S.A. Green, A.L. Hurley, N. Jochnowitz, S. Khalilieh, R.R. Miller, H. Nagabukuro, J.D. Ormes, B. Sacre-Salem, G.M. Salituro, D. Stickens, A.A. Kulick, A.T. Sanfiz, A. Stevenson, K. Villa, L.A. Wickham, B.A. Zamlynny, M. Struthers, A.E. Weber

Section B

Colorado Convention Center

Mile High Blrm 2A/2B

MEDI Award Symposium

W. B. Young, *Organizer*

J. E. Macor, *Presiding*

2:00 MEDI **250.** Phenylalkylaminome: Scaffolding for drugs of abuse, with a focus on synthetic cathinones. **R.A. Glennon**

2:45 MEDI **251. Award Address** (George and Christine Sosnovsky Award for Cancer Research sponsored by the George and Christine Sosnovsky Endowment Fund). Design and development of ligand-targeted therapies and imaging agents for multiple human diseases. **P.S. Low**, C.P. Leamon, J. Reddy, I.R. Vlahov

3:30 MEDI **252. Award Address** (George and Christine Sosnovsky Award for Cancer Research sponsored by the George and Christine Sosnovsky Endowment Fund). Personalized medicine using targeted small molecule drug conjugates and companion imaging agents for cancer therapy. **C.P. Leamon**

4:15 MEDI **253. Award Address** (Earle B. Barnes Award for Leadership in Chemical Research Management sponsored by the Dow Chemical Co. Foundation). Getting the chemistry right: Catalyzing translational innovation at NIH. **C.P. Austin**

Section C

Colorado Convention Center

Mile High Blrm 2C

General Oral Session

W. B. Young, *Organizer*

J. J. Bronson, *Presiding*

1:30 MEDI **254.** Design, synthesis, and biological evaluation of manassantin analogues for HIF-1α inhibition. **D. Kwon**, K. Park, D. Weitzel, S. Lee, T. Stephenson, C. Lee, J. Chi, R. Mook, M. Dewhirst, Y. Lee, J. Hong

1:50 MEDI **255.** First discovery of a single digit nanomolar small molecule protein-protein interaction blocker. L.K. Petersen, F. Sloek, P. Blakskjaer, L. Larsen, J. Holmkvist, A.B. Christensen, J. Rasmussen-Dietvorst, T. Hansen, **N. Hansen**

2:10 MEDI **256.** Discovery of the mGlu5 receptor NAM HTL14242 by fragment based drug discovery. M. Congreve, S.J. Aves, K.A. Bennett, J.A. Christopher, A.S. Doré, J.C. Patel, B. Tehan, F.H. Marshall

2:30 MEDI **257.** Small molecules targeting XBP-1s expression in CLL. **J.R. Del Valle**, S. Ranatunga, C. Kang, C. Hu

2:50 MEDI **258.** Stabilized cyclopropane analogs of the spliceosome Inhibitor FD-895. **M.D. Burkart**

3:10 MEDI **259.** Investigating aromaticity effects In the tail region of sphingosine kinase 2 selective guanidine-based inhibitors. **M.D. Congdon**, Y. Kharel, K. Lynch, W. Santos

‡ *Cooperative Cosponsorship*

3:30 MEDI **260.** Repurposing aspartic protease inhibitors as novel antimalarial agents. **M.J. Meyers**

3:50 MEDI **261.** Chemical optimization of novel inhibitor classes selectively targeting PI4KIIIbeta: A host lipid kinase crucial for enterovirus replication. **A. Leivers**, A. Maynard, A.J. Peat, E. Nartey, J. Shotwell, J. Botyanszki, J. Gobel, J. Catalano, J.F. Miller, J. Seal, L. Want, L. Shewchuk-Chapman, P.Y. Chong, P. Xiong, S. Dickerson, S. You, V.W. Tai

4:10 MEDI **262.** Variation in ADC linker composition generated from aldehyde-tagged antibodies impacts both efficacy and PK. **A.W. Garofalo**

4:30 MEDI **263.** HIV microbicide development using a combination of QSAR and structure-based approaches. **L. Guasch**, A.V. Zakharoz, M.C. Nicklaus

4:50 MEDI **264.** Dihydroquinazolines: A novel class of hOCT3 inhibitors. **M. Dukat**, X. Pan, M. Argade, K.A. Iyer, P.D. Mosier, D. Sweet

Drug Discovery

Ligand-Based

Sponsored by COMP, Cosponsored by CINF and MEDI

WEDNESDAY EVENING

Section A

Colorado Convention Center

Four Seasons Ballroom

General Poster Session

W. B. Young, *Organizer*

7:00 - 9:00

MEDI **134.** Amphipathic α-helix mimetics based on a 1,4-disubstituted 2,3,4,5-tetrahydro-1*H*-benzo[e][1,4]diazepine: Inhibition of the Mcl-1 oncoprotein. **L. Chen**, K. Jeong, S. Fletcher

MEDI **265.** Physical compatibility of co-solubilized vancomycin, piperacillin, and tazobactam in aqueous solution. **R.N. Mason**, S.C. Butler, H.N. Gray, H.S. Gray

MEDI **266.** Development and validation of RP-HPLC method for simultaneous determination of guaifenesin impurities in multidrug combinations. **R. Grigoryan**

MEDI **267.** Carbon monoxide releasing property of amine carboxyboranes. **N.N. Dingra**

MEDI **268.** Use of Fc receptor affinity separation resin to obtain high potency glycoforms (nonfucocylsated) of antiviral immunoglobulin. **A. Boesch**, G. Bolton

MEDI **269.** Structure-activity relationships of prazole fragment inhibitors of *T. vaginalis* uridine nucleoside ribohydrolase using NMR-based activity and binding assays. **T.A. Shea**, M.A. VanAlstine-Parris, B.J. Stockman

MEDI **270.** Aminomethyl spectinomycins as novel therapeutics for drug resistant respiratory tract and sexually transmitted bacterial infections. **S.L. Waidyarachchi**, D.F. Bruhn, J. Liu, D.B. Madhura, D. Shcherbakov, Z. Zheng, Y. Abdelrahman, A. Singh, C. Rathi, R. Belland, B. Meibohm, J. Rosch, E. Böttger, R.E. Lee

MEDI **271.** Targeting *Mycobacterium tuberculosis* biotin protein ligase (MtBPL): Synthesis and evaluation of nucleoside-based bisubstrate adenylation inhibitors. **M.R. Bockman**, A. Kalinda, D. Tiwari, T. De la Mora, B. Finzel, D. Schnappinger, C.C. Aldrich

MEDI **272.** Hybridization of metronidazole with natural product tetramic acids improves its antidifficile efficacy. **P.T. Cherian**, X. Wu, R.E. Lee, J. Hurdle

MEDI **273.** Lipidated cyclice gamma-AA peptides display both antimicrobial and anti-inflammatory activities. **Y. Li**, C. Smith, H. Wu, S. Padhee, H.H. Yin, J. Cai

MEDI **274.** Design and biological evaluation of novel Cdc42 inhibitors. **B.J. Aguilar**, **B. Hinckley**, S. Huo, Y. Chen, Q. Lu

MEDI **275.** Development of $\alpha_4\beta_3\gamma_2$-subtype selective ligands for $GABA_A$ receptors. **R.S. Verma**, C. Witzigmann, J.M. Cook

MEDI **276.** Quantitative structure-activity relationship (QSAR) investigations of abuse-related neurochemical and behavioral effects of para-substituted methcathinone derivatives. **F. Sakloth**, R. Kolanos, M. Barnier, P.D. Mosier, J. Partilla, M.H. Baumann, R.A. Glennon

MEDI **277.** Structure-activity studies on the α-modified analogs of the abused substance methylenedioxypyrovalerone (MDPV) as reuptake inhibitors at the dopamine transporter (DAT). **F. Sakloth**, R. Kolanos, A.D. Jain, J. Partilla, M.H. Baumann, R.A. Glennon

MEDI **278.** Synthesis, SAR, and progress toward orally available, brain penetrant P2X7R antagonists for the treatment of neuroinflammatory disorders. **C. Chrovian**

MEDI **279.** Structure-activity relationships of iminoheterocyclic BACE1 inhibitors: Discovery of MK-8931 for the treatment of Alzheimer's disease. **J.D. Scott**, S.W. Li, X. Chen, K. Cox, J. Cumming, M. Forman, E.J. Gilbert, W.J. Greenlee, R. Hodgson, C. Huang, L. Hyde, Y. Jin, U. Iserloh, I. Kazakevich, R. Kuvelkar, G. Li, X. Liang, J. Misiaszek, P. Orth, E.M. Parker, C. Strickland, J.H. Voigt, H. Wang, B. Werner, J. Wong, M.E. Kennedy, A.W. Stamford

MEDI **280.** Robust and efficient amination route toward the development of N-substituted piperazines as serotonergic ligands for autism spectrum disorder. **J. Dhuguru**, S.W. Goldstein, A. Khalil, O.M. Ghoneim

MEDI **281.** Computational approach for performing medchem transformations within a 3D active site. **M.R. Goldsmith**

MEDI **282.** Applying extended Huckel theory to pharmacophore modeling. **A. Deschenes**

MEDI **283.** Exploring the role of solvation in drug design and optimization. **M.L. Drummond**, J. Truchon, C. Williams, P. Labute

MEDI **284.** Performance of structure based and ligand based virtual screening methods for ten selected anticancer targets. **C. Selvam**, T. Ramasamy

MEDI **285.** Scaffold hopping: Balancing novelty, accessibility, and physicochemical properties. **T. Cheeseright**, S. Tomásio, P. Tosco, M. Mackey

MEDI **286.** Discovery of KSI-6666, a novel S1P1 antagonist for the treatment of autoimmune disease. **Y. Ohsawa**, **H. Inoue**, T. Suzuki, Y. Maruyama, K. Ohno, N. Arisaka, S. Muto, Y. Okuhara, M. Hayashi, A. Yamamoto, K. Kaidoh, H. Mukaiyama, M. Hiratochi

MEDI **287.** Discovery of a new indole-based group IVA cytosolic phospholipase A_2 inhibitor as a promising drug candidate for treatment of respiratory diseases. **T. Tomoo**, T. Nakatsuka, T. Katayama, Y. Hayashi, Y. Fujieda, M. Terakawa, K. Nagahira

MEDI **288.** Controlled-release mechanism for sulfur mustard anti-inflammatory drugs based on polyamine platform. C.J. Lacey, J. Saxena, **C.D. Guillon**, G.M. Composto, L.B. Joseph, D.E. Heck, J.D. Laskin, N.D. Heindel

MEDI **289.** Synthesis and anti-inflammatory activity of three nitro chalcones. **A. Gómez** Rivera, C.E. Lobato Garcia, H. Aguilar Mariscal, N. Romero Ceronio

MEDI **290.** Microwave assisted synthesis, pharmacological activities, and molecular docking studies of Ethyl 2-substituted-4-(2-thienyl) thiazole-5-acetates. **M. Attimarad**, M.A. Khedr, B.E. AlDubaib

MEDI **291.** Toward a bioisosteric alkahest: Targeting the human dehydroorotate dehydrogenase (hDHODH) by a scaffold hopping bioisosteric approach using hydroxylated pentaatomic heterocycles. **M.L. Lolli**, A.C. Pippione, S. Sainas, S. Mensa, M. Giorgis, M. Piccinini, E. Lupino, S. Al-Kadaraghi, D. Boschi

MEDI **292.** Discovery of thienopyrimidinones as a new series of potent phosphodiesterase 7 inhibitors. **Y. Endo**, K. Kawai, T. Asano, S. Amano, K. Sawada, K. Ogura, N. Ueo, N. Takahashi, Y. Sonoda, M. Nagai, N. Kamei

MEDI **293.** Development of fluorescent affinity probes for the $P2Y_{14}$G protein-coupled receptor. **E. Kiselev**, M. Barrett, E. Hammes, V. Katritch, R. Balasubramanian, A. Yin, S. Paoletta, C. Weitzer, Q. Zhao, R. Stevens, T. Harden, K. Jacobson

MEDI **294.** Design, evolution, and in vivo profile of a novel series of GPBAR 1 agonists for the treatment of diabetes and metabolic syndrome. **R. Kurukulasuriya**, S.K. Shah, J. Dellureficio, S. Fung, L. Guo, J. Szewczyk, M. Trujillo, R.P. Nargund, W.K. Hagmann, A. Pocai, R.J. Devita

MEDI **295.** Withdrawn.

MEDI **296.** Benzothiazolyl substituted iminothiazolidinones and benzamido-oxothiazolidines as potent and partly selective aldose reductase inhibitors. **J. Iqbal**

MEDI **297.** Design and bioevaluation of novel human 4-hydroxyphenylpyruvate dioxygenase inhibitors. **H. Lin**, G. Yang, W. Yang

MEDI **298.** Targeting integrin $\alpha_v\beta_3$ receptors with multivalent RGD peptidomimetics. **J.L. Teh**, R.N. Hanson, S. Sridhar

MEDI **299.** Design, synthesis, topoisomerase I and II inhibitory activity, cytotoxicity, and structure-activity relationship study of novel 2-phenyl-4-aryl indenopyridines. **G. Bist**, T.M. Kadayat, T. Thapa Magar, A. Shrestha, Y. Kwon, E. Lee

MEDI **300.** Importance of side chain orientation on large macrocycles: Structure activity relationship of sanguinamide B analogs on colon cancer HCT-116 cells. **A. Pietkiewicz**, H. Wahyudi, J. McConnell, S. McAlpine

MEDI **301.** Synthesis, characterization, and in vitro anticancer activity of quinolylmethyl- and napthylmethyl-substituted imidazolium salts. **P.O. Wagers**, M. DeBord, M.J. Panzner, C. Tessier, W.J. Youngs

MEDI **302.** Development of novel casein kinase 1 nhibitors. **R.L. Schroeder**, N.A. Pham, P. Tram, T. Stone, K. Nguyen, J. Geathers, D.Q. Nguyen, E. Skripnikova, M.R. Bratton, J. Sridhar

MEDI **303.** Synthesis and biological evaluation of novel naphthoquinones as HER2 inhibitors for the treatment of trastuzumab resistant breast cancer. **R.L. Schroeder**, M.E. Sfondouris, M.R. Bratton, N.A. Pham, P. Tram, T. Stone, K. Nguyen, J. Geathers, D.Q. Nguyen, C.L. Stevens, F.E. Jones, J. Sridhar

MEDI **304.** Anthracenyl isoxazole amides (AIMs) stabilize quadruplex DNA structures in telomeric and c-MYC promotor sequences. **S. Stump**, M.J. Weaver, N.S. Duncan, A.K. Kearns, N.R. Natale, H.D. Beall

MEDI **305.** Design, synthesis, and biological screening of novel estrone analogs toward treatment of hepatocellular carcinoma. **M. Mahnashi**

MEDI **306.** Synthesis, structure-activity relationship (SAR) study, and mode of action study of cationic triazole analogs of 1,4-naphthoquinone: A new class of highly potent anticancer agent. **J.P. Shrestha**, C.T. Chang

MEDI **307.** ZMPSTE24 protease inhibitors as senescence agonists for cancer chemotherapy. **D. Xanthopoulos**, A. Matralis, H. de Vries, G. Huot, G. Ferbeyre, Y.S. Tsantrizos

MEDI **308.** Thio-sugars can sensitize human cervixadenocarcinoma (Hela) cancer cells to Bleomycin and ROS generator. J. Sarnik, A. Czubatka, T. Poplawski, **Z.J. Witczak**

MEDI **309.** Low glucose level enhances the cytotoxicity of CARB-pharmacophore to cancer cells. A. Czubatka, J. Sarnik, T. Poplawski, Z.J. Witczak

MEDI **310.** N,N'-bisquinolylmethyl-2-alkyl and N-quinolylmethyl-N'-naphthylmethyl-2-alkyl substituted imidazolium salts as potential therapeutics for the treatment of lung cancer: Synthesis, characterization, and in vitro anticancer activity. **M. DeBord**, P.O. Wagers, M.J. Panzner, C. Tessier, W.J. Youngs

MEDI **311.** 2,4-Diaryl-indenopyridine derivatives: Design, synthesis, topoisomerase I and II inhibition, cytotoxicity, and structure-activity relationship study. **T. Thapa Magar**, T.M. Kadayat, G. Bist, A. Shrestha, Y. Kwon, E. Lee

MEDI **312.** Mechanistic studies of imidazolium salts as antitumor agents. **M.R. Southerland**, P.O. Wagers, M. DeBord, K.L. Shelton, L. Shriver, S.M. Paruchuri, C. Tessier, M.J. Panzner, W.J. Youngs

MEDI **313.** Design, synthesis, and in vitro anticancer activities the 7-chloro-6-fluoro-N-subsituted-2-phenylquinoline-4-carboxamide derivatives. **A.P. Patel**, H.G. Bhatt

MEDI **314.** Synthesis of pyrazole derivatives as potential cytotoxic agents. **T. Rowe**, **J. Brider**, M. Branscum, M.A. Alam

MEDI **315.** Synthesis of curcumin mimics with substituted triazolyl groups and their sensitization effect of TRAIL against brain cancer cells. **S. Lee**, S. Oh, D. Kwon, Y. Park, W. Shin

MEDI **316.** 10-oxy-anthracenyl isoxazole amides (AIMs) as potential G-quadruplex stabilizing antitumor agents. **N.S. Duncan**, N.R. Natale, H.D. Beall

MEDI **317.** Ferrocenyl derivatives as promising scaffolds for anticancer and antileishmanial agents. **S. Zaib**, J. Iqbal, M. Hassan, F. Macaev, A.K. Powell

MEDI **318.** Improved efficacy for a novel class of G-quadruplex binding anti-tumor agents. **M.J. Weaver**, N.R. Natale

MEDI **319.** Design, synthesis, and antineoplastic evaluation of isoform selective inhibitors of AKR1C3. **K. Verma**, T. Zhang, T.M. Penning, P.C. Trippier

MEDI **320.** Discovery and development of a series of irreversible EGFR_T790M 7H-pyrrolo[2,3-d]pyrimidine inhibitors with high selectivity over EGFR wild type. **S. Planken**, S.K. Nair, J.C. Kath, J. Lafontaine, S. Weinrich, H.K. Cheng, S.C. Sutton, T.O. Johnson, M. Zientek, A. Nagata, K. Gajiwala, J. Solowiej, B.W. Murray, M. Yin, M. Hemkens

MEDI **321.** Synthesis of PF-06459988; a next generation irreversible EGFR_T790M inhibitor for resistant non-small cell lung cancer. **K.T. Tran**, D.C. Behenna, S. Cho-Schultz, S. Kephart, J. Matthews, S.K. Nair, M.A. Ornelas, S.T. Orr, M.A. Pairish, P. Richardson, D.T. Richter, N. Sach, H. Shen, S.C. Sutton, R. Zhou

MEDI **322.** Synthesis of warhead containing scaffolds on irreversible 7H-pyrrolo[2,3-d] pyrimidine EGFR T790M inhibitors. **J.J. Matthews**, S.E. Kephart, R. Zhou, M.A. Pairish, D. Behenna, S. Cho-Schultz, S.K. Nair, M.A. Ornelas, S.T. Orr, D.T. Richter, H. Shen, S.C. Sutton, K.T. Tran

MEDI **323.** Exploring EGFR kinase-ligand interactions for optimizing dual action inhibitors. C. Williams, A. Ajamian, **P. Kamya**, B. Jean-Claude, Z. Rachid

MEDI **324.** Fully automated radiosynthesis of [11C]AZD8931 as a new PET agent for imaging of EGFR, HER2 and HER3 signaling. **M. Wang**, M. Gao, Q. Zheng

MEDI **325.** Synthesis of carbon-11-labeled aminoalkylindole derivatives as new candidate CBR radioligands for PET imaging of alcohol abuse. M. Gao, A. Gao, **M. Wang**, Q. Zheng

MEDI **326.** Development of isoform selective compounds for Grp94 inhibition. **S. Mishra**

MEDI **327.** Targeting Hsp90: Development of C-terminal inhibitors. **M. Anyika**

MEDI **328.** Deuterated dabrafenib (BRAF kinase inhibitor): Metabolism and pharmacokinetics. **J.M. Ralph**, L.E. Richards-Peterson, T. Wilde, D. Bershas, E.A. Minthorn, A. Kaura, M. Bleam, S. Laquerre, M. Arnone, C. Manning, J.L. Adams

MEDI **329.** Combination therapy with epothilone and aurora kinase inhibitors induces a novel form of cell death. **L. Woods**, R.E. Taylor, K.T. Vaughan

MEDI **330.** Identification of 2-(4-benzamidophenyl)-7-phenyl-5H-benzo[c]pyrimido[4,5-e]azepines as potent aurora kinase inhibitors. **R.E. Gershman**, S.G. Stroud, D.A. Janowick, T.B. Sells, M. Rezaei, C.F. Claiborne, S.J. Critchley

MEDI **331.** Rational design of ALK2 small molecule inhibitors for treatment of fibrodysplasia ossificans progressiva (FOP). **Y.L. Luo**, A. Alsamarah

MEDI **332.** Discovery and SAR exploration of a novel series 8-oxo-8,9-dihydro-7H-purine-6-carboxamides as mTOR kinase inhibitors. **P. Papa**

MEDI **333.** Discovery of substituted morpholinothiophene and morpholinothiazole carboxylic acids as selective inhibitors of PI3Kb kinase. **Z. Shi**, D. Cardin, J. Chouitar, J. Ecsedy, K. Galvin, R. Griffin, P. Hales, M. Hirose, T. Hu, N. Natasha Iartchouk, D.A. Janowick, Y. Kawakita, M. Rezaei, T. Sells, M. Smith, S. Stroud, L. Takaoka, S. Vyskocil, D. Deborah Wysong, T. Xu, W. Zhang

MEDI **334.** Inhibition of the inositol phosphatase SHIP utilizing quinoline-based small molecules. C.M. Russo, A.A. Adhikari, D.R. Wallach, R. Brooks, F. Sandra, A.N. Balch, W.G. Kerr, **J.D. Chisholm**

MEDI **335.** Disruption of STAT3 phosphorylation by novel pyrimidino-thiazinones, PI3K-α and δ inhibitors. **B. Akula**, D. Subbaiah, M.R. Mallireddigari, S. Cosenza, V. Bharathi, V. Pallela, G. Panda, . Reddy, M. Reddy

MEDI **336.** Structure based design, synthesis, and anticancer evaluation of human neutrophil elastase inhibitors. Q. Sun, Y. Li, J. Li, W. Yang, **G. Yang**

MEDI **337.** Synthesis and biological evaluation of potential isoform-selective benzimidazole-4-carboxamide inhibitors of poly(ADP-ribose)polymerases. **J. Pickles**, C. Cano, B. Golding, S. Harnor, S. Jackson, H. Newell, J. Travers, R. Griffin

MEDI **338.** Novel strategies for improving the pharmacological properties of platinum-acridine anticancer agents. **S. Ding**, A. Pickard, G. Kucera, U. Bierbach

MEDI **339.** Labeling of TSPO PET radioligands by [18F]fluorination of diarylsulfoxide precursors. **F.G. Simeon**, E. Barresi, S. Lu, S. Taliani, F. Da Settimo, V.W. Pike

MEDI **340.** Red blood cell-mediated photodynamic therapy for improved cancer treatment. **W. Tang**, J. Xie, Z. Zhen

MEDI **341.** Molecular modeling studies of choline acetyltransferase inhibitors as potential PET probes. **R. Kumar**, T. Darreh-Shori

MEDI **342.** Target identification and mechanism elucidation of chalcones' cytotoxicity via photoaffinity probes. **B. Zhou**, X. Yu, C. Zhuang, P. Jiang, S.S. Wickramaratne, Y. Lin, J. Lü, C. Xing

MEDI **343.** Activity-based probe for acyl protein thioesterases. **Y. Chen**, M. Zompa, R. Bisiewicz, C.T. Seto

MEDI **344.** Design and application of lipid probes for proteomic characterization of protein binding partners. **S. Eni**, M. Best, S. Mattern-Schain, K. Tscherch

MEDI **345.** Design and synthesis of novel fluorinated amines. **P. Mykhailiuk**

MEDI **346.** Synthesis of conformationally restricted scaffolds by double-Mannich reaction of cyclic ketones. **P. Mykhailiuk**

MEDI **347.** Synthesis of novel unique pyrrolidines by [3+2]-cycloaddition of azomethine ylides with electron-deficient alkenes. **P. Mykhailiuk**

MEDI **348.** Affinity selection-mass spectrometry screening: Development and validation of a 384-well ultrafiltration format for drug discovery. **R.E. Williamson**, D. Terry, G. Roth

MEDI **349.** Plasma treatment of dentin surfaces for improving dental composite restoration bonding. X. Dong, M. Cheng, Y. Wang, H. Li, **Q. Yu**

MEDI **350.** Synthesis and evaluation of inhibitors of the salicylate synthase (MbtI) involved in siderophore biosynthesis in *mycobacterium tuberculosis*. **F. Liu**, Z. Liu

MEDI **351.** Large scale storage stability analysis of molecules in the MLSMR. **C. Laggner**, Y. Shayo, C. Hendarto, C.R. Johnson, C.R. Loomis

MEDI **352.** Development of novel nitrogen based heterocyclic antibiotic advjuvants. **R.E. Furlani**, C. Melander

NUCL

Division of Nuclear Chemistry and Technology

J. C. Braley and D. E. Hobart, *Program Chairs*

SOCIAL EVENTS:

Social Hour, 6:30 PM: Mon

BUSINESS MEETINGS:

NUCL Executive Business Meeting, 5:30 PM: Sun

NUCL Business Meeting, 5:30 PM: Mon

SUNDAY MORNING

Section A

Embassy Suites Denver–Downtown Convention Center

Crestone Ballroom A

Glenn T. Seaborg Award for Nuclear Chemistry: Symposium in Honor of Heino Nitsche

C. Duellman, T. Fanghänel, D. E. Hobart, A. Kersting, R. Wilson, *Organizers, Presiding*

8:30 NUCL **1.** Studies of the thermodynamics of actinide reactions: A tribute to Heino Nitsche. **K.L. Nash**

8:50 NUCL **2.** Treatment of contaminated water at Fukushima. D. Hobbs, R. Peterson, **K. Yamaguichi**, M. Yamamoto

9:20 NUCL **3.** Thermodynamics and predicting actinide behavior in repository science. **D.T. Reed**

9:40 NUCL **4.** Spatially resolved characterization techniques for next generation nuclear forensics signature development. J.M. Schwantes, **L. Sweet**, E. Buck, T.J. Johnson, D.D. Reilly, D. Abrecht, E. Mausolf

10:10 Intermission.

10:30 NUCL **5.** Investigation of silica-grafted CMPO-modified calix[4]arenes for radionuclide separations. **E.M. May**, Y. Wanglee, A. Solovyov, Y. Matvieiev, A.S. Katz, V. Kalchenko, H. Nitsche

10:50 NUCL **6.** Interactions of plutonium and ordered mesoporous materials. **T. Parsons-Moss**, D. Olive, S. Jones, J. Wang, D. Zhao, Z. Dai, M. Zavarin, A. Kersting, H. Nitsche

11:10 NUCL **7.** FIONA: A new mass analyzer for superheavy elements. **N. Esker**, J.M. Gates, G.K. Pang, K.E. Gregorich, H. Nitsche

11:30 NUCL **8.** Solid-phase extractants for sequestration and separation of actinides and lanthanides. **J. Shusterman**, A. Bruchet, H. Mason, E.C. Uribe, H. Nitsche

11:50 NUCL **9.** DTRA basic research for combating weapons of mass destruction. **S. Wilk**

Uranium in Seawater

Sorbents and Analysis

Sponsored by I&EC, Cosponsored by CEI, MPPG‡ and NUCL

SUNDAY AFTERNOON

Section A

Embassy Suites Denver–Downtown Convention Center

Crestone Ballroom A

Glenn T. Seaborg Award for Nuclear Chemistry: Symposium in Honor of Heino Nitsche

C. Duellman, T. Fanghänel, D. E. Hobart, A. Kersting, R. Wilson, *Organizers, Presiding*

1:20 NUCL **10.** Scientific contributions of Heino Nitsche to actinide and transactinide chemistry. **C. Düllmann**, R. Wilson

1:40 NUCL **11.** Heavy element studies at Berkeley. **K.E. Gregorich**

2:10 NUCL **12.** Impact of $[Ca_2\ UO_2\ (CO_3)_3]$ aq.-complex formation on environmental behavior of uranium. **G. Bernhard**, G. Geipel, V. Brendler

2:40 NUCL **13.** Molecular scale investigations towards actinide retention at mineral surfaces. **H. Geckeis**

3:10 Intermission.

3:30 NUCL **14.** Applications of molten salts in nuclear technology. **T. Fanghänel**, O. Beneš, J. Glatz, R. Konings, R. Malmbeck, P. Souček

4:00 NUCL **15.** Advances in the production and chemistry of the heaviest elements. **A. Tuerler**

4:30 NUCL **16.** Laser-induced spectroscopy of actinides: From simple metal systems to species in living cells. **G.C. Geipel**

5:00 NUCL **17.** Toward A and Z identification of superheavy elements. **J.M. Gates**

5:30 NUCL **18.** Chronology of 239/240Pu and of 236U in the Miaergou glacier from eastern Tien Shan, China. **H.W. Gaeggeler**, S. Hou, C. Wang, M. Christl, S. Maxeiner, H. Synal, C. Vockenhuber

Section B

Embassy Suites Denver–Downtown Convention Center

Crestone Ballroom B

Nuclear Forensics

Fission Product Studies

A. Klingensmith, R. S. Rundberg, *Organizers*

T. A. Bredeweg, *Organizer, Presiding*

1:00 NUCL **19.** Energy dependence of fission product yields from 235U, 238U and 239Pu for incident neutron energies between 0.5 and 14.8 MeV. **M. Gooden**, C. Arnold, T.A. Bredeweg, J. Wilhelmy, D. Vieira, A. Tonchev, M.A. Stoyer, W. Tornow

1:25 NUCL **20.** Measurement of fission product yields and nuclear reaction crossSections using mono-energetic neutrons from a dense plasma focus. **R.S. Rundberg**

1:50 NUCL **21.** Fission product chain yields from fission spectrum irradiations at NCERC. T.A. Bredeweg, **K.R. Jackman**, A.C. Olson, S.M. Bowen, A. Schake, S.A. Kozimor

2:15 NUCL **22.** SPIDER: New instrument for fission mass yield measurements. **K.C. Meierbachtol**, F. Tovesson, C. Arnold, T.A. Bredeweg, M. Devlin, M. Jandel, J. Lestone, R. Nelson, A. Sierk, D. Shields, M. White, A. Hecht, R. Blakeley

2:40 NUCL **23.** Relative fission product yield determination in varying neutron environments. **M. Koehl**, J. Braley

Section B

Embassy Suites Denver–Downtown Convention Center

Crestone Ballroom B

Nuclear Forensics

Separations

T. A. Bredeweg, A. Klingensmith, *Organizers*

R. S. Rundberg, *Organizer, Presiding*

3:20 NUCL **24.** Synthesis of rapid separation targets by hydrothermal methods. **J.M. Dorhout**, K. Czerwinski

3:45 NUCL **25.** Thermochromatographic separations of volatile rare earth compounds for nuclear forensics analysis. **J.D. Auxier**, S.A. Stratz, D.E. Hanson, M.L. Marsh, A.V. Jones, H.L. Hall

4:10 NUCL **26.** Synthesis and characterization of Ln[fod]$_4$ and Ln[dpm]$_4$ compounds for the development of rapid gas-phase separation methods. **S.A. Stratz**, J.D. Auxier, M.L. Marsh, D. Hanson, A.V. Jones, H.L. Hall

4:35 NUCL **27.** Determination of decontamination factor for various radioisotopes during the PUREX process of irradiated DUO_2. **T.K. Bhardwaj**, P. Mendoza, R. Du, M. Bencomo, J. Allred, M. Swinney, C.M. Folden, S. Chirayath

5:00 NUCL **28.** Source facility determination based on PUREX process trace metal signatures. **A. Baldwin**, J.C. Braley

Uranium in Seawater

Sorbents and Analysis

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MONDAY MORNING

Section A

Embassy Suites Denver–Downtown Convention Center

Crestone Ballroom A

Glenn T. Seaborg Award for Nuclear Chemistry: Symposium in Honor of Heino Nitsche

C. Duellman, T. Fanghänel, D. E. Hobart, A. Kersting, R. Wilson, *Organizers, Presiding*

8:10 NUCL **29.** Actinide sorption to aluminum (hydr)oxides: Influence of sorption site acidity. **T. Baumer**, P.E. Kay, A. Ko, A.E. Hixon

8:30 NUCL **30.** Pu transport mechanisms in the environment: Field evidence, conceptual models, and experimental data. **M. Zavarin**, J. Begg, C. Joseph, P. Zhao, A. Kersting

8:50 NUCL **31.** Separating uranyl nanoclusters using ultrafiltration membranes. **M. Sharifironizi**, C.R. Andrews, J.E. Syzmanowski, G.E. Sigmon, W.A. Phillip, P.C. Burns

9:10 NUCL **32.** Superheavy element discovery and chemistry program at LLNL. **D.A. Shaughnessy**, R. Henderson, K. Moody, N. Gharibyan, J. Despotopulos

9:30 Intermission.

9:50 NUCL **33.** Biotransformation of plutonium. **T. Ohnuki**, A.J. Francis

10:10 NUCL **34.** Plutonium hydrolysis and condensation. **L. Soderholm**, S. Skanthakumar

10:40 NUCL **35.** Role of multinucleon transfer reactions in making neutron-rich transactinide nuclei. **W. Loveland**, R. Yanez, S. Barrett

11:00 NUCL **36.** Relativistic quantum theory for chemical identification of the heaviest elements. **V. Pershina**

11:30 NUCL **37.** Heino Nitsche's contributions to the understanding of Pu reactions at mineral:water interfaces and their implications on present reactive transport modeling. **B.A. Powell**, D. Kaplan

Section B

Embassy Suites Denver–Downtown Convention Center

Crestone Ballroom B

Nuclear Forensics

Surrogates

T. A. Bredeweg, R. S. Rundberg, *Organizers*

A. Klingensmith, *Organizer, Presiding*

8:15 NUCL **38.** Mass transport in aerodynamic fallout glass from a near-surface nuclear explosion. **D. Weisz**, S.G. Prussin, K. Knight, B. Jacobsen, N.E. Marks, I.D. Hutcheon

8:40 NUCL **39.** Constraints on fallout melt glass formation from a near-surface nuclear test. **G.R. Eppich**, K.B. Knight, G. Spriggs, I.D. Hutcheon

9:05 NUCL **40.** Production of activation species for use with realistic surrogate debris materials. **B.B. Bandong**

‡ *Cooperative Cosponsorship*

9:30 NUCL **41.** Forensic analysis of urban nuclear melt glass surrogates. **A.V. Giminaro**, J.P. Auxier, J.A. Gill, S.A. Stratz, C.J. Oldham, H.L. Hall

Section B

Embassy Suites Denver–Downtown Convention Center

Crestone Ballroom B

Nuclear Forensics

Surrogates

A. Klingensmith, R. S. Rundberg, *Organizers*

T. A. Bredeweg, *Organizer, Presiding*

10:10 NUCL **42.** Controlled pore glass materials as use for a surrogate nuclear explosion debris (SNED) material. **A.J. Carman**, B. Valenzuela, M.V. Snyder, M. Endres, M. Liezers, A. Prinke, G.C. Eiden

10:35 NUCL **43.** Surrogate nuclear explosion debris methods: ICP-fluidized bed reactor and agglomerated laser melt material. **M. Endres**, M. Liezers, G. Eiden, A.J. Carman

11:00 NUCL **44.** Radiochemistry for the production of a realistic post-det surrogate debris. **N. Gharibyan**, K. Moody, P. Grant, S. Tumey, T. Brown, K. Roberts, D. Shaughnessy

Uranium in Seawater

Sorbents and Analysis

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MONDAY AFTERNOON

Section A

Embassy Suites Denver–Downtown Convention Center

Crestone Ballroom A

Glenn T. Seaborg Award for Nuclear Chemistry: Symposium in Honor of Heino Nitsche

C. Duellman, T. Fanghänel, D. E. Hobart, A. Kersting, R. Wilson, *Organizers, Presiding*

1:20 NUCL **45.** Behavior of U(VI) silicate minerals and Np(V)-doped U(VI) silicates. **N. Wall**, S.B. Clark

1:40 NUCL **46.** Production and decay studies of 265Sg for chemical studies of seaborgium using the gas-filled recoil ion separator GARIS at RIKEN. **H. Haba**

2:10 NUCL **47.** Recent advances in uranium cluster chemistry research. **P.C. Burns**

2:40 NUCL **48.** Use of projectiles with Z ≥ 20 to produce heavy and superheavy elements. **C.M. Folden**

3:10 Intermission.

3:30 NUCL **49.** Second break in the actinide series occurs at californium. **T.E. Albrecht-Schmitt**

4:00 NUCL **50.** Heavy element studies at the University of Nevada Las Vegas. **R. Sudowe**, J. Despotopulos, J. Rolfes

4:20 NUCL **51.** Plutonium speciation during interaction with argillaceous rocks. **T. Reich**

4:50 NUCL **52.** X-ray spectroscopy characterisation of radionuclide-NOM interaction. **M.A. Denecke**

5:20 NUCL **53.** Plutonium uptake by mammalian cells. **M.P. Jensen**, B. Aryal, T. Paunesku, G. Woloschak

Section B

Embassy Suites Denver–Downtown Convention Center

Crestone Ballroom B

Nuclear Forensics

Spectroscopic Methods

T. A. Bredeweg, A. Klingensmith, *Organizers*

R. S. Rundberg, *Organizer, Presiding*

1:00 NUCL **54.** Spectroscopic signatures for forensic sciences. **N. Wozniak**, S.M. Clegg, K. Czerwinski, G.L. Wagner, M.P. Wilkerson

1:25 NUCL **55.** Calibration of femtosecond laser ablation inductively coupled plasma mass spectrometer using a thermal inkjet picofluidic system for sensitive isotopic nuclear material characterization. **G.J. Havrilla**, K.G. McIntosh, J. Gonzalez, D. Oropeza, R. Russo, M.S. Morey

1:50 NUCL **56.** FIER: A method for forensic attribution of fissile mixtures using beta-delayed gamma-ray signatures. **E. Matthews**, B.L. Goldblum, B.J. Quiter

2:15 NUCL **57.** Considerations when using scanning electron microscopy for nuclear forensics. **A.L. Tamasi**, G.L. Wagner, B. Scott, J.R. Walensky, M.P. Wilkerson

Section B

Embassy Suites Denver–Downtown Convention Center

Crestone Ballroom B

Nuclear Forensics

Other

T. A. Bredeweg, R. S. Rundberg, *Organizers*

A. Klingensmith, *Organizer, Presiding*

2:55 NUCL **58.** Electrochemistry of a modified-hematite film electrode for the detection of rhenium as a technetium analog. **L. Gribat**, **H. Beyenal**, **N. Wall**

3:20 NUCL **59.** Stability constants and total dissolution of Tc(IV) and DTPA complexes. **T. Omoto**, N.A. Wall

3:45 NUCL **60.** Cathodoluminescent signatures of neutron irradiation. **G.F. Peaslee**, D.K. Silletti, S. Brokus, J. Buscaglia

4:10 NUCL **61.** Applications for nuclear forensics at the National Ignition Facility. **D.A. Shaughnessy**, K. Moody, N. Gharibyan, P. Grant, C. Yeamans, K. Holliday, J. Despotopulos

4:35 NUCL **62.** Boron-rich benzene and pyrene derivatives for the detection of thermal neutrons. **H. Yemam**, A. Mahl, U. Koldemir, U. Greife, A. Sellinger

5:00 NUCL **63.** Plutonium speciation Influence on the 22Na yield from the 19F[α,n] reaction. **W.M. Kerlin**, J.D. Despotopulos, D.D. Reilly, R. Sudowe, K. Czerwinski

TUESDAY MORNING

Section A

Embassy Suites Denver–Downtown Convention Center

Crestone Ballroom A

50th Anniversary of the NUCL Division

T. E. Albrecht-Schmitt, J. Auxier II, D. E. Hobart, D. S. Peterson, D. A. Shaughnessy, D. K. Shuh, *Organizers*

J. C. Braley, *Organizer, Presiding*

8:00 NUCL **64.** Division of Nuclear Chemistry and Technology 50th Anniversary celebration. **D.E. Hobart**

8:30 NUCL **65.** Division of Nuclear Chemistry and Technology (1990-2015). **D.C. Hoffman**

9:00 NUCL **66.** Heavy element chemistry at Berkeley: A distinguished history with a promising future. **D.K. Shuh**

9:20 NUCL **67.** Heavy element chemistry and separations science at Argonne National Laboratory: A current perspective. J.V. Beitz, **L. Soderholm**

9:40 NUCL **68.** Decades of progress in actinide solution chemistry in NUCL/DNCT. **K.L. Nash**

10:00 Intermission.

10:20 NUCL **69.** Fifty years of heavy element science: Understanding their elemental states. **R. Haire**

10:50 NUCL **70.** NUCL and the ACS/DOE summer school in nuclear chemistry: A historical perspective. **P.A. Baisden**

11:10 NUCL **71.** Helping build a future nuclear forensics and radiochemistry workforce: Education efforts within the Seaborg Institute at Lawrence Livermore National Laboratory. **A. Kersting**

11:30 NUCL **72.** Thirty years of bridging the gap: The ACS Summer Schools in Nuclear and Radiochemistry. **J.D. Robertson**

11:50 NUCL **73.** NUCL Division strategic plan. **P.F. Mantica**

Uranium in Seawater

Sorbents and Analysis

Sponsored by I&EC, Cosponsored by CEI, MPPG‡ and NUCL

TUESDAY AFTERNOON

Section A

Embassy Suites Denver–Downtown Convention Center

Crestone Ballroom A

50th Anniversary of the NUCL Division

J. Auxier II, D. S. Peterson, D. A. Shaughnessy, D. K. Shuh, *Organizers*

T. E. Albrecht-Schmitt, D. E. Hobart, *Organizers, Presiding*

1:00 NUCL **74.** Thermodynamics of actinide solution chemistry: Complexation by alpha-hydroxy organic acids in mixed solvent systems. **S.B. Clark**

1:20 NUCL **75.** EMSL radiochemistry annex: A new international user-facility for the study of radiological samples. **N.J. Hess**

1:40 NUCL **76.** Radiochemistry at Los Alamos National Laboratory: Past, present, and future. **D.S. Peterson**

2:00 NUCL **77.** The Radiochemistry Center of Excellence at the University of Tennessee. **H.L. Hall**

2:20 NUCL **78.** Molecular electronic structure theory applied to heavy-element chemistry: Some past accomplishments, present challenges, and future opportunities. **B.E. Bursten**

2:40 NUCL **79.** Savannah River National Laboratory and [NUCL] a joint history. **M.G. Bronikowski**

3:00 Intermission.

3:20 NUCL **80.** Online chemistry research at Texas A&M University. **C.M. Folden**

3:40 NUCL **81.** Protactinium: Chemistry at the intersection of the 5f and 6d elements. **R. Wilson**, S. De Sio, V. Vallet

4:00 NUCL **82.** Radiotracers for biological, environmental, and medical applications. **S.S. Jurisson**

4:20 NUCL **83.** Recent advances in molecular f-element chemistry centered on TRU elements. **J.L. McDonald**, A. Gaunt

4:40 NUCL **84.** High field and high frequency EPR study of isotypic herterobimetallics. **K. Diefenbach**, T.E. Albrecht-Schmitt

5:00 NUCL **85.** Microstructural characterization of structural alloys for nuclear energy applications. **M. Li**

5:20 NUCL **86.** Optimization and characterization of a molecular plating technique for homogenous thin film samples. **A. Roman**, R.S. Rundberg

WEDNESDAY MORNING

Section A

Embassy Suites Denver–Downtown Convention Center

Crestone Ballroom A

50th Anniversary of the NUCL Division

T. E. Albrecht-Schmitt, J. Auxier II, J. C. Braley, D. E. Hobart, D. S. Peterson, *Organizers*

D. A. Shaughnessy, D. K. Shuh, *Organizers, Presiding*

8:00 NUCL **87.** Fission and the DNCT. W. Loveland

8:20 NUCL **88.** Nuclear shape triaxiality in neutron-rich niobium isotopes. **J.O. Rasmussen**, Y.X. Luo, Y. Liu

8:40 NUCL **89.** Exploiting fast neutrons: From nuclear structure to neutrinoless double-beta decay. **S.W. Yates**

9:00 NUCL **90.** New opportunity: Coincident spectroscopy in neutron-deficient actinides. **O.R. Gothe**, K.E. Gregorich, B. Baartman, P. Fallon, N. Esker, J.T. Kwarsick, A. Machiavelli, P. Mudder, D. Olive, G.K. Pang, J. Rissanen, H. Nitsche

9:20 NUCL **91.** Comparing nuclear counting statistics with the network statistics. S.E. Beach, **T.M. Semkow**, D.J. Remling

9:40 NUCL **92.** Working toward measurement of nuclear structure in superheavy elements. **K.E. Gregorich**

10:00 Intermission.

10:20 NUCL **93.** Response of actinide materials to highly ionizing radiation. **R.C. Ewing**

10:40 NUCL **94.** Reductive routes to low-oxidation states actinide materials. **T.E. Albrecht-Schmitt**

11:00 NUCL **95.** Determination of Pu in spent nuclear fuel: Results from field testing of high resolution X-ray (hiRX). **G.J. Havrilla**, K.G. McIntosh, R. Gilmore, D. Missimer, M. Holland

11:20 NUCL **96.** Accumulation of specific nuclides by fish bodies in Fukushima-Ken (Prefecture) EEZ (Exclusive Economic Zone), Japan in November 2012. **H. Katsura**

11:40 NUCL **97.** Cost effective tank waste characterization at the Savannah River site. **S.H. Reboul**, D.P. Diprete, J.M. Pareizs, F.G. Smith, R.H. Young

Section B

Embassy Suites Denver–Downtown Convention Center

Crestone Ballroom B

Convergence of Theory & Experiment in Heavy Element Chemistry

A. P. Sattelberger, D. K. Shuh, L. Soderholm, *Organizers, Presiding*

8:20 NUCL **98.** Elucidation of redox properties, structures, and bonding for cerium and uranium complexes through DFT and experiment. **E.J. Schelter**

8:40 NUCL **99.** Water adsorption on AnO_2 (An = U, Np, Pu) surfaces. J.P. Wellington, A. Kerridge, **N. Kaltsoyannis**

9:00 NUCL **100.** Evaluation of the coordination chemistry and reactivity of trimethylsilylanilido and phosphinimide complexes of U and Th. **R.K. Thomson**

9:20 NUCL **101.** Structure and stability of uranyl(VI) and uranium(VI) imido complexes with high-nitrogen ligands. **K.A. Maerzke**, N. Henson, J. Veauthier, J.L. Kiplinger

9:40 NUCL **102.** Bonding and magnetism in tris-cyclopentadienyl neodymium and uranium complexes and their isocyanide adduct. **W.W. Lukens**, R.A. Andersen, N.M. Edelstein, P. Yang, M. Speldrich

10:00 Intermission.

10:20 NUCL **103.** Experimental and theoretical determinations of covalency in d- and f-block metal oxides. **S.G. Minasian**, E.R. Batista, C. Booth, J.M. Keith, W.W. Lukens, S.A. Kozimor, R.L. Martin, D. Nordlund, D.K. Shuh, D. Sokaras, T. Tyliszczak, X. Wen, T. Weng

10:40 NUCL **104.** Strong correlations and covalency in actinide materials. **R.L. Martin**

11:00 NUCL **105.** Toward controlling the formation of cation-cation interactions in neptunyl(V) compounds. **G. Jin**, S. Skanthakumar

Technical program information known at press time.
The official technical program for the 249th ACS National Meeting is available at:
www.acs.org/denver2015

11:20 NUCL **106.** Combined structural characterization, raman spectroscopy, and theory to promote an enhanced understanding of aqueous speciation. **T. Forbes**, M.C. Basile, J. de Groot

11:40 NUCL **107.** Characterisation of actinide selective N-donor extractants using spectroscopic and quantum theoretical methods. **M.A. Denecke**

WEDNESDAY AFTERNOON

Section A

Embassy Suites Denver–Downtown Convention Center

Crestone Ballroom A

50th Anniversary of the NUCL Division

T. A. Albrecht, J. C. Braley, D. E. Hobart, D. A. Shaughnessy, D. K. Shuh, *Organizers*

J. Auxier II, D. S. Peterson, *Organizers, Presiding*

1:00 NUCL **108.** Actinide interactions with aminopolycarboxyates: Heavy element curiosities. **J. Braley**

1:20 NUCL **109.** Advances in organometallic chemistry at the bottom of the periodic table. **J.L. Kiplinger**

1:40 NUCL **110.** Use of molecular dynamics to evaluate tributyl phosphate and diamylamyl phosphonate containing systems. M. Servis, **J.C. Braley**, D. Wu

2:00 NUCL **111.** Historical overview of radioisotope thermoelectric generators. **C.E. Whiting**

2:20 NUCL **112.** Characterization of actinide reactivity and speciation at mineral:water interfaces. **B.A. Powell**, S.L. Estes, D. Kaplan, A. Kersting, M. Zavarin

2:40 NUCL **113.** Enhanced immobilization of iodine by biochar in soil-water system. **D. Zhang**, L. Wang, H. Zhao

3:00 NUCL **114.** Studies on the thermodynamics of trivalent lanthanide/actinide extraction by tri-*n*-octylphosphine oxide and bis(2-ethylhexyl) phosphoric acid. **T.S. Grimes**, P.R. Zalupski, L.R. Martin

3:20 Intermission.

3:40 NUCL **115.** Specific recognition and enhanced luminescence sensitization of trivalent actinides. **R.J. Abergel**, B.E. Allred, M. Sturzbecher-Hoehne, A. Daleo

4:00 NUCL **116.** Minor actinide separations using a combination of a dithiophosphinic acid and a synergist. **D.R. Peterman**, P.R. Zalupski, J.R. Klaehn

4:20 NUCL **117.** Probing for differences in the electronic properties of actinides and lanthanides using 1,10-phenanthroline-2,9-dicarboxylic acid. **S.K. Cary**, T.E. Albrecht-Schmitt

4:40 NUCL **118.** Structural and electronic variations in *f*-block containing plumbite clusters. **J.T. Stritzinger**, K. Pace, T.E. Albrecht-Schmitt

5:00 NUCL **119.** Supramolecular coordination polymers of lanthanide and actinide metals featuring the 1,8-naphthalimide tecton. **A. Leitner**, D.L. Reger, M.D. Smith

5:20 NUCL **120.** Ionothermal flux syntheses of isomorphous metalloborate clusters. **G. Parker**, A.L. Chown, T.E. Albrecht-Schmitt

Section B

Embassy Suites Denver–Downtown Convention Center

Crestone Ballroom B

Convergence of Theory & Experiment in Heavy Element Chemistry

D. L. Clark, A. P. Sattelberger, D. K. Shuh, L. Soderholm, *Organizers, Presiding*

1:20 NUCL **121.** Correlation between single-atom adsorption enthalpies and solid-state properties. H.W. Gaeggeler

1:40 NUCL **122.** Predicting the redox potentials of actinide complexes (An=U, Np, Pu) using first-principles. W. Huang, J. Li, **P. Yang**

2:00 NUCL **123.** Actinide chemistry in the gas phase: A fruitful interplay between experiment and theory. **J.K. Gibson**

2:20 NUCL **124.** Exploring the highest oxidation state in actinide compounds. J. Li

2:40 NUCL **125.** Spectroscopy and structure of the simplest actinide bonds. **M.C. Heaven**, J. Bartlett, R. VanGundy

3:00 NUCL **126.** Experimental and quantum chemical studies of alkali-ion promoted formation of uranyl(VI) peroxide rings and a comparison with similar reactions in12-crown-5 and 15-crown-5 systems. **V. Vallet**, P. Zanonato, P. Di Bernardo, Z. Szabo, I. Grenthe

3:20 Intermission.

3:40 NUCL **127.** Integration of computational modeling and experiments in actinide chemistry. **W. Dejong**, S. Odoh, Y. Gong, J.K. Gibson

4:00 NUCL **128.** Toward accurate ab initio thermochemistry for molecules containing f-block elements. **K.A. Peterson**, D.A. Dixon

4:20 NUCL **129.** Reactivity of aqueous thorium(IV) and plutonium(IV) clusters. **M. Vasiliu**, K. Knope, L. Soderholm, D.A. Dixon

4:40 NUCL **130.** Tetravalent actinide-small organic molecule containing compounds. **K.E. Knope**

5:00 NUCL **131.** Theoretical study of the electronic spectrum of the UO and UO+ molecules. R. Tyagi, Z. Zhang, **R.M. Pitzer**

5:20 NUCL **132.** Solution and gas phase solvation of f-element ions in binary water/methanol solutions. **M. Kelley**, A.E. Clark, S.B. Clark

THURSDAY MORNING

Section B

Embassy Suites Denver–Downtown Convention Center

Crestone Ballroom B

Convergence of Theory & Experiment in Heavy Element Chemistry

D. L. Clark, A. P. Sattelberger, D. K. Shuh, L. Soderholm, *Organizers, Presiding*

8:20 NUCL **133.** Computational studies of actinide and metal oxides, fluorides, and chlorides. **D.A. Dixon**, K.A. Peterson

8:40 NUCL **134.** Combining theory with experiment to understand aggregation in solvent extraction systems for heavy element separations. **R.J. Ellis**, B. Qiao, T. Demars

9:00 NUCL **135.** Role of ionic solute vs. amphiphilic solute on local interfacial properties. **Y. Ghadar**

9:20 NUCL **136.** Examining covalency in actinide complexes with soft donor ligands and metal-ligand multiple bonding. **J.R. Walensky**, A. Behrle

9:40 NUCL **137.** Revealing the hydration of thorium(IV) with combined techniques involving EXAFS, HEXS and molecular dynamics simulations. **F. Réal**, V. Vallet, M. Masella, Y. Hu, S. Skanthakumar, L. Soderholm

10:00 Intermission.

10:20 NUCL **138.** Effects of strong π-donors on actinides: bent uranyl(VI) and molecular Pu(IV). **M. Silver**

10:40 NUCL **139.** Covalency in f-element materials probed with ligand K-edge X-ray absorption spectroscopy. **E.R. Batista**

11:00 NUCL **140.** Solvation thermodynamics of trivalent actinide (An=U, Np and Pu) ions using polarizable force field. **P. Parmar**, Y. Ghadar, A.E. Clark

11:20 NUCL **141.** Divergence between plutonium and americium in oxoanion materials. **T.E. Albrecht-Schmitt**

11:40 NUCL **142.** Combined theoretical and experimental study of the binding features of the super uranyl-binding protein. **L. Gagliardi**, S. Odoh, G. Bondarevsky, J. Karpus, C. He, Q. Cui, R. Spezia

ORGN

Division of Organic Chemistry

M. C. McIntosh and R. D. Broene, *Program Chairs*

SUNDAY MORNING

Section C

Colorado Convention Center

Rooms 704/706

New Reactions and Methodology

M. C. McIntosh, *Organizer*

P. Willoughby, *Presiding*

8:00 ORGN **1.** New synthetic approaches to biologically active amino containing natural Ppoducts: Total synthesis of oxybenzophenanthridines. **E.D. Calder**, F.I. McGonagle, A.H. Harkiss, G.A. McGonagle, S.A. Sharif, A. Sutherland

8:20 ORGN **2.** Development of complexity generating and stereoselective carbon carbon bond forming reactions. **B.J. Cowen**

8:40 ORGN **3.** Rh(III)-catalyzed C-H activation of N-enoxyphthalimides. **T. Piou**, T. Rovis

9:00 ORGN **4.** Regioselective C-H activation of azine *N*-oxides in arylation and dimerization. **D.E. Stephens**, J. Lakey-Beitia, A.C. Atesin, T. Atesin, G. Chavez, H. Arman, O. Larionov

9:20 ORGN **5.** Butyrolactone synthesis via polar radical crossover cycloaddition reactions: Diastereoselective synthesis of methylenolactocin and protolichesterinic acid. **M. Zeller**, M. Riener, D.A. Nicewicz

9:40 ORGN **6.** A K_2CO_3 mediated regioselective synthesis of indole/pyrrole-fused 1,4-oxazines: An unexpected indole-fused azlactone synthesis. **J. Vandavasi**, W. Hu, J. Wang

10:00 ORGN **7.** Metal- and reagent-free highly selective anodic cross-coupling reaction. **D.R. Waldvogel**, B. Elsler, D. Schollmeyer, K. Dyballa, R. Franke

10:20 ORGN **8.** Surprising organic synthesis: Serendipitous discovery of a novel cascade process. J.A. Simanis, E.L. Woodall, C.M. Law, C.G. Hamaker, J.R. Goodell, **T.A. Mitchell**

10:40 ORGN **9.** Near-IR uncaging chemistry: discovery, and applications. M.J. Schnermann

11:00 ORGN **10.** Synthesis of *N*-phthalimido-*O*-acyl-*N*,*O*-acetals from aldehydes and their conversion into ⊠-branched phthalimides. **P.H. Willoughby**, R.N. Enright, L.T. Henningsen, L.I. Wurtz, E.R. Cliff, J.L. Grinde

11:20 ORGN **11.** Pentadehydro-Diels-Alder (PDDA) reaction Part 2: Cycloadditions of allenynes with nitriles to give pyridine derivatives. **R. Naredla**, T. Wang, T.R. Hoye

Section D

Colorado Convention Center

Room 708

Asymmetric Reactions and Syntheses

M. C. McIntosh, *Organizer*

E. S. Spahn, *Presiding*

8:00 ORGN **12.** Insights into the enantioselectivity of monoprotected amino acid assisted C–H activation reaction. **G. Cheng**, P. Chen, T. Sun, J. Yu, X. Zhang, **Y. Wu**

8:20 ORGN **13.** Enantiodivergent hydrovinylation reaction. S. Biswas, J.P. Page, T. RajanBabu

8:40 ORGN **14.** Asymmetric hydrovinylation of siloxydienes: Making enantio-pure nucleophilic synthons. **S. Biswas**, J.P. Page, T. RajanBabu

9:00 ORGN **15.** Expedient synthesis of chiral polysubstituted 1,4-oxazepanes. M. Bezanson, **J. Pottel**, N. Moitessier

9:20 ORGN **16.** New strategy for the asymmetric conjugate addition of acetylenes to activated olefins via sequential palladium and copper catalysis. B.M. Trost, **J.T. Masters**, B.R. Taft, J.G. Lumb

9:40 ORGN **17.** Development of an enantio- and diastereoselective Simmons-Smith bromocyclopropanation reaction and mechanistic considerations. **S. Taillemaud**, N. Diercxsens, A. Gagnon, A.B. Charette

10:00 ORGN **18.** Kinetic resolution of 2-aryl cyclohexanols via asymmetric silylation. L. Wang, **R. Akhani**, S.L. Wiskur

10:20 ORGN **19.** Efficient synthesis of enantiopure lignin models and their catalytic oxidation using cobalt-Schiff base complexes. **C. Njiojob**, J.J. Bozell, B.K. Long

10:40 ORGN **20.** Development of an asymmetric synthesis of Letermovir exploiting a novel PTC–catalyzed aza-Michael reaction. **G.R. Humphrey**, Z. Song, S. Dalby, B. Xiang, T. Andreani, K.M. Belyk, D. Tschaen

11:00 ORGN **21.** Phosphonate-directed catalytic asymmetric hydroboration. **S. Chakrabarty**, **R. Carr**, J.M. Takacs

11:20 ORGN **22.** Toward the reproducibility of CuIPhEt hydrosilylations. E.S. Spahn, **M.C. McIntosh**, R.E. Gawley

Section E

Colorado Convention Center

Room 702

Materials, Devices and Switches

M. C. McIntosh, *Organizer*

D. J. Dibble, *Presiding*

8:00 ORGN **23.** Multiscale simulations of morphology and charge-transport in oligothiophenes. **S.A. Lopez,** I. Yavuz, L. Zhang, B.P. Cherniawski, A.L. Briseno, K.N. Houk

8:20 ORGN **24.** Withdrawn.

8:40 ORGN **25.** New organic conjugated molecules toward semiconducting and light-emitting materials. **D. Zhang**

9:00 ORGN **26.** Graphene oxide coupled metal oxide nanosheets incorporating small organic molecules for n-type and p-type field effective transistors (FETs). **M. Samal,** N. Barange, K. Yun

9:20 ORGN **27.** Tunable electronic and spintronic properties in highly conjugated multi[(porphinato)metal] oligomers. **R.C. Bruce**, R. Wang, M.J. Therien, W. You

9:40 ORGN **28.** Protein-based protonic transistors. **D.D. Ordinario**, L. Phan, J. Jocson, T. Nguyen, A.A. Gorodetsky

10:00 ORGN **29.** Synthesis and electrochemical characterization of oligonucleotide-inspired organic nanowires. **A. Mazaheripour,** N. Hüsken, J. Jocson, A.M. Burke, A.A. Gorodetsky

10:20 ORGN **30.** Better than metals: Cyanostar macrocycles stabilize and switch organic anion radicals. **C. Benson,** A.H. Flood

10:40 ORGN **31.** Withdrawn.

11:00 ORGN **32.** Chemistry of boron-doped graphene flakes. **S. Yamaguchi**

SUNDAY AFTERNOON

Section A

Colorado Convention Center

Four Seasons Ballroom 2&3

Ronald Breslow Award for Achievement in Biomimetic Chemistry: Symposium in Honor of Eric T. Kool

K. Walker, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 ORGN **33.** Mimicry of protein tertiary structures by expanding beyond natural constraints of covalent connectivity in biological sequences. **W.S. Horne**

1:50 ORGN **34.** Carbene and nitrene transfer reactions catalyzed by engineered hemoproteins. **R. Fasan**

2:35 ORGN **35.** Looking beneath the surface to determine what makes DNA damage deleterious. **M.M. Greenberg**

‡ *Cooperative Cosponsorship*

3:20 Introduction of Awardee.

3:25 ORGN 36. Award Address (Ronald Breslow Award for Achievement in Biomimetic Chemistry sponsored by the Ronald Breslow Award Endowment). Designer DNA bases: Probing molecules and mechanisms in biology. **E.T. Kool**

Section B

Colorado Convention Center
Four Seasons Ballroom 1

Development of Direct C-H Functionalization Processes towards the Synthesis of Biologically Active Compounds

J. Mousseau, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 ORGN 37. C–H functionalization: Can we leverage cutting-edge synthetic methods to enhance drug discovery? **A.F. Stepan**

1:35 ORGN 38. C-H bond functionalization cascades for the synthesis of complex heterocycles. **J.A. Ellman**

2:25 ORGN 39. Selective functionalization of alkyl and aryl c-h bonds — installation of temporary functional groups. **J.F. Hartwig**

3:15 ORGN 40. High-throughput experimentation methods in the development of direct functionalization reactions. **L. Campeau**

4:05 ORGN 41. Studies in natural poduct synthesis. **P.S. Baran**

Section C

Colorado Convention Center
Rooms 704/706

New Reactions and Methodology

M. C. McIntosh, *Organizer*
S. Blakey, *Presiding*

1:20 ORGN 42. Development of Corey-Seebach *umpolung* reagents in palladium-catalyzed cross-coupling reactions. **S. Baker Dockrey**, J.R. Schmink

1:40 ORGN 43. Palladium-catalyzed decarboxylative C–C bond formation of secondary benzyl electrophiles. **S.N. Mendis**, J.A. Tunge

2:00 ORGN 44. Withdrawn.

2:20 ORGN 45. Catalyst development for enantioselective atom transfer C-H functionalization reactions. **S. Blakey**

2:40 ORGN 46. Triphenylphosphine promoted hydroalkoxylation of divinyl sulfone: An ol-ene "Click" reaction? **S. Strasser**, C. Slugovc, I. Hanghofer, A. Eder

3:00 ORGN 47. N Boc amines to oxazolidinones via Pd(II)/Bis-sulfoxide/Brønsted acid co-catalyzed allylic C–H oxidation. **T.J. Osberger**, M.C. White

3:20 ORGN 48. Photoredox catalysis in a complex pharmaceutical setting. **J. Douglas**, K.P. Cole, C. Stephenson

3:40 ORGN 49. Rhodium (I) catalyzed carbon-carbon bond activation: Decarbonylation of ynones. **R. Whittaker**, G. Dong

4:00 ORGN 50. New dehydrative glycosylation with phosphonium anhydrides. **L. Dockery**, R. Dyapa, M.A. Walczak

4:20 ORGN 51. Epoxide approach towards the synthesis of the polypropionate acid moiety of dolabriferol. **K. Morales**, J.A. Prieto

4:40 ORGN 52. One-pot tandem cyclization of alkynes to generate polycyclic products. R.A. Carmichael, A. O'Loughlin, **W.A. Chalifoux**

Section D

Colorado Convention Center
Room 708

Asymmetric Reactions and Syntheses

M. C. McIntosh, *Organizer*
D. Coltart, *Presiding*

1:00 ORGN 53. Methodological study of a proposed, asymmetric Rauhut-Currier reaction/aldol condensation and current efforts to synthesize the anticancer agent xenitorin A. **J.E. Dander**, B. Chandler

1:20 ORGN 54. Catalytic, stereoselective vicinal difunctionalization of alkenes. **S.T. Eey**, A.J. Cresswell, S.E. Denmark

1:40 ORGN 55. Lewis base catalyzed, enantioselective, intramolecular sulfenoamination of olefins. **H. Chi**, S.E. Denmark

2:00 ORGN 56. Progress and efforts toward the asymmetric total synthesis of antascomicin B. **B. Walker**, M.C. McIntosh

2:20 ORGN 57. Enantioselective [2+2] cycloadditions using visible light photocatalysis. **K.L. Skubi**, J. Du, D.M. Schultz, T.P. Yoon

2:40 ORGN 58. Pd(II)/Brønsted acid catalyzed enantioselective oxidative carbocyclization-borylation of enallenes. **T. Jiang**, T. Bartholomeyzik, J. Mazuela, J. Willersinn, J. Bäckvall

3:00 ORGN 59. Asymmetric synthesis of piperidines by zinc-catalyzed [4+2] cycloaddition of 1-azadienes and nitro-alkenes. **C. Chu**, D. Dalton, T. Rovis

3:20 ORGN 60. Organocatalyzed enantioselective conjugate addition of heteroaryl and aryl trifluoroborates and application to the synthesis of discoipyrrole D. **J. Shih**, T.S. Nguyen, J. May

3:40 ORGN 61. Highly enantioselective preparation of chiral amines by direct asymmetric hydrogenation of ketoximes and by direct asymmetric reductive amination of ketones. **P. Ryberg**

4:00 ORGN 62. Highly efficient enantioselective hydrogenation of *N*-alkyl-pyridinium salts with an iridium-phosphole catalyst. **Y. Chen**, M. Chang, Y. Huang, S. Liu, S.W. Krska, I.W. Davies, X. Zhang

4:20 ORGN 63. Development of iridium (III) bis(imidazolinyl)phenyl complexes for enantioselective atom transfer C–H functionalization with acceptor-only metallocarbenes. **N.M. Weldy**, C. Owens, A. Schafer, C. Herting, S. Blakey

4:40 ORGN 64. Umpolung approach to the asymmetric α-alkylation of aldehydes and ketones. **D.M. Coltart**

Section E

Colorado Convention Center
Room 702

Nanomaterials

Chemistry of Fullerenes

M. C. McIntosh, *Organizer*
C. C. Kirkpatrick, *Presiding*

1:30 ORGN 65. Chemical sensing with porous molecular crystals. **C.H. Hendon**, A. Walsh

1:50 ORGN 66. Shape-persistent macrocycles conjugated with biomacromolecules and nanoparticles. **K.D. Okochi, D. Domaille, J. Cha, W. Zhang**

2:10 ORGN 67. Extension of air stability in organic light-emitting diodes using MoS_2 and WS_2 synthesized by chemical vapor deposition. **K. Kwon**, C. Kim, L. Quyet, S. Kim, H. Jang

2:30 ORGN 68. How to get selective organo(hydro)fullerenes through Rh/organoboron combination. **A. Poater**, J. Martínez, M. Solà

2:50 ORGN 69. Exploiting the unique properties of carbon nanotubes for unprecedented biological applications. **C.J. Serpell**, B.G. Davis

3:10 ORGN 70. High level computational study of C60-X- systems (X=F-,Cl-,Br-) using LPNO-CEPA/1/CBS and MP2/CBS variants. **B. Welch**, C.C. Kirkpatrick

3:30 ORGN 71. Computational studies of the interaction between carbon nanotubes and aromatic species: Energy components and SAPT methods. **C.C. Kirkpatrick**, P. Bruce-Vanderpuije

SUNDAY EVENING

Section A

Colorado Convention Center
Hall C

Asymmetric Reactions and Syntheses; Chemistry of Fullerenes, Carbon Nanotubes, and Graphene; Materials, Devices and Switches; Nanomaterials; Physical Organic Chemistry: Calculations, Mechanisms, Photochemistry, and High-Energy Species; Total Synthesis of Complex Molecules

R. D. Broene, *Organizer*

8:00 - 10:00

ORGN 72. Chiral transfer in nucleophilic reactions using chiral ionic liquids. **H.M. Thorfinnson, M.D. Mosher ORGN 73.** Asymmetric synthesis of β-amino nitriles via Mannich reactions of silyl ketene imines. **J. Zhao**, X. Feng

ORGN 74. Asymmetric synthesis of spiro-epoxyoxindoles by the catalytic Darzens reaction of isatins with phenacyl bromides. **Y. Kuang**, X. Feng

ORGN 75. Asymmetric synthesis of 2,3-dihydroquinolin-4-one derivatives catalyzed by a chiral bisguanidium salt. **X. Xiao**, X. Feng

ORGN 76. Stereoselective preparation of 3,5-disubstituted pyrrolidine-3-carboxylic acids as catalysts in asymmetric Aldol and Mannich reactions. **H. Kotapati**, J. Robinson, D.S. Masterson

ORGN 77. Catalytic asymmetric synthesis of tetrahydroquinolines via tandem 1,5-hydride transfer/Ring closure. **W. Cao**, L. Lin, X. Feng

ORGN 78. Catalytic asymmetric [3 + 2] cycloadditions about oxiranes by C–C bond cleavage of epoxides. **L. Lin**, W. Chen, X. Feng

ORGN 79. Reactions of $KPPh_2$ with cyclopalladated complexes containing an (sp_3)C—Pd bond. **G.C. Dickmu**, I.P. Smoliakova

ORGN 80. Synthesis of a transition state analog for mechanistic study of catalytic enantioselective reactions. **X. Wang**, L. Morrill, D.G. Alberg, G.E. Hofmeister

ORGN 81. Silylation-based kinetic resolution of 2-aryl cyclohexanols. **L. Wang**, R. Akhani, S.L. Wiskur

ORGN 82. Synthesis of all carbon quaternary aldehydes by palladium catalyzed asymmetric allylic alkylation (Pd-AAA): Toward the synthesis of Horsfiline. **M. Asad**, M. Hossain

ORGN 83. Withdrawn.

ORGN 84. β-D-carbafructopyranosyl-1,2-diamine-derived salen emerges as a promising new chiral ligand from a miniaturized enzymatic screen (ISES). K.R. Karukurichi, **X. Fei, R.A. Swyka**, S. Broussy, W. Shen, S. Dey, S.K. Roy, D.B. Berkowitz

ORGN 85. *N,N'*-dioxide–scandium(III)-catalyzed asymmetric Friedel–Crafts reactions of phenol derivatives. **S. Bai**, X. Feng

ORGN 86. Synthesis and reaction of silyloxy vinylketene iron complexes. **O. Kool**, Y. Guo

ORGN 87. Hydrogen bond mediated enantioselective catalysis by Werner complexes. **S.K. Ghosh**, J.A. Gladysz

ORGN 88. Synthesis of chiral sultines and derivatives: Investigation of the effect of sulfur atom in the helicity of phenyl rings. **D.R. Viernes**, C.S. Jungong, V.S. Kandula, C.K. Wach, A.G. Goos, D.J. Kerwood, D.C. Dittmer

ORGN 89. Asymmetric isomerization of alkynyl to allenyl aldehydes bearing a traceless organo-manganese η2-auxiliary. **A. Roy**, B. Bhat

ORGN 90. Catalytic asymmetric intermolecular Stetter raction of aldehydes and α,β-unsaturated ketones. **D. Flanigan**, T. Rovis

ORGN 91. Construction of trifluoromethylated all carbon quaternary stereocenters using Friedel-Crafts alkylation of arenes. **H. Subramanian**, M.P. Sibi

ORGN 92. Development of novel carboxylate-containing N-heterocyclic carbenes and their application towards new and enhanced chemical transformations. **A. Munoz**, T. Rovis

ORGN 93. Effect of added acid on the diastereoselective synthesis of chiral β-substituted [3.3.0]-bicyclic lactams. P.T. Buonora, **H. Abriam**, L. Ung, D. Nugyen

ORGN 94. Studies on the synthesis of terpene-derived chiral ketone and iminium salt catalysts for asymmetric olefin epoxidation. **K.R. Overly**, C. Williams, J. Bouchard, A. Trainor

ORGN 95. Catalytic enantioselective synthesis of 2-aryl chromenes. **B. Zeng**, K. Scheidt

ORGN 96. Rapid synthesis of 3,3′ bis-arylated BINOL derivatives using a C–H borylation in situ Suzuki–Miyaura coupling sequence. **I. Ahmed**, D.A. Clark

ORGN 97. Dynamic kinetic resolution (DKR) of atropisomers by fluxional DMAP catalysts. **G. Ma**, M.P. Sibi

ORGN 98. Aza-MIRC reactions. Asymmetric synthesis of trifluoromethyl substituted aziridines. **R. Moorthy**, M.P. Sibi

ORGN 99. Stereodynamic catalysts: Bidirectional enantioselectivity controlled by temperature. **G. Storch**, O. Trapp

ORGN 100. Synthesis of arylamine tribenzopentaphenes and investigation of their hole mobility. **B.A. Alameddine, C.K. Luscombe, T. Jenny**

ORGN 101. Synthetic tuning of the electronic properties of fused-ring oligothiophenes. **M.J. Kleinsasser**, C.B. McCausland, E.J. Uzelac, S.C. Rasmussen

ORGN 102. Bent-core 6-oxoverdazyls — a new class of mesogens. **S. Ciastek**, M. Jasinski, D. Pociecha, H. Monobe, J. Szczytko, P. Kaszynski

ORGN 103. Polar liquid crystals based on pyridinium zwitterions of the [*closo*-1-CB_9H_{10}]$^-$ and [*closo*-1-$CB_{11}H_{12}$]$^-$ anions. **J.G. Pecyna**, B. Ringstrand, P. Kaszynski

ORGN 104. Synthesis of photoreleasable protecting groups. **M.L. Hunsley**, S.M. Reed

ORGN 105. Colorimetric investigation of responsive catechol-based coatings inspired by melanin. **S.L. Lewandowski**, L.M. Choban, S.A. Flatt, J.M. Belitsky

ORGN 106. Hydrogen peroxide sensing for reproductive health. **M.S. Purdey**, E.P. Schartner, T.M. Monro, R.J. Aitken, J.G. Thompson, A.D. Abell

ORGN 107. Reversible switching of chiral DNA-templated metalloporphyrin nanoassemblies. **S. Tannir**, G. Sargsyan, M. Balaz

ORGN 108. Design and synthesis of a new switchable [2]rotaxane with a rhodamine B and pyrene as two fluorescent stoppers. J. Shi, **X. Bao**

ORGN 109. Synthesis of crosslinked membranes based on polyvinyl alcohol and naphthalene diimides. **R. Altamimi**

ORGN 110. Formulation of conductive carbon aerogels from polysaccharide-based sources. **A. Jauregui**, B.R. Luginbuhl, B.D. Cutler, C.C. Browder

ORGN 111. Electrical optimization of agar-derived carbon aerogels for use in structural electric double-layer capacitors. **B.R. Luginbuhl**, B.D. Cutler, A. Jauregui, C.C. Browder

ORGN 112. Naphthalene diimide based materials with adjustable redox potentials for organic lithium ion batteries. **G. Vadehra**, R.P. Maloney, B. Dunn, M.A. Garcia-Garibay

ORGN 113. Thermoluminescent boron compounds: Synthesis, characterization, and photophysical properties. **A.A. Molina Paredes**, B. Muñoz

ORGN 114. Small molecular donor-acceptor dyads as additives for organic photovoltaics. **D. Chavis**, J. Strain, H.P. Rathnayake

ORGN 115. Fused arenes-based molecular systems as additives for organic photovoltaics. **D. Patel**, R. Neesu, H.P. Rathnayake

ORGN 116. Mechanochromic luminescent heteroaromatic difluoroboron β-diketonate complexes. **M. Kolpaczynska**, W. Morris, C.A. DeRosa, C.L. Fraser

ORGN **117.** Novel route to synthesize polymers containing single mechanical bond. **U. Choudhary**, B.H. Northrop

ORGN **118.** Synthesis and photochemical properties of bis (4'-azo-4" (5)substituted dibenzo-18-crown-6) carboxylic acid derivatives. **R. Khatmullin**

ORGN **119.** Poly(1,4-phenylene vinylene) derivatives with ether substituents to improve polymer solubility for use in organic light-emitting diode (OLED) devices. **C.A. Young**, T. Lee

ORGN **120.** Novel ionic liquid crystals based on nitrile functionalized imidazolium. **T.A. Sanders**, L. Douce, B. Heinrich

ORGN **121.** Preparations and self-assembly study of gold nanoparticles composited with discotic organic molecules. **Y. Mi**, P. Liang, D. Wang, Z. Yang

ORGN **122.** Proton-electron dual responsive system of ferrocene-bound nickelladithiolene. **A. Tanushi**, T. Kusamoto, Y. Hattori, K. Takada, H. Nishihara

ORGN **123.** Substituent and solvent effects: Examining acidity via infrared spectroscopy. **J.E. Buhle**, M. Samet, S.R. Kass

ORGN **124.** Mechanism and stereoselectivity of an isothiourea-catalyzed [2,3]-rearrangement: Control via electrostatics and orbital Interactions. **D.M. Walden**, T.H. West, R.C. Johnston, A.D. Smith, P.H. Cheong

ORGN **125.** Computational study of diaryliodonium reagents for heteroatom arylation reactions. **J. Buchanan**, S.K. Sundalam, D.R. Stuart, P.H. Cheong

ORGN **126.** Highly efficient and selective epoxidation catalyzed by iron corrole complexes and iodobenzene diacetate. **T. Chen**, K. Kwong, W. Luo, A.C. Carver, R. Zhang

ORGN **127.** Visible light-promoted selective sulfoxidations catalyzed by ruthenium porphyrins with iodobenzene diacetate. **W. Luo**, T. Chen, Z. Yuan, A.C. Carver, R. Zhang

ORGN **128.** Synthetic and mechanistic studies of catalytic oxidations by manganeses(III) porphyrins and iodobenzene diacetate. **K. Kwong**, T. Chen, W. Luo, R. Zhang

ORGN **129.** Synthesis and photophysical studies of two lophine derivatives with electron-donating groups on the aryl ring in the 2-position. T. Le, T. Hamada, J. Rimby, **R.A. Isovitsch**

ORGN **130.** Kinetics of retro-hetero-Diels-Alder reactions to model controlled release from novel sulfonamide drug-polymer conjugates. **C.S. Erkkila, N.A. Yakelis**

ORGN **131.** Phenylchlorocarbene additions to diarylcyclooctynes and diarylcyclooctenes. **E. Dalchand**, S. Tsuno, A. Scorese, K. Francisco, C. Buzard, D.C. Merrer

ORGN **132.** Getting beyond frontier molecular orbital theory to predict regioselectivity of nucleophilic aromatic photosubstitution reactions. **G.G. Wubbels**

ORGN **133.** Computational investigations into stereoselective alkylation reactions: Evidence for torsional and Curtin–Hammett control. **A.M. Harned**

ORGN **134.** Radical viologen organic spin cross over materials. **M.J. Juetten**, A. Winter

ORGN **135.** Density functional theory treatment of substituent effects on the amide-acetal Claisen rearrangement. **M. Hartley**, G.W. Daub, R.J. Cave

ORGN **136.** Computational mechanistic study on hexadehydro-Diels-Alder reactions. **L.R. Furan**, K.T. Kuwata

ORGN **137.** Fluoro-amide and fluoro-sulfonamide gauche effects: An experimental study. **B.U. Emenike**

ORGN **138.** Abnormal substrates give "abnormal" products: Competition between classical Diels–Alder vs. hexadehydro-Diels–Alder (HDDA) reactions. **Q. Luu Nguyen**, B. Baire, T.R. Hoye

ORGN **139.** Sterically demanding bis-(o-biphenyl)-phospine ligands in gold(I) catalysis. **C. Griebel**, D.D. Hodges, A.C. Jones

ORGN **140.** Investigation of spin coated pristine and blended organic semiconductor films containing perylene diimides: The role of molecular structure and crystal formation in blended film composition. **J.M. Szarko**, A. Austin, E. Xhakaj, S. Liu

ORGN **141.** DFT study of phosphine-borane bonds: Exploring electronic effects. **P.A. Sibbald**

ORGN **142.** Expeditious, radical pathway for sonication assisted Mitsunobu reaction of hindered secondary alcohols. **R. Florre, R. Heckler**, P. Cohn, S. Rajaraman

ORGN **143.** Mechanistic studies on the catalytic oxidative cyclization reactions of 2'-arylbenzaldehyde oxime ethers. **N.R. Armada**, J. Hofstra, B. Grassbaugh, Q. Tran, P. De Lijser

ORGN **144.** Solution photophysics of *o*-carborane carrying one or two singlet-fission chromophores (1,3-diphenylisobenzofuran). **Y. Hervault**, J. Schrauben, M. Schreiber, J.C. Johnson, J. Michl

ORGN **145.** (t-Bu)$_2$P(*o*-dimethylaminophenyl): The role of P, N ligands in gold(I) catalysis. **J. Piedad**, A.C. Jones

ORGN **146.** Experimental study of solution Ag(I)-π interactions using molecular balances. **J. Maier**, K.D. Shimizu

ORGN **147.** Revealing the carbon centered radical reactivity towards oxygen by DFT calculations. **D.M. Sriyarathne**, A.D. Gudmundsdottir

ORGN **148.** Synthesis of tetra(benzyloxy) benzenes for mass spectrometry studies. **R. Brumbaugh**, R. Taylor, R. Hark, D. Kuck, W.M. Ames, P. Schettler

ORGN **149.** Source of the puzzling effect of the primary isotope on secondary kinetic isotope effects in alcohol dehydrogenases. **J. Lefton**, J. Eilers, Y. Lu

ORGN **150.** Primary isotope dependence of secondary kinetic isotope effects in NADH/NAD+ model reactions. **M. Boroujeni**, Y. Lu

ORGN **151.** Progress toward the total synthesis of tetarimycin A. **E. Jones-Mensah**, S.H. Lusk, J. Magolan

ORGN **152.** Withdrawn.

ORGN **153.** Synthesizing and trialing triesterified monosaccharides for protected culture pest control. **H. Cavender, M.W. Fultz, M. Guetzloff**, B. Liedl

ORGN **154.** Studies into the total synthesis of the drimentine alkaloids. **S.M. Pound**, C.J. Douglas

ORGN **155.** Catalytic approach to the MH-031 lactone: Application to the synthesis of geralcin analogs. **R. Tello-Aburto**, A.N. Lucero, S. Rogelj

ORGN **156.** Progress towards the total synthesis of (-)-gilbertine. **T. Folda**, K.S. Feldman

ORGN **157.** Progress towards the synthesis of 7,20-diisocyanoadociane. **P.C. Roosen, C.D. Vanderwal**

ORGN **158.** 2,5-Cyclohexadienones as a useful launching point for the synthesis of the briarane diterpenoids. **N.G. Moon**, A.M. Harned

ORGN **159.** Total synthesis of cyanolide A. **T. Lek**, R.W. Bates

ORGN **160.** Work toward the synthesis of aspidospermine via a ring fragmentation and 1,3-dipolarcycloaddition sequence. **G. Giampa**, M. Brewer

ORGN **161.** Synthesis and biological activity of 1-aryl and 1-heteroaryl analogs of eudistomin U. **C.M. Roggero**, J. Giulietti, P. Tate, S.P. Mulcahy

ORGN **162.** Highly stereoselective total synthesis of Lagunamide A. **A. Kanner**, N. Kohnen, B. Banasik, L. Wang, M.B. Bergdahl

ORGN **163.** Preparation of isogemichalcone analogs, potential inhibitors of aromatase. **A. Angelbello, M. Morales, S. Longson, E.G. Casillas**

ORGN **164.** First enantiospecific total synthesis of macrosalhine chloride (4) and progress toward the synthesis of macroline-related indole alkaloids macrocarpine A, B, and C will be presented. **M. Rahman**, R. Jahan, R.V. Edwankar, J.R. Deschamps, J.M. Cook

ORGN **165.** Progress toward the enantioselective total syntheses of leodomycins A and B via an asymmetric vinylogous aldol strategy. **A. Chin**, J.D. Carrick

ORGN **166.** Configuration-encoded 1,5-polyol synthesis: Access to the anti,syn-1,5,7-triol within the C15-C25 fragment of tetrafibricin. **R. Friedrich**, G.K. Friestad

ORGN **167.** Progress toward the total synthesis of hippolachnin A. **M.E. McCallum**, J.L. Wood

ORGN **168.** Efficient synthesis of polycyclic skeletons of *Aspidosperma* and *Corynanthe* indole alkaloids. **Z. Angel**, E.K. Leggans

ORGN **169.** Synthesis of carbazole alkaloids via an HDDA-based strategy. **T. Wang, D. Niu, T.R. Hoye**

ORGN **170.** Synthesis of unnatural enantiomers of morphinan derivatives as toll-like receptor 4 inhibitors. **W.T. Hartwig**, T. Sammakia

ORGN **171.** Toward the total synthesis of phomoidride D. **J. Leung**, A.A. Bedermann, N. Hama, G. Murphy, C. Schneider, P. Dong, J.L. Wood

ORGN **172.** New and facile synthesis of brazilin via intramolecular alkyne-aldehyde metathesis. **Y. Jung**, I. Kim

ORGN **173.** Progress toward the total synthesis of tetrapetalone A. **H. Dhanjee, Y. Kobayashi**, T.C. McMahon, J.F. Buergler, M. Haley, J.M. Howell, J.L. Wood

ORGN **174.** Assessing the need for a trityl group as a steric buttress to initiate a Diels-Alder reaction. **C.D. Choony**

ORGN **175.** Ongoing work to prepare the anticancer agent xenitorin A. **S.M. Soars**, B. Chandler

ORGN **176.** Total synthesis of Herbarin A and B and determination of their anti-oxidant properties and toxicity in Zebra fish model. **J. Heimberger**, H. Cade, M.A. Lnu

MONDAY MORNING

Section A

Colorado Convention Center
Four Seasons Ballroom 2&3

Elias J. Corey Award for Outstanding Original Contribution in Organic Synthesis by a Young Investigator: Symposium in Honor of Jin-Quan Yu

B. B. Snider, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 ORGN **177.** Innovative methodology introduced in the total synthesis and subsequent diversification of vinblastine. **D.L. Boger**

9:20 ORGN **178.** Metal-catalyzed cross-coupling reactions of alkyl electrophiles. **G.C. Fu**

10:05 ORGN **179.** Catalytic activation of nucleophiles for selective reactions. **L. Deng**

10:50 Introduction of Awardee.

11:00 ORGN **180. Award Address** (Elias J. Corey Award for Outstanding Original Contribution in Organic Synthesis by a Young Investigator sponsored by the Pfizer Endowment Fund). Ligand-accelerated C-H activation reactions: Near and far. **J. Yu**

Section B

Colorado Convention Center
Four Seasons Ballroom 1

Miniaturization in Chemistry: (sub)-Nanoscale Synthesis, Analysis & Application

S. Dreher, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 ORGN **181.** From synthesis in flow to integrated dose-response screening in flow. **R.E. Martin**, M. Werner, C. Kuratli, R. Hochstrasser, T. Enderle, H. Vogel

8:50 ORGN **182.** From screening of (enantioselective) catalysts by integration of analysis and synthesis to the application in a pilot plant. **O. Trapp**

9:35 ORGN **183.** High-throughput high-content screening using model organisms enabled by automated microfluidics. **H. Lu**

10:20 ORGN **184.** Nanomolar scale high throughput chemistry for complex molecules synthesis. **S. Dreher**, A. Buitrago Santanilla, T. Cernak, C.J. Welch, R.M. Helmy, I.W. Davies, E. Regalado, a. pereira, P. Vachal, Z. Shi, P.G. Nantermet, M. Shevlin

11:05 ORGN **185.** Flow chemistry miniaturization and optimization. **K.F. Jensen**

Section C

Colorado Convention Center
Rooms 704/706

New Reactions and Methodology

M. C. McIntosh, *Organizer*
S. Luesse, *Presiding*

8:00 ORGN **186.** Enantioselective cycloadditions of aminoazaxylylenes photogenerated via proton transfer in aromatic imines and oxazolines offer expedited access to diverse polyheterocyclic moleculararchitectures. **O. Mukhina**, N.N. Bhuvan Kumar, D. Kuznetsov, A.G. Kutateladze*

8:20 ORGN **187.** Stereoselective homoallylation with cyclopropanated allylation reagents. **I.J. Krauss**

8:40 ORGN **188.** Efficient assembly of epoxyisoindoline derivatives through a tandem Diels-Alder Ugi-Smiles process. **S.B. Luesse**, B. Richey, K. Mason, M. Meyers, R. Poormotamed

9:00 ORGN **189.** Protodecarboxylation of unstablized carboxylic acids and malonic acid derivatives through photoredox catalysis. **J. Griffin**, M. Zeller, D.A. Nicewicz

9:20 ORGN **190.** C-H activation and C-C bond formation through cross-coupling reaction by using potassium organotrifluoroborates. **M. Al-Masum**, W. Shaban

9:40 ORGN **191.** Chiral anti-diols from alpha-oxyaldehydes. **G.A. Abeykoon**, S. Chatterjee, J.S. Chen

10:00 ORGN **192.** Multicomponent reactions in deep eutectic solvents. **S.T. Handy**

10:20 ORGN **193.** Efficient synthesis of N-alkylated amides from nitriles and alcohols catalyzed by the combination of gold and iridium complexes. **F. Li**, J. Ma, L. Lu, X. Bao

10:40 ORGN **194.** Mechanistic studies and applications of tertiary amine trapping of HDDA-generated benzynes. **S.P. Ross**, T. Hoye

11:00 ORGN **195.** Synthesis of highly functionalized aryl sulfides from HDDA-generated benzynes: Scope and mechanisms. **J. Chen, V. Palani, T.R. Hoye**

11:20 ORGN **196.** Withdrawn.

11:40 ORGN **197.** Synthesis of 6-hydroxyquinoline starting from glycerol via improved microwave-assisted modified Skraup reaction and Bamberger rearrangement. **C. Len**, N. Thiebault, H. Saggadi, D. Luart, I. Polaert, L. Estel

Section D

Colorado Convention Center
Room 708

Molecular Recognition and Self-Assembly

M. C. McIntosh, *Organizer*
J. J. Reczek, *Presiding*

9:00 ORGN **198.** Isothermal titration calorimetric analyses of the hydrophobic and Hofmeister effects. **P. Sokkalingam**, B.C. Gibb

9:20 ORGN **199.** Studies of statistically patterned two-component self-assembled monolayers. **Y. Yang**, M.B. Zimmt

9:40 ORGN **200.** Development of a molecular turing machine. **S. Varghese**, J.A. Elemans, A.E. Rowan, R. Nolte

10:00 ORGN **201.** Rapid threading of a long polyethylene glycol chain through a macrocycle in water. **E. Peck**, W. Liu, G. Spence, B. Smith

10:20 ORGN **202.** Chemosensors for redox-active biomolecules. **J. Hong**, D. Lee, J. Oh

10:40 ORGN **203.** Self-assembly of collagen mimetic nanofibers through triple-helical hybridization. **B. Sarkar**, J.D. Hartgerink

‡ *Cooperative Cosponsorship*

11:00 ORGN **204.** *C*-alkylpyrogallol[4]arenes: Robust building blocks for supramolecular organic frameworks (SOFs). **R. Patil**, H. Kumari, J.L. Atwood

11:20 ORGN **205.** Highly substituted anthracenes as self-assembly components of new donor-acceptor columnar liquid crystalline materials. **J.J. Reczek**

Section E

Colorado Convention Center
Room 702

Physical Organic Chemistry: Calculations, Mechanisms, Photochemistry, and High-Energy Species

M. C. McIntosh, *Organizer*
C. Hamann, *Presiding*

8:30 ORGN **206.** Comparison of high spin nitrene isomers with low-temperature matrix isolation spectroscopy. **K. Long**, M. Maehara, E. Mendez-Vega, D. Sander

8:50 ORGN **207.** Synthesis and characterization of di- and tri- aryl pentanes as model for conducting organic polymers. **A. Agrahari**, J. Masnovi

9:10 ORGN **208.** Experimental studies on how *meta*- and *para*-substituents influence the strength of the off-set aromatic stacking interaction. **J. Hwang**, K.D. Shimizu

9:30 ORGN **209.** Degradation of thiophenes by singlet oxygen: Insights from theoretical photochemistry. **M. Wykes**, J. Gierschner, D. Roca-Sanjuán

9:50 ORGN **210.** Withdrawn.

10:10 ORGN **211.** Do aza-*ortho*-quinone-methide mediated transformations involve aza-*ortho*-quinone-methides? **P.H. Cheong**, R.C. Johnston, M.T. Hovey, K. Scheidt

10:30 ORGN **212.** De novo catalyst design of scaffolding bifunctional catalysts for the site-selective functionalization of *trans*-1,2 diols. **R.C. Johnston**, O.M. Ogba, M.F. El Mansy, H. Yao, R.G. Carter, P.H. Cheong

10:50 ORGN **213.** Light-induced radical trapping (LIRT): A new approach to molecular photomagnetism from old principles of organic photochemistry. H. Phan, A. Dragulescu-Andrasi, K. Lekin, S.M. Winter, R.T. Oakley, **M. Shatruk**

11:10 ORGN **214.** Exploring the conformational isomerization of the humulyl cation using computational methods. **C.S. Hamann, D.J. Tantillo**

11:30 ORGN **215.** Carbenic, allenic, and propargylic nitrile imines. **C. Wentrup**

MONDAY AFTERNOON

Section A

Colorado Convention Center
Four Seasons Ballroom 2&3

Herbert C. Brown Award for Creative Research in Synthetic Methods: Symposium in Honor of Gary A. Molander

C. White, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 ORGN **216.** New allylic alkylation reactions: Asymmetric construction of acyclic quaternary carbon stereogenic centers. **P. Evans**

1:50 ORGN **217.** Straightforward strategies to access N-containing structure: Organocatalysis for the benefit of natural products. **G. Masson**

2:35 ORGN **218.** Catalysis in light and shadow. **K. Zeitler**

3:20 ORGN **219.** From alkaloids to terpenoids: New strategies and tactics for the synthesis of polycyclic natural products. **S.E. Reisman**

4:05 Introduction of Awardee.

4:10 ORGN **220. Award Address** (Herbert C. Brown Award for Creative Research in Synthetic Methods sponsored by the Purdue Borane Research Fund and the Herbert C. Brown Award Endowment). Novel mechanistic paradigm for organoboron cross-coupling. **G.A. Molander**

Section B

Colorado Convention Center
Four Seasons Ballroom 1

Synthetic Biology Applied to Natural and Unnatural Product Pathways

B. Bachmann, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 ORGN **221.** Microbial natural product discovery and diversification: New tools and applications. **J.S. Thorson**

1:55 ORGN **222.** New recipes for biocatalysis: Expanding the cytochrome P450 reaction landscape for non-natural chemistry. **E. Brustad**

2:45 Intermission.

3:00 ORGN **223.** Introduction of noncanonical amino acids into a lasso peptide, microcin J25. **F.J. Piscotta, A. Link**

3:20 ORGN **224.** Engineered biosynthesis of antimycin-type depsipeptides. **W. Zhang**

4:10 ORGN **225.** Adapting the retrograde evolution hypothesis to build new biosynthetic pathways for unatural molecules. **B.O. Bachmann**

Section C

Colorado Convention Center
Rooms 704/706

New Reactions and Methodology

M. C. McIntosh, *Organizer*
D. Bandyopadhyay, *Presiding*

1:20 ORGN **226.** Unusual rearrangement of 3-acyl-2-alkoxyfurans enabling appendage of a carbon substituent at C-2: Application to the synthesis of furanolabdanes. **C. Thibault**, J. Boukouvalas

1:40 ORGN **227.** Photochemistry of *o*-nitroarenes: Trifluoromethylated o-nitrobenzyl sytems as efficient photosynthons for selective trifluoromethylated arenes and heteroarenes. G. Prakash, K. Belligund, **T. Mathew**, G.A. Olah

2:00 ORGN **228.** Regioselective synthesis of chloro/bromostyrenes: Chloro/bromotrimethylsilane-nitrate salt as efficient reagent system. G. Prakash, **L. Gurung**, T. Mathew, G.A. Olah

2:20 ORGN **229.** Examining the scope of ISES hits: Pd-catalyzed halo- and pseudohalometalation/carbocyclization transformations. **G.G. Malik**, R.A. Swyka, G.A. Applegate, X. Fei, D.B. Berkowitz

2:40 ORGN **230.** Copper (I) catalyzed synthesis of enaminones from thioamides and α-diazocarbonyl compounds. **A. Pal**, N. Koduri, S.R. Hussaini

3:00 ORGN **231.** Site-selective aliphatic C-H halogenation using N-haloamides. **R.K. Quinn**, V.A. Schmidt, A. Brusoe, E.J. Alexanian

3:20 ORGN **232.** Transition metal catalyzed redox-triggered C-C couplings of alcohols *via* transfer hydrogenation. **B.Y. Park**, T.P. Montgomery, T. Luong, V. Garza, M.J. Krische

3:40 ORGN **233.** Intramolecular [3 + 2] cyclocondensations of alkenes with indolidenes and indolidenium cations. **I.Y. Gonzalez**, C.M. Glinkerman, K.S. Feldman

4:00 ORGN **234.** Metal-free methodology for the preparation of sterically hindered ynones and its application to the synthesis of natural products. **C. Taylor**, Y. Bolshan

4:20 ORGN **235.** Dramatic kinetic isotope effects (kie), solvent effects, and tunneling in directed ortho metallation (DOM). **M.G. Organ**, J. Farmer, E. Leeruff, R. Froese

4:40 ORGN **236.** Radical decarboxylation in micellar media for the formulation of new surfactants. **C. Len**, F. Mangin, E. Banaszak-Leonard

5:00 ORGN **237.** Microwave-assisted dehydration of polyols in aqueous media. **C. Len**, S. Le Guenic, C. Ceballos

Section D

Colorado Convention Center
Room 708

Molecular Recognition and Self-Assembly

M. C. McIntosh, *Organizer*
I. Vargas-Baca, *Presiding*

1:30 ORGN **238.** CH–π Interactions of methyl ethers as a model for carbohydrate–*N*-heteroarene interactions. **P. Li**, T.M. Parker, J. Hwang, M.D. Smith, P.J. Pellechia, D. Sherrill, K.D. Shimizu

1:50 ORGN **239.** Design and self-assembly of metallo-supramolecular structures guided by density of coordination sites. M. Wang, B. Sun, A. Cisneros, **X. Li**

2:10 ORGN **240.** Molecular dynamics simulations of stacked DNA base surrogates. C. Markegard, **A. Mazaheripour**, J. Jocson, A.M. Burke, A.A. Gorodetsky, H. Nguyen

2:30 ORGN **241.** Supramolecular polymers for active layer organization in photovoltaics. **L. Barreda**, T. Aytun, A. Ruiz-Carretero, J. Lehrman, S.I. Stupp

2:50 ORGN **242.** Overcoming static disorder within photoreactive co-crystals by vortex grinding. **R.H. Groeneman**, K.A. Kummer

3:10 ORGN **243.** Racemic hydrogels from self-assembling enantiomeric peptides: Predictions from Linus Pauling. **J.P. Schneider**

3:30 ORGN **244.** Supramolecular macrocycles self-assembled by iso-tellurazole N-oxides. P.C. Ho, J. Sinclair, L. Lee, **I. Vargas-Baca**

3:50 ORGN **245.** Regulating molecular recognition in synthetic supercontainers. **Z. Wang**, F. Dai, U. Sambasivam, Y. Qiao, A. Corbett

4:10 ORGN **246.** Peptide-based functional molecular gels. **B. Escuder Gil**, J. Miravet, M. Tena-Solsona, C. Berdugo, S. Diaz-Oltra

Section E

Colorado Convention Center
Room 702

Physical Organic Chemistry: Calculations, Mechanisms, Photochemistry, and High-Energy Species

M. C. McIntosh, *Organizer*
K. M. Miller, *Presiding*

1:30 ORGN **247.** Molecular origin of color tuning of deepwater Lake Baikal cottoid fish visual pigments. **H. Luk**, F. Montisci, F. Melaccio, N. Bhattacharyya, J. Morrow, B. Chang, F. Fanelli, M. Olivucci

1:50 ORGN **248.** On the mechanism of silver-catalyzed decarboxylative fluorination. **N.R. Patel**, R.A. Flowers

2:10 ORGN **249.** Physicochemical and thermal properties of 1,2,4-triazolium ionic liquids. **K.M. Miller**

2:30 ORGN **250.** Luminescent properties of an open-shell organic radical with high photostability. **T. Kusamoto**, Y. Hattori, H. Nishihara

2:50 ORGN **251.** Autocatalytic self-replicating micelles. **K. Bukhriakov**, S. Almahdali, V. Rodionov

3:10 ORGN **252.** Computational mechanistic investigation of a Cu(I)-catalyzed 1,3-halogen migration. **B.M. Hudson**, H. Wedler, R. Van Hoveln, D. Bates, D.J. Tantillo, J.M. Schomaker

3:30 ORGN **253.**
Intramolecular reactions of polysubstituted cyclobutenones: An in silico investigation of product specificity. **F.E. Jernigan**, L. Sun

3:50 ORGN **254.** 9-Imino-pyronin analogs: Rationally designed small-molecule fluorophores with large Stokes shifts. **P. Sebej**, P. Horvath, T. Solomek, P. Klan

4:10 ORGN **255.** Transition state *Gauche* effect controls the torquoselectivities of the electrocyclizations of Chiral 1-azatrienes. **A. Patel**, Z. Ma, J. Vella, R. Hsung, K.N. Houk

4:30 ORGN **256.** Semiempirical and QM/MM calculations of the noncovalent interactions between ATP and RecA DNA-repairing proteins. **J.H. Rodriguez**, M. Palenik, L. Beard

MONDAY EVENING

Section A

Colorado Convention Center
Halls C/D

Sci-Mix

R. D. Broene, M. C. McIntosh, *Organizers*

8:00 - 10:00
77, 81, 87, 99, 108, 116, 133, 135, 146, 162, 171. See previous listings.
330, 333, 335, 337, 377-378, 381, 394, 399, 405, 412, 418, 524, 539, 546, 555, 588, 594, 600. See subsequent listings.

TUESDAY MORNING

Section A

Colorado Convention Center
Four Seasons Ballroom 2&3

ACS Award for Creative Work in Synthetic Organic Chemistry: Symposium in Honor of F. Dean Toste

C. A. Maryanoff, *Organizer, Presiding*

8:20 Introductory Remarks.

8:25 ORGN **257.** Synthetic studies of complex natural products. **T.J. Maimone**

9:05 ORGN **258.** C—H bond aminations. **M. White**

9:45 ORGN **259.** Synthetic methods based on catalytic P(III)/P(V) cycling. **A.T. Radosevich**

10:25 ORGN **260.** Catalyst discovery with base metal heterobimetallic complexes. **N.P. Mankad**

11:05 ORGN **261. Award Address** (ACS Award for Creative Work in Synthetic Organic Chemistry sponsored by Aldrich Chemical Co., LLC). Concepts and catalysts for enantioselective reactions of carbon-carbon multiple bonds. **F. Toste**

Section B

Colorado Convention Center
Four Seasons Ballroom 1

ACS Award for Creative Invention: Symposium in Honor of Jotham W. Coe

P. L. Feldman, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 ORGN **468.** Chemical synthesis of secondary metabolites. **R.A. Shenvi**

9:25 ORGN **469.** Alcohol C-H functionalization via redox-triggered Carbonyl Addition: Borrowing hydrogen, returning carbon. **M.J. Krische**

10:15 ORGN **470.** Strategy for selective halogenation. **N.Z. Burns**

11:05 Introduction of Awardee.

11:10 ORGN **471. Award Address** (ACS Award for Creative Invention sponsored by ACS Corporation Associates). Discovery of Chantix (varenicline tartrate), an aid to smoking cessation. **J.W. Coe**

Section C

Colorado Convention Center
Rooms 704/706

New Reactions and Methodology

M. C. McIntosh, *Organizer*
M. Emmert, *Presiding*

8:00 ORGN **262.** Rh(III)-catalyzed C(sp3)H allylic functionalization of *N*-tosylamides :An unexpected formation of azabicyclic compounds. **A. Archambeau**, T. Rovis

8:20 ORGN **263.** Synthetic clays as new catalysts for aerobic oxidation. **J. Magolan**, M. Karki, H.C. Araujo, J.J. Dalton, S.D. Holmbo, L. Baker

8:40 ORGN **264.** Cerium-free Luche reduction in the presence of alumina. **E. Jones-Mensah**, L.A. Nickerson, H.J. Knox, J. Magolan

9:00 ORGN **265.** New applications of dimethylsulfoxide as a terminal oxidant. **J. Magolan**, E. Jones-Mensah, M. Karki, J.T. Schmalz

9:20 ORGN **266.** Iron catalyzed α-C-H oxidation of tertiary amines mimicking cytochrome P450 activity. **M. Emmert**

9:40 ORGN **267.** Tetrabutylammonium bromide: Catalytic abilities in C-O activation. **M. Emmert**

10:00 ORGN **268.** Catalytic olefin hydroamination with aminium radical cations: A photoredox method for direct C-N bond formation. **A. Musacchio, R.R. Knowles**

10:20 ORGN **269.** Accessing triplet nitrenes by visible light triplet sensitization of azides. **S. Scholz, E. Farney**, T.P. Yoon

10:40 ORGN **270.** 2,2,2-Trichloroethyl aryldiazoacetates as robust reagents for site-selective C–H functionalization. **D.M. Guptill**, H.M. Davies

11:00 ORGN **271.** Synthesis of bridged bicycles via additional steps of metal carbene cascade reaction. **Y. Kuo**, J. May

11:20 ORGN **272.** HOF-CH_3CN Probably the best oxygen transfer agent organic chemistry has to offer. **S. Rozen**, I. Vints, S. Potash

Section D

Colorado Convention Center
Room 708

Biologically-Related Molecules and Processes

M. C. McIntosh, *Organizer*
Y. Aye, *Presiding*

8:00 ORGN **273.** Synthesis of novel carbon monoxide releasing molecules. **T. Israsenanaayudhya**, C. Raymond, N.N. Dingra

8:20 ORGN **274.** Determination of the absolute configuration of a single enantiomer of deoxyArbutin. **A.M. Kornilov**, M.A. Delong, A.J. Stein, J.B. Williams, D.K. Van Strien, M.C. Ammerman

8:40 ORGN **275.** Synthesis and inhibition studies of a transition-state inhibitor for *Mycobacterium tuberculosis* GlgE. **S. Veleti**, J. Lindenberger, S. Thanna, D. Ronning, S.J. Sucheck

9:00 ORGN **276.** Chemical modulation of lipid bilayer membranes via copper(I)-catalyzed azide alkyne cycloaddition. **J.M. Beveridge**, M.M. Baksh, M. Finn

9:20 ORGN **277.** Syntheses of heteroatom-activated β-lactams and their evaluation as potential antibiotics and enzyme inhibitors. **K.D. Watson**, M.W. Majewski, P.L. Barker, M.J. Miller

9:40 ORGN **278.** Cell death imaging using fluorescent probes for phosphatidylserine. **K.J. Clear**, K.M. Harmatys, D.R. Rice, B.D. Smith

10:00 ORGN **279.** Generalizable platform for target- and signal-specific perturbation of a single signaling target in cells. **Y. Aye**

10:20 ORGN **280.** Selective fluorescence detection of homocysteine over cysteine using aldehyde bearing fluorophores. **A. Barve**, R.M. Strongin

10:40 ORGN **281.** Syntheses and evaluation of highly functionalized monobactams and cephalosporins as medicinally useful agents. **M.W. Majewski**, K.D. Watson, S. Cho, P.A. Miller, S.G. Franzblau, M.J. Miller

11:00 ORGN **282.** Near infrared activated cobalamin-drug conjugates for light targeted delivery. W. Smith, N. Oien, R.M. Hughes, C. Marvin, **Z. Rodgers**, J. Lee, D.S. Lawrence

11:20 ORGN **283.** Synthetic chemists to aid the community for open antimicrobial drug discovery. **M.A. Blaskovich**, J. Zuegg, A.G. Elliott, M.A. Cooper

11:40 ORGN **284.** Tropane alkaloids from the Australian proteaceous plant *Flyodia praealta*. **F. Yang**, A.R. Carroll, H. Zhao

Section E

Colorado Convention Center
Room 702

Physical Organic Chemistry: Calculations, Mechanisms, Photochemistry, and High-Energy Species

M. C. McIntosh, *Organizer*
D. B. Lawson, *Presiding*

8:30 ORGN **285.** Intramolecular Diels–Alder reactions between aromatic dienes and a benzyne dienophile: Relative reactivities of the dienes. **V. Pogula**, T. Wang, T.R. Hoye

8:50 ORGN **286.** Mechanism for reversible photodegradation of 1-substituted aminoanthraquinones doped in poly(methyl methacrylate). **S. Hung**, K. Schademan, M.D. McCluskey, K. Clays, M. Kuzyk

9:10 ORGN **287.** Synthesis and gas phase reactivity of charged σ,σ,π-tri- and σ,σ,σ,π-tetraradicals toward small organic substrates in a linear quadrupole ion trap (LQIT) mass spectrometer. **R. Kotha**, H.I. Kenttamaa

9:30 ORGN **288.** Substituent effects on the [N-X-N]+ halogen bonds. **A. Carlsson**, A. Karim, M. Bedin, J. Grafenstein, M. Erdelyi

9:50 ORGN **289.** Elucidating the role of SmI_2-water and glycol in reductions: Mechanistic studies of anthracene reduction. **T.V. Chciuk**, R.A. Flowers

10:10 ORGN **290.** Radical arylation of epoxides by low-valent titanocene complexes: Mechanistic studies and methodology development. **G. Fianu**, R.A. Flowers

10:30 ORGN **291.** Irreversible formation of high energy intermediates to achieve high yield photorelease of alcohol. **K.R. Thenna Hewa**, A.D. Gudmundsdottir, D.L. Phillips, M. Li

10:50 ORGN **292.** Two-color fluorescent dyes for "click" labeling: Design and characterization. **R.K. Meka**, M.D. Heagy

11:10 ORGN **293.** Computational studies of fluorinated biomimetic molecules. **J.J. Urban**, G.S. Kedziora, M. Hastings, N. Erxleben, R.M. Crutcher, R. Atwood

11:30 ORGN **294.** Evidence supporting a revised mechanism for the traceless Staudinger ligation of phosphino phenyl esters and aryl azides. **T.P. Kirby**, T.H. Koch

11:50 ORGN **295.** DFT density and difference density volumes of transition states. **D.B. Lawson**

TUESDAY AFTERNOON

Section A

Colorado Convention Center
Four Seasons Ballroom 2&3

Ernest Guenther Award in the Chemistry of Natural Products: Symposium in Honor of Thomas R. Hoye

P. R. Hanson, *Organizer, Presiding*

1:00 ORGN **296.** Recent studies toward the synthesis of rocaglamide and related natural products. **J.A. Porco, Jr.**

1:40 ORGN **297.** Worm language: A natural combinatorial library and a xylopyranose-based nucleoside. **F.C. Schroeder**

2:20 ORGN **298.** Strategies and tactics for chemical synthesis inspired by complex alkaloids. **R. Sarpong**

3:00 ORGN **299.** Evolution of anion relay chemistry (ARC) leading to Negishi cross-coupling without $ZnCl_2$. **A.B. Smith**

3:40 Introduction of Awardee.

3:45 ORGN **300. Award Address** (Ernest Guenther Award in the Chemistry of Natural Products sponsored by Givaudan). Natural products as drivers of discovery. **T.R. Hoye**

Section B

Colorado Convention Center
Four Seasons Ballroom 1

James Flack Norris Award in Physical Organic Chemistry: Symposium in Honor of Charles L. Perrin

L. T. Scott, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 ORGN **301.** In search of kinetically stable aryltrifluoroborates: B-18F bond formation for one-step 18F-labeling of peptides for PET imaging. **D.M. Perrin**, Z. Liu, Y. Li, R. Ting

1:45 ORGN **302.** From host-guest chemistry to the nucleosome: Studies in biomolecular recognition. **M. Waters**

2:25 ORGN **303.** Adventures in physical organic chemistry with Pd and Zn. **P.J. Walsh**

3:05 ORGN **304.** Myths and models in aromatic chemistry. **J.S. Siegel**

3:45 Introduction of Awardee.

3:50 ORGN **305. Award Address** (James Flack Norris Award in Physical Organic Chemistry sponsored by the ACS NortheasternSection). Logic behind a physical-organic chemist's research topics. **C.L. Perrin**

Section C

Colorado Convention Center
Rooms 704/706

Green Chemistry: Reactions in Alternative Media

B. H. Lipshutz, *Organizer, Presiding*

1:00 Introductory Remarks.

1:01 ORGN **306.** Fluorous chemistry meets green chemistry. **J.A. Gladysz**

1:31 ORGN **307.** Practical overview of organic synthesis in ionic liquids. **R.D. Rogers**, S.P. Kelley

2:01 ORGN **308.** Biocatalysis and biomass conversion in alternative reaction media. **R.A. Sheldon**

2:31 Intermission.

2:46 ORGN **309.** Switchable hydrophilicity solvents and switchable water: Design for applications and the environment. **P.G. Jessop**

3:16 ORGN **310.** Transitioning organic synthesis from organic solvents to water. **B.H. Lipshutz**

3:45 Intermission.

4:00 Panel Discussion.

Section D

Colorado Convention Center
Room 708

Biologically-Related Molecules and Processes

M. C. McIntosh, *Organizer*
A. T. Koppisch, *Presiding*

1:30 ORGN **311.** Discovery and synthesis of new crop protection solutions. **B.A. Lorsbach**, Z.L. Benko, T.A. Boebel, N. Breaux, K. Bryan, G. Davis, J. Epp, K.G. Meyer, J. Owen, M. Pobanz, J.M. Ruiz, M. Sullenberger, J.D. Webster, C. Yao, D. Young

1:50 ORGN **312.** Profluorogenic activatable-substrate-probes for detection and imaging of disease markers. **S.U. Hettiarachchi**, B. Prasai, R.L. McCarley

2:10 ORGN **313.** Synthesis of a novel class of proline-containing 2,5-diketopiperazine. **S. Hamedzadeh**, K. Ha, C. Hall, A. Katritzky

2:30 ORGN **314.** De novo designed peptides from a sugar amino acid are permeable to neuronal and HeLa cells. **A. Monreal**, J.P. Saludes, H. Aguilar, G. Wayman

2:50 ORGN **315.** Azasulfurylpeptide solid-phase synthesis, conformational analysis, and application as modulators of toll-like receptor inflammatory response in macrophages. S. Turcotte, K. Mellal, H. Ong, **W.D. Lubell**

3:10 ORGN **316.** Indocyanine dye cancer targeting agents. **C. Dietz**, I. Mohammad, M. Smith, Q. Zhu, A. Abuteen, F. Zhou

3:30 ORGN **317.** Synthesis and structure proof for a bioactive lipid associated with multiple sclerosis, isolated from *Porphyromons gingivalis*. **C. Dietz**, I. Mohammad, M. Smith, F. Nichols, P. Bhatt, T. Hart, I. Popiv

3:50 ORGN **318.** Dehydroshikimate dehydratase from pathogenic *Bacillus* strains: Antibiotic target and catalyst for heterologous biosynthesis of polymer precursors. K.B. Finney, I.A. Simon, A.J. Rodin, G.M. Canales, P.A. Netz, K. Hotta, C.C. Browder, D.T. Fox, **A.T. Koppisch**

4:10 ORGN **319.** Synthesis of intermediates of loline biosynthesis pathway. **M. Bhardwaj**, J. Pan, R.B. Grossman, C.L. Schardl

Section E

Colorado Convention Center
Room 702

Metal-Mediated Reactions and Syntheses

M. C. McIntosh, *Organizer*
M. G. Organ, *Presiding*

1:30 ORGN **320.** Selective carbamates synthesis by copper catalyzed oxidative coupling of formamides with salicylaldehydes. **B.D. Barve**, Y. Wu, M. El-Shazly, D. Chuang, Y. Cheng, J. Wang, F. Chang

1:50 ORGN **321.** Copper(I) ladder complexes and their use in organic synthesis. **B. Buckley**

2:10 ORGN **322.** Development of copper catalysts for photoredox reactions. **K.H. Jensen**

2:30 ORGN **323.** Synthesis of diaryl sulfones at room temperature: Cu-catalyzed cross-couplings of arylsulfonyl chlorides with arylboronic acids. **X. Lei**, F. Hu

2:50 ORGN **324.** Soft propargylic deprotonation: Designed ligand enables Au-catalyzed isomerization of alkynes to 1,3-dienes. **Z. Wang**, Y. Wang, L. Zhang

3:10 ORGN **325.** Key mechanistic features of Ni-catalyzed C-H/C-O biaryl coupling of azoles and naphthalen-2-yl pivalates. H. Xu, K. Muto, J. Yamaguchi, C. Zhao, K. Itami, **J. Musaev**

3:30 ORGN **326.** New co-catalyst strategy: Cobalt and nickel-catalyzed cross-electrophile coupling of benzyl mesylates and aryl halides. L.K. Ackerman, **L. Anka-Lufford**, M. Naodovic

3:50 ORGN **327.** Selective Negishi coupling of secondary alkylzinc reagents to aromatics: Solving the 5-membered ring heterocycle problem. **M.G. Organ**, B. Atwater, M. Pompeo, J. Farmer, D. Mitchell, M.J. Rodriguez, R. Froese

4:10 ORGN **328.** Mono arylation of primary amines and ammonia using specially designed Pd-NHC complexes. **M.G. Organ**, R. Rucker, S. Sharif, C. Lombardi, N. Chandrasoma, D. Mitchell, M.J. Rodriguez, R. Froese

TUESDAY EVENING

Section A

Colorado Convention Center
Hall C

Biologically-Related Molecules and Processes; Chemistry of Natural Resources; Metal-Mediated Reactions and Syntheses; Molecular Recognition and Self-Assembly; Peptides, Proteins, and Amino Acids

R. D. Broene, *Organizer*

8:00 - 10:00

ORGN **329.** Synthesis and antibacterial study of Schiff bases from 2,2'-bipyridyl-5,5'-dialdehyde. **M.R. Hoq**, M.R. Karim

ORGN **330.** Fluorescent triazaborolopyridinium dyes for cross metathesis labeling. **R.R. Sapkota**, M. Garcia, K.P. Dandamudi, T.M. Schaub, J.B. Arterburn

ORGN **331.** Synthesis and kinetic investigation of differently substituted chalcones. **I. Janser**, R. Gopagani

ORGN **332.** Platinum (IV) prodrugs: A simultaneous release of cisplatin and a glutathione S-transferase inhibitor. **N. Pilli**, I. Janser

‡ *Cooperative Cosponsorship*

ORGN **333.** Proposed revision of the absolute structure of mandelalide B based on computational methods. **K.M. Snyder**, R.G. Carter, K.L. McPhail, P.H. Cheong

ORGN **334.** Efficient synthesis of *l*-sirenin and its evaluation as CatSper channel agonist in human sperm. **S. Syeda**, E.J. Carlson, R. Francis, J. Hawkinson, G.I. Georg

ORGN **335.** Improved syntheses of BET inhibitor JQ1. **S. Syeda**, S.R. Jakkaraj, G.I. Georg

ORGN **336.** Allenic Pauson-Khand approach to bicyclo[5.3.0]decadienones and novel guaianolides. **S.M. Wells**, K.M. Brummond

ORGN **337.** Withdrawn.

ORGN **338.** Synthesis of modified nucleosides for the preparation of ribonucleic guanidine. **R. Van Ostrand**, A. Awad

ORGN **339.** Synthesis, cytotoxicity, and DNA-binding studies of the natural product eudistomin U. **J. Giulietti**, P. Tate, C.M. Roggero, S.P. Mulcahy

ORGN **340.** Modulating the reactivity of guaianolide analogs through modifications to the lactone ring. **P.A. Jackson**, K.M. Brummond

ORGN **341.** Progress on the design and synthesis of alternate substrates and inhibitors of indole-3-glycerol phosphate synthase. **R. Barrows**, D. Konas

ORGN **342.** Synthesis of derivatives of the natural product radicinin that inhibit the plant pathogen *Xylella fastidiosa*. **M.J. Steinhaus, J.M. Reader**, M.J. Rouffet, T.J. Aldrich, P. Rolshausen, M.C. Roper, K.N. Maloney

ORGN **343.** Development of a photochromic drug delivery system: Storage and release of nitroxyl. **K.P. Schultz**, D. Spivey, E.K. Loya, J. Kellon, L. Taylor

ORGN **344.** 9-Phenylethynyl pyronin analogs: Near infrared emitting fluorophores for imaging. **P. Sebej**, T. Pastierik, J. Medalova, P. Stacko, P. Klan

ORGN **345.** Design and synthesis of dopamine analogs for analysis in SULT1A3. **J.C. Rote**, G.E. Bailey, M. Cafiero, L.W. Peterson

ORGN **346.** Conformational analysis of aplyronine A. **D. McKenzie**, C. Nicholson

ORGN **347.** Conformational analysis of FD-895: Measuring flexibility and rigidity of different dihedral angles in the ring. **S. Jackson**, C. Nicholson

ORGN **348.** Development of inhibitors of petrobactin biosynthesis: Dehydroshikimate dehydratase as a target for anti-anthrax therapeutics. **I.A. Simon**, A. Rodin, P.A. Netz, D. Fox, A.T. Koppisch, C.C. Browder

ORGN **349.** Testing two conformational search methods of Aplyronine C. **T. Hutchinson**, C. Nicholson

ORGN **350.** Development of nonhydrolyzable inositol pyrophosphate analogs and their application in the identification of inositol pyrophosphate binding partners. **A. Hager**, D. Fiedler

ORGN **351.** Stereocontrolled total synthesis of pro-resolving lipid mediators derived from docosahexaenoic acid. **S.J. Glynn**, J.W. Winkler, C.N. Serhan, N.A. Petasis

ORGN **352.** Incorporation of 3β-modified fluorescent cholesterols into liposomal and mycobacterial membranes. A.N. Wercholuk, **J.L. Stanley**, E.S. Anderson, W.E. Allen

ORGN **353.** Recognition of bacterial lipid headgroups by fluorescent crown ether-naphthalimides. **S.R. Marshall**, J.L. Stanley, W.E. Allen

ORGN **354.** Installation of metal-binding functionality at lysine residues via azide-alkyne "click chemistry". **M.R. Baucom, D.P. Farrell, A.L. Sargent, W.E. Allen**

ORGN **355.** Improving the metal-binding efficiency of heterocyclic compounds targeting metal ion-dependent enzyme of hepatitis C virus. **A.M. Naanaa, R. Chen**, B. Smith, R. Wong, D.N. Ward

ORGN **356.** Synthetic strategies to control bacterial virulence. S.R. Dunbar, K. March, **M.A. Bertucci**

ORGN **357.** Effects of exposure of phthalates to chlorinated drinking water. M. Neyrat, H. Kim, T. Corbet, **L. Li**, K. Yeung

ORGN **358.** Direct carbon-carbon bond formation from diaryl-λ3-iodanes and (hetero) aryl borates: Redefining formal S_NAr reactivity with carbon nucleophiles. **K. Jayatissa**, D.R. Stuart

ORGN **359.** Kinetic analysis of the transesterification of soybean oil and methanol catalyzed by N-heterocyclic carbenes. H. Palencia, **D.L. Broxterman**

ORGN **360.** From glycerol to gasoline: A new approach for the utilization of a renewable source. **J. Gmeiner**, V. Tran, O. Trapp

ORGN **361.** Use of polarimetry in studying the isomerization of bittering agents in beer: The effects of temperature, pH, ultra-violet light, and solvents on the conversion of humulone to isohumulone. **S. Johnson**, M.D. Mosher

ORGN **362.** Palladium-mediated tandem cyclization-coupling reactions of β,γ-unsaturated oximes. **J. Mikesell**, M.D. Mosher

ORGN **363.** New diastereoselective synthesis of (E)-trisubsrituted alkenes containing trimethylsilylmethyl and p-methoxyphenyl moities via organoboranes. **N.G. Bhat**

ORGN **364.** Reaction of (Z)-1-bromo-1-alkenylboronate esters with allylmagnesium bromide followed by Suzuki coupling with p-methylbromobenzene. **N.G. Bhat**

ORGN **365.** Thiourea hydrogen-bond donors to promote the reductive Heck reaction. **C. Anderson**, T.M. Locascio, J.A. Tunge

ORGN **366.** Solution and X-ray crystal structures of lithium pinacolone enolate solvated by HMPA. **J. Guang**, P.G. Williard

ORGN **367.** 1,2-Boryl migration empowers regiodivergent synthesis of borylated furans. **R. Kazem Shiroodi**, O. Koleda, V. Gevorgyan

ORGN **368.** Tetrahedral oxo-Sn catalyst. **E.V. Beletskiy**, Z. Shen, M.V. Riofski, X. Hou, J. Gallagher, J.T. Miller, Y. Wu, M.C. Kung, H.H. Kung

ORGN **369.** Rhodium(I)-catalyzed enantioselective intramolecular hydroacylation of 4-allenals. **Y. Oonishi,** A. Hosotani, T. Yokoe, Y. Sato

ORGN **370.** Magnetic-metal nanocatalysts for sustainable organic transformations. **A. Rathi**, M. Gawande, R.S. Varma, R. Zboril

ORGN **371.** Recyclable soluble palladium N-heterocyclic carbene star polymer. **K. Bukhriakov**, C. Mugemana, V. Rodionov

ORGN **372.** Electronic effects of intramolecular [2+2+2] cyclizations toward β-carbolines. **M. O'Donnell**, J.G. Varelas, S. Khanal, S.P. Mulcahy

ORGN **373.** Palladium-catalyzed one-pot reactions towards β-carbolines. **J.G. Varelas**, M. O'Donnell, S. Khanal, S.P. Mulcahy

ORGN **375.** Oxygen-mediated coupling of silicon and boron compounds. E. Costello, P. Kirby, C. Lindsey, C. McNamara, **J. Hershberger**

ORGN **376.** C-H insertions in oxidative gold catalysis: Expedient synthesis of bicyclic dihydropyran-3-ones from In situ-generated α-oxo gold carbenes through the relay of vinyl cation intermediates. **Z. Zheng**, L. Zhang

ORGN **380.** Effect of ligand Ssructure in cycloisomerization reactions of enynes catalyzed by heterobimetallic Ti-Pt complexes. **R. Stokes**, M. Talley, W. Walker, D. Michaelis

ORGN **381.** Negishi-type cross-coupling arylation of selected carbamates. **B.K. Sharp**, R.E. Gawley

ORGN **382.** Enyne cycloisomerization reactions catalyzed by heterobimetallic Ti–Pt complexes. **M. Talley**, R. Stokes, W. Walker, D. Michaelis

ORGN **384.** Gold-catalyzed synthesis of cyclic ethers and lactones. **J. Dotson**, R.D. Lyski, J.R. Vyvyan

ORGN **385.** Influence of Biphenylphosphine Stabilization on Catalyst Structure and Reactivity. **W. Zhou**, A.C. Jones

ORGN **386.** Ruthenium catalyzed CN bond formation from alcohols and various nitrogen sources. **S. Hong**

ORGN **387.** Phosphine-free palladium-catalyzed direct double arylation of pyrroles with aryl iodides on water. **Y.K. Chung**, H. Bae, B. Cho

ORGN **388.** Kinetic and thermodynamic solubility of pyrazinamide cocrystals. **E.J. Johnson**, H. Abourahma

ORGN **389.** Progress in the synthesis and characterization of a resorcin[4]arene-based heterodimer. **E.G. Morado**, L.M. Tunstad

ORGN **390.** Phosphate-coordination directed assemblies: From modeling to laboratory validation. **C. Jia**, B.P. Hay, R. Custelcean

ORGN **391.** Synthesis and characterization of a covalently assembled molecular capsule for guest encapsulation. **E.S. Garcia**, L.M. Tunstad

ORGN **392.** Divalent peptide recognition mediated by an auxiliary guest. **H. Lee**, N. Petukhov, Z.T. Ball, A.R. Urbach

ORGN **393.** Covalent modification of a calixarene-capped azobenzene for increased solubility in polar media. **P.A. Bonvallet**, V.C. Iungerich, A. Steiger, T.J. Horst

ORGN **394.** Selective modification of emission intensity in a rhodamine-anthraquinone macrocycle. **M. Hoffman**, P.N. Basa, K. Mariappan, O. Schmidt, A.G. Sykes

ORGN **395.** Investigation the cleavage of Si-O bond in trimethylsilyl ether for quantitative measurement of fluoride. G. Kim, **H. Cao**

ORGN **396.** Chiral channels in molecular co-crystals: Unexpected structures that arise from the co-crystallization of 2,4,6-tris(4-X-phenyl)arenes. **R. Wiscons**, H. Lai, M. Zeller, J. Rowsell

ORGN **397.** Carboxylated polyphenylarenes: A new family of tunable porous organic crystal. **H.W. Lai**, R.A. Wiscons, M. Zeller, J.L. Rowsell

ORGN **398.** 2,2′-Linked sulfonated dicalix[4]arene as a component in supramolecular species. J.L. Fantini, **E.D. Cosco**

ORGN **399.** Depolymerization as an amplification method for analyte-triggered gelation. **D.M. Zurcher, A.J. McNeil**

ORGN **400.** Supermolecular catalysis via metal-organic supercontainers (MOSCs). Y. **Qiao**, Z. Wang

ORGN **401.** Chiral auxiliary/organocatalyst porphyrin hybrids: Modular hosts for chiral recognition. **J.G. Naizer**, M. Atyah Alqurafi, P. Battles, L. Mwangi, K. Truong, S.D. Starnes

ORGN **402.** Novel electron-rich anthracene components in modular donor-acceptor columnar liquid crystals. **A. Gray Be, J.J. Reczek**

ORGN **403.** Synthesis of a dual fluorescence probe for the G4 quadruplex. **T. Wermer**, A. Do, M.D. Heagy

ORGN **404.** Aromatic guests for cubic M8L6 metallocages. **H. Castillo**, J.D. Thoburn

ORGN **405.** Dibridgehead diphosphine dioxide cages: Syntheses and unusual structural features. **S. Kharel**, J. Bluemel, J.A. Gladysz

ORGN **406.** Impact of H-bonding and chirality on the self-assembly (and morphology) of mono and disubstituted ferrocenyl-peptide-conjugates. **B. Adhikari, C. Singh**, H. Kraatz

ORGN **407.** Modulating rhodamine B isomerization in metal-organic supercontainers. **A. Corbett**, Z. Wang, F. Dai, U. Sambasivam

ORGN **408.** Synthesis of a 1-aza-9-crown-3-substituted coumarin for fluorescence sensing of metal ions. **X. Zhang, C.J. Forsythe**, D.L. Nutbrown

ORGN **409.** Quinoline-based turn-on sensors for fluoride. **X. Zhou**, C. Stains

ORGN **410.** Synthesis of enantiomeric enriched disubstituted C_α-methyl-γ- and δ-unnatural amino acids analogs. **E.R. Vogel**, D.S. Masterson

ORGN **411.** Photodynamics of azobenzene-dipeptide (Pz-dipeptide) conjugates. **C.T. Brown, S.K. Rastogi, W.J. Brittain**

ORGN **412.** Mechanism and stereocontrol models in peptide-catalyzed acylations. **O.M. Ogba**, P.H. Cheong

ORGN **413.** Synthesis and conformational studies of hybrid α-aminoxy/cyclic β2,3-aminoxy peptides. **K. An**, S. Dai, D. Yang

ORGN **414.** Circular dichroism studies of hybrid cell penetrating – collagen peptides. **C. Hu**, K. Slowinska

ORGN **415.** New coupling and cyclization strategy for peptide synthesis via chemoselective three-fragment hydroxyproline ligation. **J.W. McDaniel**, K. Ha, C. Hall

ORGN **416.** Synthesis of four isomers of 5-hydroxypipecolic acid by intramolecular cyclization of epoxides derived from 2-amino-5-hexenoic acid. **S. Krishna Murthy**, T. Moriguchi, A. Tsuge

ORGN **417.** Synthesis of *ortho*-fluorine derivatives of phenylazobenzyloxycarbonyl(pz)-Pro-Leu for photodynamic study. **S.K. Rastogi**, C.T. Brown, W.J. Brittain

ORGN **418.** Pyrophosphorylation of peptides and proteins using phosphorimidazolides. **A.M. Marmelstein**

ORGN **419.** Characterization of a hydrophobic peptoid which interacts with beta-sheet proteins. **T.M. Lutz-Rechtin**, J.P. Turner, S.L. Servoss

ORGN **420.** Development of a highly regioselective *N*-2 arylation of indazole carboxamides: Application toward the synthesis of MK-4827 (Niraparib). **M.E. Scott**

WEDNESDAY MORNING

Section A

Colorado Convention Center

Four Seasons Ballroom 2&3

National Fresenius Award: Symposium in Honor of Abigail G. Doyle

Cosponsored by WCC

J. Aube, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 ORGN **421.** New approaches to the analysis of asymmetric catalytic processes. **M.S. Sigman**

9:25 ORGN **422.** Proton-coupled electron transfer in organic synthesis and asymmetric catalysis. **R.R. Knowles**

10:15 ORGN **423.** Functionalization of C—H bonds. **M. White**

11:05 Introduction of Awardee.

11:10 ORGN **424. Award Address** (National Fresenius Award sponsored by Phi Lambda Upsilon, the National Chemistry Honor Society). New Csp3-electrophiles for Ni-catalyzed cross coupling. **A.G. Doyle**

Section B

Colorado Convention Center

Four Seasons Ballroom 1

Total Synthesis of Complex Molecules

M. C. McIntosh, K. Walker, *Organizers*

N. Choony, *Presiding*

8:20 ORGN **425.** Expedient approach to bicyclic nucleosides: Precursors to nucleic acid modifications for antisense technology. **N.K. Narayanan**, A.M. Dmytrejchuk, B.L. Merner

8:40 ORGN **426.** Organocatalytic and protecting-group-free synthesis of (+)-artemone. **S.P. Wetzler, B.C. Fielder, D.A. Vosburg**

9:00 ORGN **427.** Use of triphenylchloromethane (trityl chloride) as a steric buttress to enhance Diels Alder cycloaddition reactions. **N. Choony**

9:20 ORGN **428.** Synthesis of bis(indole) alkaloids from *Arundo donax*. **A. Ferreira**, C. Beaudry

9:40 ORGN **429.** Syntheses of acyclic polyhalogenated *Plocamium* monoterpenes and evaluation of activity for solid tumors. **C.V. Vogel**, H. Pietraszkiewicz, O.M. Sabry, W.H. Gerwick, F.A. Valeriote, C.D. Vanderwal

10:00 ORGN **430.** Case for a spontaneous, Diels-Alderase-free dimerization as the key step in the biosynthesis of (±)–paracaseolide A. **T. Wang**, T.R. Hoye

10:20 ORGN **431.** Total synthesis of leiodermatolide. **S. Williams**, K. Ng, I. Paterson

10:40 ORGN **432.** Withdrawn.

11:00 ORGN **433.** Total synthesis of aflastatin A. D.A. Evans, **J.J. Beiger**, E. Kattnig, P.H. Fuller, J.M. Young, J.D. Burch, F. Glorius, J. Zhang, W.C. Trenkle, D.A. Thaisrivongs

11:20 ORGN **434.** Efficient and concise syntheses of spiroisoxazolines: Progress toward first total synthesis of 11-deoxyfistularin-3. **P. Das, A.T. Hamme II**

11:40 ORGN **435.** Phytochemical study of the genus *Piper*: Synthesis and photoreactivity of chromene natural products. **T.T. Nguyen, C.S. Jeffrey**

12:00 ORGN **436.** Total synthesis of 6-deoxypladienolide D and assessment of splicing inhibitory activity in a mutant SF3B1 cancer cell line. K. Arai, S. Buonamici, B. Chan, L. Corson, A. Endo, B. Gerard, M. Hao, C. Karr, K. Kira, L. Lee, X. Liu, J.T. Lowe, T. Luo, L.A. Marcaurelle, Y. Mizui, M. Nevalainen, M.W. O'Shea, E. Park, S. Perino, S. Prajapati, M. Shan, P.G. Smith, P. Tivitmahaisoon, J.Y. Wang, M. Warmuth, K. Wu, L. Yu, H. Zhang, G. Zheng, **G.F. Keaney**

Section C

Colorado Convention Center
Rooms 704/706

New Reactions and Methodology

M. C. McIntosh, *Organizer*
B. L. Ashfeld, *Presiding*

8:00 ORGN **437.** Synthesis of 5, 6, 7, and 8-membered oxacycles by silver and gold catalysis. **R. Tata, M. Harmata**

8:20 ORGN **438.** From carbon to cancer: The impact of reaction development on natural products and designed materials synthesis. **B.L. Ashfeld**, A. Chavannavar, E. White

8:40 ORGN **439.** Transition metal catalyzed reactions for the functionalization of cubane and triptycene scaffolds. **M.O. Senge**

9:00 ORGN **440.** Enantioselective N-heterocyclic carbene-catalyzed β-hydroxylation of enals using nitroarenes: An atom transfer reaction that proceeds via single electron transfer. **N.A. White**, T. Rovis

9:20 ORGN **441.** Rh(III)-catalyzed synthesis of 2,3-dihydropyridines initiated by C-H activation. **F. Romanov Michailidis**, T. Rovis

9:40 ORGN **442.** Highly active multidentate molybdenum (VI) catalysts for alkyne metathesis. **H. Yang**, C. Zhu, W. Zhang

10:00 ORGN **443.** Chemo-enzymatic synthesis of key intermediates (*S*)-γ-hydroxymethyl-α,β-butenolide and (*S*)-γ-hydroxymethyl-γ-butyrolactone *via* lipase-mediated Baeyer-Villiger oxidation of levoglucosenone. A.L. Flourat, A.A. Peru, A.R. Teixeira, F. Brunissen, **F. Allais**

10:20 ORGN **444.** Synthesis of functionalized benzenoid macrocycles: Templates for carbon nanotube synthesis. **B.L. Merner**, N.K. Mitra, R. Meudom, S. Iqbal

10:40 ORGN **445.** Pentadehydro-Diels-Alder (PDDA) reaction.Part 1: Cycloisomerization of triynes to a,3-dehydrotoluene derivatives and their trapping reactions. **T. Wang,** R. Naredla, **T.R. Hoye**

11:00 ORGN **446.** Automated simultaneous catalyst screening and cross-coupling reaction optimization in a continuous-flow microreactor system. **B.J. Reizman**, K.F. Jensen

11:20 ORGN **447.** Flow chemistry for sustainable chemical manufacturing. **M.G. Organ**, D. Mallik, M. Tilley, K. Somerville, G. Li, A. Khadra, M.A. McGuire, K. Nalivela, D. Daly

Section D

Colorado Convention Center
Room 708

Heterocycles and Aromatics

M. C. McIntosh, *Organizer*
L. Silverberg, *Presiding*

8:00 ORGN **448.** Pd-catalyzed iterative *bis*-amination of functionalized dihalo-1,2,4-triazinyl substituted heterocycles. **S. Tai**, S.V. Marchi, E.J. Dover, J.D. Carrick

8:20 ORGN **449.** Development of an expedient process for the multikilogram synthesis of CHK1 inhibitor GDC-0425. **A. Stumpf**

8:40 ORGN **450.** Benzo[*a*]imidazo[2,1,5-*cd*] indolizines as tunable heterocyclic fluorophores: Synthesis and applications. **E. Levesque**, L. Constantineau-Forget, G. Pelletier, W.S. Bechara, A.B. Charette

9:20 ORGN **451.** Accessing diverse polyheterocycle-fused diketopiperazines via cycloadditions of photogenerated azaxyxylenes. **N.N. Bhuvan Kumar**, D.M. Kuznetsov, A.G. Kutateladze*

9:40 ORGN **452.** Prospective energetic materials derived from 4, 4'-bi(5-nitro-1, 2, 3-2*H*-triazole). **C. He**, J.M. Shreeve

10:00 ORGN **453.** Synthesis, photochemical, and electrochemical characterization of N,N'-dimethyl-5,10-diaza[5]helicene bistetrafluoroborate and other helical viologens. **X. Zhang**, E.L. Clennan

10:20 ORGN **454.** Highly efficient synthesis of HIV NNRTI doravirine. **D.R. Gauthier, Jr**

10:40 ORGN **455.** Synthesis of organo nitrogen compounds and heterocycles via catalytic allylic C-H amination. **S. Murru**, R. Srivastava

11:00 ORGN **456.** Studies on cyclic six- and seven-membered 2, 3-diaryl-1, 3-thiaza-4-ones. **L.J. Silverberg**, H.P. Yennawar, J. Tierney, C.N. Pacheco, K.C. Cannon, A.F. Lagalante, J.T. Bachert, L.M. Baker, J. Bayliff, R.V. Bendinsky, A.S. Cali, L. Chen, A.D. Cooper, D.J. Coyle, J.R. Dahl, M.J. Minehan, C.R. Mroz, H. Singh, Y. Xie

11:20 ORGN **457.** Thiazole chemistry toward a second generation EML4-ALK inhibitor. **G. Smith**

11:40 ORGN **458.** Withdrawn.

Section E

Colorado Convention Center
Room 702

Metal-Mediated Reactions and Syntheses

M. C. McIntosh, *Organizer*
S. P. Mulcahy, *Presiding*

8:30 ORGN **459.** Stereospecific nickel-catalyzed cross-coupling of benzylic ethers with Grignard reagents. **A. Johnson**, I.M. Yonova, L.W. Erickson, M.A. Greene, C.A. Osborne, E.R. Jarvo

8:50 ORGN **460.** Efficient catalytic system for Ru-catalyzed C-H arylation: A practical synthesis of a pharmaceutical. **M. Seki**

9:10 ORGN **461.** Terminal olefins to chromans, isochromans, and pyrans via allylic C–H oxidation. **S. Ammann**, G. Rice, M.C. White

9:30 ORGN **462.** Intramolecular metalloaminations of *N,N*-dimethylhydrazinoalkenes. **A. Smith**, B. Sunsdahl, T. Livinghouse

9:50 ORGN **463.** Mechanistic study of gold(I)-catalyzed alkene addition reaction. **Y. Zhu**, E.M. Petryna, A.C. Jones

10:10 ORGN **464.** Efficient palladium-catalyzed reactions toward complex nitrogen-containing heterocycles. **S.P. Mulcahy**

10:30 ORGN **465.** Catalyst-transfer direct arylation: Selectivity and potential initiators. **H. Johnson**, T. Schwochert, J. Enders, A. Olivares, T. Hougen, K. Woods, L. Lawrence, J.F. Tannaci

10:50 ORGN **466.** Efficient synthesis of polysubstituted cyclopentadienyl ligands for Rh(III) catalysis. **N. Semakul**, T. Rovis

11:10 ORGN **467.** BINAP-based metal-organic framework catalysts for asymmetric reactions. **T. Sawano**, J. Falkowski, T. Zhang, G. Tsun, Y. Chen, N.C. Thacker, A.R. McIsaac, J.V. Lockard, W. Lin

WEDNESDAY AFTERNOON

Section C

Colorado Convention Center
Rooms 704/706

Peptides, Proteins, and Amino Acids

M. C. McIntosh, *Organizer*
J. Haseltine, *Presiding*

1:00 ORGN **472.** Remodeling of bacterial cell surfaces using unnatural D-amino acids. **M.M. Pires**

1:20 ORGN **473.** N-terminal modification for traceless expressed protein ligations. **E.J. Petersson**

1:40 ORGN **474.** Lanthipeptides with diverse ring topologies are generated by ProcM under kinetic control. **S. Mukherjee**, Y. Yu, W.A. van der Donk

2:00 ORGN **475.** Synthesis and responsive self-assembly of boronic acid-functionalized peptides. **B.H. Jones**, A. Martinez, J. Wheeler, D.R. Wheeler, E. Spoerke

2:20 ORGN **476.** Orally bioavailable cyclic peptides. **D.S. Nielsen**, H.N. Hoang, R. Lohman, D.P. Fairlie

2:40 ORGN **477.** Bioinspired strategy for the ribosomal synthesis of thioether-bridged macrocyclic peptides in bacteria. **N. Bionda**, R. Fasan

3:00 ORGN **478.** Comparing methods for the solution-state synthesis of dipeptide and tripeptide esters. O. Sugahara, I.L. Beltran, J.T. Bauer, **J.N. Haseltine**

3:20 ORGN **479.** Synthesis and applications of peptides with C-terminal esters to studies of protein prenylation. **M.D. Distefano**, V. Diaz-Rodriguez, J.S. Vervacke

3:40 ORGN **480.** Development of 4-hydroxyproline ligation for coupling of peptide fragments. **K. Ha**

4:00 ORGN **481.** Constrained *N*-amino peptide derivatives for conformational scanning applications. **J.R. Del Valle**, C. Kang, S. Ranatunga

Section D

Colorado Convention Center
Room 708

Heterocycles and Aromatics

M. C. McIntosh, *Organizer*
C. Santini, *Presiding*

1:00 ORGN **482.** Porphyrin synthesis by grinding. **T.D. Hamilton**, D. Cordero, V.S. Hoelscher, T. Sabol, Q. Su

1:20 ORGN **483.** Synthesis and reactions of 2-oxo-*p*-*tert*-butyltetramethoxycalix[4] arene. **J.L. Fantini**, I.M. Delahunty, K.P. Klatt

1:40 ORGN **484.** Dearomative (3+2) cycloadditions of aza-oxyallyl cation intermediates and indoles. **A. Acharya**, C.S. Jeffrey

2:20 ORGN **485.** Trifluoromethyl heterocyclic compounds: Synthesis and characterization. **K.P. Castro**, A.M. Pluntze, I.V. Kuvychko, E. Bukovsky, T. Clikeman, Y. Chen, S.H. Strauss, O.V. Boltalina

2:40 ORGN **486.** Modular approach to crowded benzoquinolines. **A. Mazaheripour**, D.E. Laidlaw, R. Lopez, D.J. Dibble, M. Umerani, Y. Park, A.A. Gorodetsky

3:00 ORGN **487.** Gram scale total synthesis of veranamine. **J. Magolan**, H.C. Araujo, S.D. Holmbo, R. Gautam

3:20 ORGN **488.** Gold-catalyzed cyclizations of cis-enediynes: Insights into the nature of gold–aryne interactions. **Y. Wang**, A. Yepremyan, S. Ghorai, R. Todd, D.H. Aue, L. Zhang

3:40 ORGN **489.** Analysis of PAH(CF_3)*n*:PAH charge transfer complexes. **E.V. Bukovsky**, K.P. Castro, L. San, T. Clikeman, I.V. Kuvychko, O. Boltalina, S.H. Strauss, Y. Chen

4:00 ORGN **490.** New approaches in *N*-heterocycle construction and applications toward industrially relevant materials. **D. Pena**, A. Chavannavar, B.L. Ashfeld

4:20 ORGN **491.** Oxidative 1,2 and 1,4-diamination of olefins using simple urea derivatives. **D. Anumandla**, C.S. Jeffrey

4:40 ORGN **492.** Transition-metal mediated cycloaddition reactions of chiral diaziridines for the diastereoselective synthesis of N-containing heterocycles. **G. Moura-Letts**

Section E

Colorado Convention Center
Room 702

Metal-Mediated Reactions and Syntheses

M. C. McIntosh, *Organizer*
B. Michel, *Presiding*

1:30 ORGN **493.** Palladium-catalyzed intramolecular oxidative coupling of nitrogen heteroaromatics with unactivated arenes in the synthesis of fused N-heterocycles. **J. Laha**, N. Dayal, K. Jethava

1:50 ORGN **494.** Stereoselective synthesis of allenyl alcohols using an organo-manganese η2-auxiliary: A new entry to furofuranone natural products. **A. Roy**, B. Bhat

2:10 ORGN **495.** Mechanistic studies of isocyanide promoted Buchner insertion reactions with Ruthenium-based metathesis catalysts. **J.R. Griffiths**, E.J. Hofman, J.B. Keister, S.T. Diver

2:30 ORGN **496.** Gold-catalyzed 1,3-transposition of ynones. **R. Kazem Shiroodi**, M. Soltani, V. Gevorgyan

2:50 ORGN **497.** Withdrawn.

3:10 ORGN **498.** Novel catalytic reactivities of PN3-pincer complexes. **K. Huang**

3:30 ORGN **499.** Rhodium-catalyst controlled carbenoid and vinylogous reactions of vinyldiazoacetates and silyl ketene acetals. **S. Negretti**, H.M. Davies

3:50 ORGN **500.** Overcome inherent regioselectivity in oxidative gold catalysis: A desulfonylation approach. **H. Chen**, L. Zhang

4:10 ORGN **501.** Powerful fluoroalkoxy molybdenum(V) reagent for the selective oxidative arene coupling reaction. **M. Schubert**, J. Leppin, K.M. Wehming, D. Schollmeyer, D. Heinze, D.R. Waldvogel

WEDNESDAY EVENING

Section A

Colorado Convention Center
Four Seasons Ballroom

Heterocycles and Aromatics; New Reactions and Methodology

R. D. Broene, *Organizer*

7:00 - 9:00

ORGN **374.** Air-stable palladium precatalyst for forylation of arylhalides with HBpin and experimental evidences on cationic metathesis mechanism. **X. Pu**, T. Colacot

ORGN **377.** Iridium precatalysts for the C–H borylation of heterocycles. **P. Gildner**, C. Seechurn, S. Vilvanathan, T. Colacot

ORGN **378.** In depth understanding of palladium acetate. **W.A. Carole**, A. DeAngelis, T. Colacot

ORGN **379.** Highly active pi-allyl Pd-precatalysts for challenging cross-coupling reactions. **A. DeAngelis**, R. Chow, C. Seechurn, T. Colacot

ORGN **383.** Heck and Sonogashira coupling of aryl and heteroaryl chlorides using L2Pd(0) and L2Pd(II) catalysts: Understanding the structure–activity relationships. **H. Li**, X. Pu, T. Colacot

‡ *Cooperative Cosponsorship*

ORGN **502.** High-load, hybrid ROMP reagents/scavengers/ligands immobilized on silica and Co/C magnetic nanoparticles for their application in sequestration and parallel synthesis. **S. Faisal**, P.K. Maity, A. Brandhofer, P.C. Kearney, D.S. Stoianova, O. Reiser, R.N. Grass, P.R. Hanson

ORGN **503.** Synthesis of Tröger's base-derived ligands. **C.S. Hampton**, M. Harmata

ORGN **504.** Synthesis of dibenz[c,h]acridines as potential G-quadruplex ligands. **K. Eickelman**, **K. Jara**, M.D. Mosher

ORGN **505.** 9-Arylacridine atropisomers. **B. Redlinger**, M.D. Mosher

ORGN **506.** Synthesis of 3,4,5-trisubstituted isoxazolines. **T.N. Leighton, K. Henson**, M.D. Mosher

ORGN **507.** QSAR analysis of O-substituted 9-hydroxylaminoacridines. **A. Carlson**, A. Lavianetskaya, M.D. Mosher

ORGN **508.** Photocyclodehydrofluorination. **K.E. Ivey**, Z. Li, R.J. Twieg

ORGN **509.** Benzimidazol-2-one scaffolds derived from unique domino processes centered upon elegant benzodiazepine ring rearrangements. **G. Martinez-Ariza**, Z. Xu, A.P. Cappelli, C. Hulme

ORGN **510.** Inverse-demand Diels-Alder of bis-(4-pyridyl)-1,2,4,5 tetrazine with alkenes and carbonyl under catalytic and non-catalytic conditions. **M.A. Max**, J. Wilson

ORGN **511.** Cross coupling of iodo-substituted aurones. **Z.E. Taylor**, S.T. Handy

ORGN **512.** Direct C-H functionalization of arenes in reactions with nitroalkanes and nitroalkenes in polyphosphoric acids. A. Aksenov, A.N. Smirnov, **N.A. Aksenov**, I.V. Aksenova, **M.A. Rubin**

ORGN **513.** Heterocycles: An enhancement in the ferrocenyl derivatives pharmacophores. **J.C. Aponte-Santini**, I. Montes Gonzalez, S. Abdul-Hadi-Martínez, F.J. Correa-Delgado, D.J. Sanabria Rios, M.D. García Maldonado, A.R. Guadalupe Quiñones, F.T. Halaweish, **A.E. Serrano Brizuela, E.E. Colón Lorenzo**

ORGN **514.** Approaches to the synthesis of C1-substituted carbapenems. **T.Q. Nguyen**, W. Chai, J. Gu, K. Cook, E. Kim, S.E. Goetz, M. Chepuru, M. Cox, P. Nguyen, H. Raja, P. Magistrado, F. Michael, P. Oelschlaeger, J.W. Janc, J.D. Buynak

ORGN **515.** Copper(I) catalyzed reaction of 1-bromo-2-iodobenzene with 1,2-cyclohexanedione as a potential route to 2,3-dihydrodibenzo[*b,d*]furan-4(1*H*)-one. D.A. Hunt, **J. Bocanegra**

ORGN **516.** Synthesis, photochemical and electrochemical characterization of a series of new phenanthrenyl viologens. **T. Bakupog, E.L. Clennan**

ORGN **517.** Air stable polycyclic aromatic hydrocarbons with strong electron accepting properties. **L.K. San**, E.V. Bukovsky, T.T. Clikeman, S. Deng, X. Wang, Y. Chen, O.V. Boltalina, S.H. Strauss

ORGN **518.** Alternative routes to phenanthroline-based diones. K.A. Pacheco, **D.J. Covelli,** C.M. Bresch

ORGN **519.** Optimization of the synthesis of 2,4,6-trimethylphenyl-1,10-phenanthroline and its derivatives. K.A. Pacheco, **D.B. Burgess**

ORGN **520.** Synthesis of neo-confused porphyrins. **A.S. Almejbel**, T.D. Lash

ORGN **521.** Efficient methods of synthesizing benzyl azetidines. **C. Ochoa**, L.M. Bradley

ORGN **522.** Synthesis of pyrazol-1-yl-benzenesulfonamides. **M. Belcher, B. Torok, R. Dembinski**

ORGN **523.** Mono- and bis- phenylpropargyl imidazolidinium cations: Structure and reduction behavior. **G. Soper**, B.M. Barry, W.L. McClennan, K. Robertson, J. Hurmalainen, T. Roemmele, H. Tuononen, R.T. Boere, J.D. Masuda, J.A. Clyburne

ORGN **524.** Perfluoroalkyl and cyano derivatives of perylene diimides as novel electron acceptors for advanced electronics. **T. Clikeman, E.V. Bukovsky**, G. Rumbles, O. Boltalina, S.H. Strauss

ORGN **525.** Synthesis of carbaporphyrinoid systems using a carbatripyrrin methodology. **L.M. Stateman**, T.D. Lash

ORGN **526.** Photoinduced oxidative cyclizations of o-arylalkynyloximes. **M. Ko**, W. Kim, P. De Lijser

ORGN **527.** Synthesis and characterization of ferrocenyl chalcones salts derivatives as potential antibacterial agents. **S.M. Delgado-Rivera**, R.E. Colón-Morillo, I.D. Montes-González, M.D. García Maldonado, A.R. Guadalupe Quiñones, D.J. Sanabria Rios, Y. Rivera-Tores, R. Gutiérrez

ORGN **528.** Methods for *N*-alkylation of benzylidene oxindoles. **A.M. Lock**, K.W. Cox, K.J. Knisley, D.M. Ketcha

ORGN **529.** New phenothiazinium derivatives for potential use in photodynamic therapy (PDT) and dye-sensitized solar cells (DSSC). **I. Kady**, N. Mehraban, S. Fanah

ORGN **530.** *C*-Arylation of triazoles: Synthesis of novel vinyl triazole-fused sultams. **A.J. Cassity**, J. Jun, N. Asad, N. Windmon, A. Diepenbrock, P.R. Hanson

ORGN **531.** Efforts toward decorated azepine derivatives through a photochemical formal [5+2] cycloaddition. **S.M. Thullen**, D.M. Rubush, T. Rovis

ORGN **532.** Synthesis of 1*H*-1,2,3-triazole esters and acids. **C.R. Butler**, A. Arroyave, K. McGee, A.M. Schoffstall

ORGN **533.** Ultrasound-assisted green synthesis of diversely substituted oxindoles. **D. Bandyopadhyay**, O.M. Rodriguez, I.M. Chapa, A. Zavala, B.K. Banik

ORGN **534.** Organocatalyzed green synthesis of *bis*-benzopyrazines: An entry to novel heteroaromatics. **D. Bandyopadhyay**, J.A. Perez, H.R. Cardenas, B.K. Banik

ORGN **535.** Proxy-PET building blocks as a design element for library synthesis. **L.J. Mallin**, H. de Kraker, S.S. Huthmacher, D.M. Ketcha

ORGN **536.** Efficient synthesis of 1,3,4-oxadiazoles promoted by NH_4Cl. **K.K. Gnanasekaran**, B. Nammalwar, M. Murie, R.A. Bunce

ORGN **537.** Ring size and substitution effects in the tandem reduction-lactamization of *ortho*-substituted nitroarenes. **R.A. Bunce**, B. Nammalwar, J.T. Hiett

ORGN **538.** Efficient synthesis of substituted 3-oxoindoline-1-carbonitriles using mesoporous silica MCM-41. B. Nammalwar, **N.P. Muddala**, M. Murie, R.A. Bunce

ORGN **539.** Synthetic studies on guaipyridine alkaloids: Intramolecular Heck approach. **B. Woldehaimanot**, P.M. Shelton, J.R. Vyvyan

ORGN **540.** Mechanistic studies on the Pechmann condensation reaction with fluorine-substituted reactants. **M.A. Vanalstine-Parris**, J. DeGrote, S. Tyndall, K. Wong

ORGN **541.** Withdrawn.

ORGN **542.** One-pot synthesis of indole-4,9-diones from naphthoquinone. **J.D. Guerra,** Q.H. Luu, **C.M. Castaneda, M.A. Martinez**, S. Mito

ORGN **543.** Efficient preparation of pyridinyl-1,2,4-triazines via telescoped condensation with diversely functionalized 1,2-dicarbonyls. **S.V. Marchi**, J.D. Carrick

ORGN **544.** Study on the palladium-catalyzed Friedel-Crafts-type allylic arylations and aryl etherifications of phenols. **C.A. Discolo**, A.G. Graves, D.R. Deardorff

ORGN **545.** Progress on the preparation of 3,5-disubstituted 2-isoxazolines. **N. Schiltz, E. Van Meter**, M.D. Mosher

ORGN **546.** Hypoiodite mediated stoichometric or catalytic cyclopropanation of alkenes with malononitrile. **A. Yoshimura**, J. Fuchs, T.N. Jones, V.V. Zhdankin

ORGN **547.** Development of an alternative energy synthetic pathway to ibuprofen through the use of solar irradiation as the sole heat source. **B. Agee**, G. Mullins, D.J. Swartling

ORGN **548.** Visible-light mediated synthesis of constrained cyclic-peptides from phenacyl protected cysteine residues. **R.C. McAtee**, T.M. Monos, C.R. Stephenson

ORGN **549.** Cycloaddition reactions of *N*-vinyl nitrones with ketenes and ketenimines. **K. Chando**, R.E. Michael, T. Sammakia

ORGN **550.** Synthesis and base-mediated rearrangement of cis-1-hydroxy-2-(2-oxoethanyl)cyclopropanes: Approach to hydroxycyclopropane peptidomimetics. **C.K. Zercher**, I. Taschner, M. Mower, P. Moran, Y.M. Bhogadhi, R. Chhetri, K. Bala

ORGN **551.** Stereoselective samarium diiodide promoted carbon carbon bond forming reactions. **C. Aretz**, H. Escobedo, B.J. Cowen

ORGN **552.** Diversity oriented wynthesis of quinoline scaffolds employing acetal substrates in the Doebner–Miller reaction. **G. Rahman**, S.D. Pegan, B.J. Cowen

ORGN **553.** Sulfonic acids as catalysts for carbon carbon bond forming reactions. B.J. Cowen, **J. Miao**

ORGN **554.** Iodination of potassium organotrifluoroborates and tributyl(aryl) stannanes using iron(III) chloride/sodium iodide. D.W. Blevins, **G.W. Kabalka**, M. Yao, L. Yong

ORGN **555.** Catalytic functionalization of unactivated sp3 C–H bonds through intramolecular oxygen nucleophiles affording cyclic ethers. **S.J. Thompson**, G. Dong

ORGN **556.** Ligand- and proton-source effects in samarium(II)-mediated elimination/isomerization reactions of alllylic benzoates. **A.M. Wright**, G.W. O'Neil

ORGN **557.** Ring-closing metathesis reactions of acyloxysulfones: Synthesis of γ-alkylidene butenolides. **I. Phan**, G. Gilbert, G.W. O'Neil

ORGN **558.** Regiocontrolled palladium-catalyzed domino synthesis of *N*-sulfonyl dihydrophenanthridines and dihydrodibenzo[*c,e*]azepines. **N. Dayal**, R. Jain, K. Patel, J.K. Laha

ORGN **559.** New quinazolin-2-yl-guanidines for medicinal chemistry approaches to neuropsychiatric disorders. **S. Ibrahim**, G. Obenauf, J.K. Britt, A. Pieper, G.K. Friestad

ORGN **560.** Photogenerated diketopiperazine-spiro-oxiranes as versatile synthons for accessing diverse polyheterocyclic scaffolds. **D.M. Kuznetsov**, N.N. Bhuvan Kumar, A.G. Kutateladze*

ORGN **561.** Practical, scalable synthesis of carbohydrate based oxepines. R **Vannam**, M.W. Peczuh

ORGN **562.** Reaction of 1,2-cyclohexanedione with diols. An unexpected aromatization reaction. **A.E. Solinski, D.A. Hunt**

ORGN **563.** Mechanistic studies into the reaction of aldehydes with *N*-acylphthalimides. **R.N. Enright**, L.T. Henningsen, P.H. Willoughby

ORGN **564.** Investigation of oxidopyrylium [5+2] cycloaddition conjugate-addition cascade sequences. **C. Law**, C.R. Zwick, J. Simanis, E.L. Woodall, J.R. Goodell, T.A. Mitchell

ORGN **565.** Lithium-promoted reaction of aldehydes with *N*-acylphthalimides. **L.T. Henningsen**, R.J. Enright, P.H. Willoughby

ORGN **566.** Intramolecular cycloadditions of photogenerated Azaxylylanes as key steps in the diversity-oriented synthesis of novel N,O,S-polyheterocycles. **W. Umstead**, O. Mukhina, A.G. Kutateladze

ORGN **567.** Development of palladium-catalyzed directed alkene difunctionalization reactions. **S.L. Moss, L. Xu, B.W. Michel**

ORGN **568.** Formation and reactions of benzyl azetidine compounds. **S.C. Allen**, L.M. Bradley

ORGN **569.** Toward the development of greener synthetic methods involving modified Knoevenagel–Doebner reaction. **K. Banerjee, M. Collins**

ORGN **570.** Mechanistic studies on selective monohydrolysis of symmetric diesters with the use of dynamic light scattering. **S. Niwayama,** Y. Hiraga

ORGN **571.** Regio- and stereoselective additions to enynes containing an organo-manganese auxiliary leading to highly substituted allenyl aldehyde products. **E. Nagy**, A. Roy, S.D. Lepore

ORGN **572.** Palladium-catalyzed microwave heated cross-coupling of organotrifluoroborates and metal fluoride. **R.L. Welch**, M. Al-Masum

ORGN **573.** Pd-catalyzed cross-coupling reaction of styryltrifluoroborates with activated alkynes and alkanes. **W. Shaban**, M. Al-Masum

ORGN **574.** Cu-catalyzed one-pot electrophilic amination with heteroarylaluminum reagents. **H. Yoon**, Y. Lee

ORGN **575.** Synthesis of fluorinated homoallylic compounds via ring-opening nucleophilic fluorination of methylene cyclopropanes (MCP) . **A. Boateng**, O. Okoromoba, G.B. Hammond

ORGN **576.** Exploring the reactivity of hexadehydro-Diels–Alder (HDDA)-generated benzynes with acids. **M.K. Haj**, P. Willoughby, T.R. Hoye

ORGN **577.** Synthesis of 2F-HAT discotic liquid crystal via PCDHF approach. **Z. Li**, R.J. Twieg

ORGN **578.** Green and scalable synthesis of γ-hydroxybutenolides via aerobic oxidation of 2-silyloxyfurans. **M. Jean**, N. Bruneau-Latour, J. Boukouvalas

ORGN **579.** Photochemistry of trifluoromethylated 2-nitrobenzyl alcohols. G. Prakash, **K. Bellingund**, T. Mathew, G.A. Olah

ORGN **580.** Development and deployment of a new methoxyvinyl cation equivalent. C.D. McCune, **M.L. Beio**, J.A. Friest, S. Ginotra, D.B. Berkowitz

ORGN **581.** Amine conjugate addition to α,β-unsaturated olefins promoted by NHC-Cu catalyst. **S. Kim**, Y. Lee

ORGN **582.** Allyl-substituted nitrophenols in the Passerini-Smiles reaction. **C. Summers**, K. Hausman, S.B. Luesse

ORGN **583.** Peroxide electrophiles for C-O bond formation. **A. Horn**

ORGN **584.** Phosphorus-based tether methods in the synthesis of complex polyols. **J.L. Markley**, P.R. Hanson

ORGN **585.** Amine and isocyanide variation in the Ugi-Smiles Diels-Alder tandem process. **K. Mason**, M. Meyers, B. Richey, S.B. Luesse

ORGN **586.** Examining the use of conjugated, heterocyclic aldehydes in the Ugi-Smiles reaction. **M. Meyers**, K. Mason, B. Richey, S.B. Luesse

ORGN **587.** N-hetereocyclic carbene catalyzed synthesis of 2-aryl-Indoles. **M.T. Hovey**, C. Check, A.F. Sipher, K. Scheidt

ORGN **588.** Synthesis of novel β-keto-sultams: Tetramic acid analogs and their derivatives. **J. Jun**, M. Hur, P.R. Hanson, T. Atkinson

ORGN **589.** Synthesis of pyrazolopyranopyrimidines under controlled microwave exposure: An eco-friendly approach. **D. Bandyopadhyay**, C.L. Gibbs

ORGN **590.** One-pot four-component synthesis of pyranopyrazoles under microwave irradiation: A green procedure. **D. Bandyopadhyay**, M. Pena-Agudelo

ORGN **591.** Rh(III)-catalyzed cyclopropanation initiated by C-H activation: Using ligand design to direct diastereoselectivity. **H. Rubin**, T. Piou, T. Rovis

ORGN **592.** One pot tandem Diels-Alder/Nazarov cyclization. **R.A. Carmichael**, W. Chalifoux

ORGN **593.** Neat boron trifluoride etherates as reagents for efficient esterification of carboxylic acids and derivatives. **C.J. Cueto**, R.R. Hark

ORGN **594.** Mn-mediated radical-polar crossover annulation employing a leaving group in the N-acylhydrazone radical acceptor. **K.A. Slater**, G.K. Friestad

ORGN **595.** Exploration of imine-based Ugi-Smiles reaction. **R. Poormotamed**

ORGN **596.** Rapid, protecting-group free route to acyl pyrrolidines using imines as substrates in the aza-Cope rearrangement—Mannich cyclization. **H.A. Lindsay**, A. Oudeif, J.M. Reder, B. Yambrosic

ORGN **597.** Synthesis of 2-indolinones through microwave-assisted intramolecular transamidation derived from a multicomponent coupling cascade process. **A. Maddirala**, P.R. Andreana

ORGN **598.** Ring opening chemistry of epoxides with new carbon nucleophiles for the synthesis of novel γ-lactones and γ-lactams. **A. Kumar**

ORGN **599.** Toward the miniaturization of chemical library synthesis to the sub-micromole scale using functionalized high loading magnetic nanoparticles. **P.C. Kearney**, P.K. Maity, S. Faisal, P.R. Hanson

ORGN **600.** Ligand-controlled, tunable silver-catalyzed C–H amination. **J.M. Alderson**, A.M. Phelps, R. Scamp, N.S. Dolan, J.M. Schomaker

ORGN **601.** Asymmetric β hydroxylation and amidation of enals via N heterocyclic carbene catalysis. **C. Hosier**, N.A. White, T. Rovis

ORGN **602.** Solid phase catalysts for the synthesis of α-aryl carboxylic acids. **W.E. Brenzovich**, A. Denton, R. Kohinke, B.R. Craig, D. Moore

ORGN **603.** Synthesis of N-heterocycles via transition metal-catalyzed C-H activation. **K.E. Ruhl**, T. Hyster, T. Rovis

ORGN **604.** New catalytic methods for N-heterocycle synthesis by late transition metal-mediated C-H bond activation. **P. Kilaru**, P. Zhao

ORGN **605.** Substituted 5,6,11,12-tetradehydrodibenzo[a,e] cyclooctenes: Syntheses, properties, and DFT studies of substituted Sondheimer diynes. **F. Xu**, A. Orita, J. Otera

PHYS

Division of Physical Chemistry

E.L. Sibert, *Program Chair*

OTHER SYMPOSIA OF INTEREST:

ACS Award for Computers in Chemical and Pharmaceutical Research honoring David Case *(see COMP, Mon, Tue)*

Electronic Structure Methods for Highly Polarizable Systems *(see COMP, Sun, Mon)*

Computational Design, Discovery and Optimization of Organic Semiconductor Materials *(see COMP, Sun, Mon)*

Quantum Chemistry *(see COMP, Sun, Mon, Tue, Wed)*

Molecular Mechanics: Force Field Development *(see COMP, Mon)*

Computational Chemistry In The Undergraduate Curriculum: What Is Working And How Do We Assess It? *(see CHED, Wed)*

SUNDAY MORNING

Section A

Colorado Convention Center
Room 501

Atmospheric Chemistry: Transformations of Matter in the Troposphere

New Particle Formation and Growth

M. Freedman, *Organizer*
D. Cziczo, *Organizer, Presiding*
J. Pierce, *Presiding*

8:00 Introductory Remarks.

8:05 PHYS **1.** Aerosol nucleation and growth in the CLOUD experiment at CERN. **J. Curtius**

8:45 PHYS **2.** Contribution of human related sources to indoor volatile organic compounds. **S. Liu**, R. Li, R. Wild, J. Krechmer, S. Thompson, C. Warneke, J.A. de Gouw, S.S. Brown, S. Miller, J.L. Jimenez, P. Ziemann

9:05 PHYS **3.** Global climate impact of sulpher-plume chemistry and particle formation. **J. Pierce**, R. Stevens

9:30 Intermission.

9:45 PHYS **4.** Mechanisms of formation and growth of particles in air. **B.J. Finlayson Pitts**

10:50 PHYS **5.** Detection of low-volatility gas-phase organic compounds from the OH-initiated oxidation of isoprene hydroxyhydroperoxide and their relevance to organic aerosol production. **J. Krechmer**, M. Coggan, J.B. Nowak, J. Kimmel, H. Stark, P. Massoli, J.T. Jayne, J.D. Crounse, T.B. Nguyen, P. Wennberg, J.H. Seinfeld, D.R. Worsnop, J.L. Jimenez, M. Canagaratna

10:25 PHYS **6.** Nanoparticle growth by carbonaceous matter. **M.V. Johnston**

11:10 PHYS **7.** Interplay between secondary organic aerosol chemistry, phase state, and growth dynamics. **R.A. Zaveri**, J. Shilling, A. Zelenyuk-Imre, J. Liu, J. Wilson, A. Laskin, B. Wang, J. Fast, R. Easter, J. Wang, C. Kuang, J.A. Thornton, A. Setyan, Q. Zhang, T.B. Onasch, D.R. Worsnop

Section B

Colorado Convention Center
Room 502

Carbon in the Galaxy: The Formation of Complex Organics from the Outflow of Carbon Stars & Their Evolution

Organic Molecules in Carbon Star Outflows

L. J. Allamandola, T. J. Lee, *Organizers*
J. Oomens, *Presiding*

8:00 PHYS **8.** Lifecycle of cosmic carbon. **A. Tielens**

8:35 PHYS **9.** Molecular content of carbon-rich evolved stars and the carbon balance from observations at all wavelengths. **P. Chernicharo**

9:10 PHYS **10.** Formation of complex organics and carbonaceous grains in the outflow of carbon stars: A laboratory study. **F. Salama**

9:45 Intermission.

10:15 PHYS **11.** Synthesis of pure and N-substituted cyclic hydrocarbons (e.g. pyrimidine) via gas-phase ion-molecule reactions. **P.P. Bera,** R. Peverati, M.P. Head-Gordon, T.J. Lee

10:50 PHYS **12.** Computational rovibrational spectroscopy and applications to astrochemistry. **R.C. Fortenberry**, X. Huang, W. Morgan, R.A. Theis, T. Crawford, T.J. Lee

11:15 PHYS **13.** Multiple excited states of PANH anions using informed orbital descriptions. **M.L. Theis**, A. Candian, A. Tielens, T.J. Lee, R.C. Fortenberry

Section C

Colorado Convention Center
Room 503

Computational Chemical Dynamics: Advancing our Understanding of Chemical Processes in Gas-Phase, Biomolecular & Condensed-Phase Systems: A Symposium in Honor of Donald Truhlar

Accurate Energies for Dynamics

Cosponsored by COMP

J. Gao, B. C. Garrett, B. Mennucci, *Organizers*
M. S. Gordon, *Presiding*

8:00 PHYS **14.** Potential energy surfaces for dynamics calculations. **D.G. Truhlar**

8:30 PHYS **15.** Strategies towards dynamic and non-dynamic electron correlation. **A.K. Wilson**

9:00 PHYS **16.** Dissecting the effect of morphology on the rates of singlet fission: Insights from theory. **A. Krylov**

9:20 PHYS **17.** Aerobic oxidation of methanol to formic acid on Au_8^-: Benchmark analysis based on completely renormalized coupled-cluster and density functional theory calculations. **P. Piecuch,** J.A. Hansen, M. Ehara

9:40 Intermission.

10:00 PHYS **18.** Complications in potential energy surfaces for molecules involving second row elements. **T.H. Dunning**

10:30 PHYS **19.** Dynamics of curved carbon π systems. **K.K. Baldridge**

11:00 PHYS **20.** Mag-walking Monte Carlo and density functional theory calculations of interaction energies in ammonium halide clusters. **R.Q. Topper**, J.J. Biswakarma, V. Ciocoi

11:20 PHYS **21.** Analysis of changes in bonding patterns along reaction paths in terms of molecule-intrinsic quasi-atomic orbitals. **K. Ruedenberg**, A.C. West, M.W. Schmidt, M.S. Gordon

Section D

Colorado Convention Center
Room 504

Role of Membrane in Amyloid-Formation & the Pathogenicity of Amyloid Disease

Amyloid β: Structures and Molecular Interactions

Cosponsored by COLL and COMP

J. C. Lee, J. E. Straub, *Organizers*
J. E. Shea, *Presiding*

8:00 Introductory Remarks.

8:05 PHYS **22.** High resolution insights on the membrane mediated amyloid aggregation. **A. Ramamoorthy**

8:45 PHYS **23.** Modulation of molecular interactions of Alzheimer's Aβ peptide fibrils and oligomers with lipid membranes. F. Tofoleanu, B. Brooks, **N. Buchete**

9:25 PHYS **24.** Interaction of A-beta with model lipid membranes. **P.S. Cremer**

9:45 Intermission.

10:05 PHYS **25.** Determining the structural ensemble of intrinsically disordered disease peptides: Applications to Alzheimer's disease biology in solution and membrane. **T.L. Head-Gordon**

10:45 PHYS **26.** Revealing the interplay between amyloid-β and membranes through molecular simulations. **B. Strodel**

11:25 PHYS **27.** Structural studies of the membrane disruption pathways induced by β-amyloid peptides in Alzheimer's disease. **W. Qiang**, R.D. Akinlolu, M. Nam, N. Shu, D. Delgado

Section E

Colorado Convention Center
Room 507

Modeling Complex Biomolecules: From Structure to Dynamics & Function

Advances in Simulation Methodology

Cosponsored by COMP

A. E. Garcia, *Organizer*
G. Hummer, *Organizer, Presiding*

8:00 PHYS **28.** Sense and nonsense when performing and interpreting molecular dynamics simulations of biomolecular systems. **W. van Gunsteren**

8:35 PHYS **29.** Potential function as a variable: Advances in using simulations of multiple states to solve hard biomolecular problems. **M.R. Shirts**

9:10 PHYS **30.** TRAM: Optimal estimation of trajectory data from multiple thermodynamic states. **F. Noe**

9:45 PHYS **31.** Exact milestoning. **R. Elber**

10:20 PHYS **32.** Fluorescent proteins as pH sensors: Insights from constant pH molecular dynamics. **E.N. Laricheva**, C.L. Brooks

10:55 PHYS **33.** Molecular multipole models for complex biomolecules. **T. Ichiye**

Section F

Colorado Convention Center
Room 505

Modeling Excited States of Complex Systems

Complex Materials and Molecules

Cosponsored by COMP

B. G. Levine, S. A. Varganov, *Organizers*
H. Jaeger, *Presiding*

8:00 PHYS **34.** Photoinduced proton-coupled electron transfer in solution: Quantum mechanical/molecular mechanical nonadiabatic dynamics. **S. Hammes-Schiffer**

8:40 PHYS **35.** Energy transfer in closely packed Si quantum dots: The role of surface defects. **S.V. Kilina**

9:20 PHYS **36.** Cheap models for electronic transitions and their application to lead-halide perovskites. **J. Parkhill**

9:40 Intermission.

10:00 PHYS **37.** Modeling artificial and natural light harvesting systems with DFT. **E. Jakubikova**

10:40 PHYS **38.** Photodissociation dynamics of phenol. **X. Xu**, J. Zheng, K. Yang, D.G. Truhlar

11:20 PHYS **39.** Computational photochemistry of thioanisole. **S.L. Li**, D.G. Truhlar

11:40 PHYS **40.** Time-dependent density functional theory study of the excited state energy landscape of gold phosphine thiolate complexes. **E.B. Guidez**, C.M. Aikens

Section G

Colorado Convention Center
Room 506

Probing Nano-Plasmonic Phenomena at the Single Molecule, Single Electron, & Single Photon Level

D. J. Masiello, *Organizer*
S. Link, K. A. Willets, *Organizers, Presiding*

8:00 PHYS **41.** Ultrafast photoelectron imaging microscopy of plasmonic nanoparticles. **D.J. Nesbitt**

8:35 PHYS **42.** Tuning the acoustic frequency of a gold nanodisk through its adhesion layer. **W. Chang**, F. Wen, D. Chakraborty, M. Su, Y. Zhang, B. Shuang, P.J. Nordlander, J. Sader, N.J. Halas, S. Link

8:55 PHYS **43.** Coherent plasmonics for ultrasensitive and single molecule sensing. **N.J. Halas**

9:30 PHYS **44.** Probing ground-state single-electron self-exchange across a molecule-metal interface and molecule-substrate electronic coupling by simultaneous spectroscopic and topographic Near-field SERS Imaging. Y. Wang, P. Sevinc, Y. He, **H. Lu**

9:50 PHYS **45.** Using STEM/EELS to probe energy transfer in plasmon-enhanced solar devices. **J.P. Camden**

10:25 PHYS **46.** Use of electron microscopy to probe quantum plasmonics, hot electrons and energy transport in hybrid nanoparticle/semiconductor systems. **C. Cherqui**

10:45 PHYS **47.** Cathodoluminescence-activated nano-imaging by resonant energy transfer. **N.S. Ginsberg**, C.G. Bischak, C. Hetherington, Z. Wang, J. Precht, D. Kaz, C. Stachelrodt, D. Schlom

Section H

Colorado Convention Center
Room 607

Design of Materials and Chemical Processes: The Genomic Approach

Recent Advances in Computational Methods

L. Gagliardi, B. Smit, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 PHYS **48.** Self-interaction correction to density-functional approximations with unitary invariance. **M.R. Pederson**

8:35 PHYS **49.** Toward rational design of small molecule adsorption in open-site metal-organic frameworks with density functional theory. **J. Neaton**

9:05 PHYS **50.** New density functionals obtained by a genome-scale search approach to functional design. N. Mardirossian, **M.P. Head-Gordon**

9:35 PHYS **51.** Mechanism of C–H bond activation of C_2H_6 by iron(IV)–oxo sites in magnesium-diluted Fe_2(dobdc). **P. Verma**, K.D. Vogiatzis, N. Planas, J. Borycz, D. Xiao, J.R. Long, L. Gagliardi, D.G. Truhlar

‡ *Cooperative Cosponsorship*

9:55 Intermission.

10:15 PHYS **52.** Enantioselective adsorption in zeolites and metal-organic frameworks. R. Bueno-Perez, A. Martín-Calvo, P. Gómez-Alvarez, J. Gutiérrez-Sevillano, P. Merkling, T. Vlugt, T. van Erp, D. Dubbeldam, **S. Calero**

10:45 PHYS **53.** New computational tools for modeling metal-organic frameworks. **F. Paesani**

11:15 PHYS **54.** Computational materials design of co-polymers for organic electronics. **R.E. Larsen**, T.W. Kemper, S. Sides, P. Graf, D.C. Olson

Computational Design, Discovery and Optimization of Organic Semiconductor Materials

Sponsored by COMP, Cosponsored by PHYS

Electronic Structure Methods for Highly Polarizable Systems

Dynamics

Sponsored by COMP, Cosponsored by PHYS

SUNDAY AFTERNOON

Section A

Colorado Convention Center
Room 501

Atmospheric Chemistry: Transformations of Matter in the Troposphere

Ice Nucleation

M. Freedman, *Organizer*
D. Cziczo, *Organizer, Presiding*
J. Lu, *Presiding*

1:30 PHYS **59.** Nucleation of ice: A molecular perspective. **V. Molinero**

2:10 PHYS **60.** Homogeneous freezing of single submicron to micron-sized water and hydrocarbon aerosol droplets levitated in a Bessel beam trap. **J.W. Lu**, M. Isenor, R. Signorell

2:30 PHYS **61.** Ice formation in ultracold cirrus. **E. Moyer**, K. Lamb, B. Clouser, L. Sarkozy, M. Bolot, O. Moehler, H. Saathoff, V. Ebert

2:55 PHYS **62.** Ice nucleation in clouds: Sensitivities to physicochemical IN properties and cloud microphysics. **B. Ervens**, G. Feingold

3:20 Intermission.

3:35 PHYS **63.** Atmospheric ice nucleating particles from the sea surface microlayer. **B. Murray**, T.W. Wilson, L. Ladino, P. Alpert, M. Breckels, I. Brooks, J.A. Huffman, C. Judd, W.P. Kilthau, R. Mason, G. McFiggans, L. Miller, J. Najera, E. Polishchuk, S. Rae, S. Corinne, M. Si, T. Whale, J. Wong, O. Wurl, J. Yakobi, J.P. Abbatt, J.Y. Aller, A.K. Bertram, D.A. Knopf

4:15 PHYS **64.** Contact-induced efflorescence of amorphous inorganic microparticles. **R.D. Davis**, S. Lance, J.A. Gordon, S.B. Ushijima, M. Tolbert

4:35 PHYS **65.** Studies of the abundance and compositions of organic ice nucleating particles in the atmosphere. **P.J. DeMott**, T.C. Hill, C.S. McCluskey, E.J. Levin, K.J. Suski, O. Laskina, Y. Tobo, D.B. Collins, C. Sultana, C. Lee, G. Cornwell, H. Al-Mashat, M. Santander, C.M. Beall, F. Malfatti, R. Mason, D. Pham, N.G. Swoboda-Colberg, V.H. Grassian, R. Moffet, A.K. Bertram, K.A. Prather, S. Kreidenweis

5:00 PHYS **66.** Atmospheric ice nucleation: Microspectroscopic imaging and characterization of individually identified ice nucleating particles. **D.A. Knopf**, P. Alpert, B. Wang, W.P. Kilthau, D. Bothe, R.E. O'Brien, S.T. Kelly, A. Laskin, M.K. Gilles, J.Y. Aller

Section B

Colorado Convention Center
Room 502

Carbon in the Galaxy: The Formation of Complex Organics from the Outflow of Carbon Stars & Their Evolution

Organic Molecules in Carbon Star Outflows

L. J. Allamandola, T. J. Lee, *Organizers*
F. Salama, *Presiding*

1:30 PHYS **67.** Observations of organic molecules in carbon-rich proto-planetary nebulae and planetary nebulae. **E. Peeters**

2:05 PHYS **68.** Dust formation in carbon stars. **I. Cherchneff**

2:40 PHYS **69.** Ion chemistry of cyclic aromatics and interactions with polar molecules leading to the formation of complex organics in the gas phase and on ice grains. **M. El-Shall**

3:15 Intermission.

3:45 PHYS **70.** Laboratory infrared spectroscopy of 'hard-to-get' ionized polyaromatics. **J. Oomens**

4:20 PHYS **71.** Carbonaceous dust and fullerenes in evolved stars. **J. Cami**

4:45 PHYS **72.** Quantum chemical studies of interstellar organic molecules: Formation mechanisms, spectroscopic signatures, and properties. **T.J. Lee**

Section C

Colorado Convention Center
Room 503

Computational Chemical Dynamics: Advancing our Understanding of Chemical Processes in Gas-Phase, Biomolecular & Condensed-Phase Systems: A Symposium in Honor of Donald Truhlar

Gas-Phase Kinetics and Dynamics

Cosponsored by COMP

J. Gao, B. C. Garrett, B. Mennucci, *Organizers*
G. C. Schatz, *Presiding*

1:30 PHYS **73.** Mode-, bond- and stereo-selective bimolecular reactions. **K. Liu**

2:00 PHYS **74.** Sudden vector projection model: Mode specificity and bond selectivity made easy. **H. Guo**

2:30 PHYS **75.** Mixed quantum/classical theory for rotationally and vibrationally inelastic scattering. **D. Babikov**

2:50 PHYS **76.** Sum over histories representation for chemical kinetics. **R.T. Skodje**

3:10 Intermission.

3:30 PHYS **77.** Resonances in chemical reactions. **X. Yang**

4:00 PHYS **78.** Reaction dynamics on ab initio potential energy surfaces. **J.M. Bowman**, Y. Wang, Z. Homayoon, R. Conte, P. Houston

4:30 PHYS **79.** Improved semiclassical tunneling. **A.F. Wagner**

4:50 PHYS **80.** Alkyl CH stretch vibrations as a probe local environment. **E.L. Sibert**, D.P. Tabor, N. Kidwell, J.C. Dean, T.S. Zwier

Section D

Colorado Convention Center
Room 504

Role of Membrane in Amyloid-Formation & the Pathogenicity of Amyloid Disease

Amyloid Precursor Protein, Origin of Amyloid β

Cosponsored by COLL and COMP

J. C. Lee, J. E. Straub, *Organizers*
M. T. Zanni, *Presiding*

1:30 PHYS **81.** Structure, dimerization, and cholesterol binding of the amyloid precursor protein transmembrane C99 domain and amyloidogenesis. **C.R. Sanders**

2:10 PHYS **82.** Impact of membrane composition on the structure, stability, and processing of the transmembrane domain of the amyloid precursor p. **L. Dominguez**, L. Foster, J.E. Straub, D. Thirumalai

2:50 PHYS **83.** Conformational changes induced by the A21G Flemish mutation in the amyloid precursor protein lead to increased Aβ secretion in Alzheimer's disease. **T. Tang**, Y. Hu, P. Kienlen-Campard, L. El Haylani, M. Decock, J. Van Hees, Z. Fu, J. Ocatve, S. Constantinescu, S.O. Smith

3:10 Intermission.

3:30 PHYS **84.** Titration of charged residues in the context of membrane bilayers; A constant pH molecular dynamics study. **A. Panahi**, C.L. Brooks

3:50 PHYS **85.** Dimerization of a transmembrane peptide from amyloid precursor protein. **S. Meredith**

4:30 PHYS **86.** Multiscale molecular dynamics simulations of transmembrane structures of amyloid precursor protein in biological membrane. **Y. Sugita**

Section E

Colorado Convention Center
Room 507

Modeling Complex Biomolecules: From Structure to Dynamics & Function

Classical and Quantum Descriptions of Protein Function

Cosponsored by COMP

G. Hummer, *Organizer*
A. E. Garcia, *Organizer, Presiding*

1:30 PHYS **87.** Proton-coupled electron transfer in soybean lipoxygenase: Hydrogen tunneling and conformational motions. **S. Hammes-Schiffer**

2:05 PHYS **88.** Activation mechanisms in RAF kinase dimers. **E. Rosta**

2:40 PHYS **89.** Ab initio QM/MM simulations point to an alternative mechanism for the AlkB catalyzed repair of 1-methyl adenine. D. Fang, **G.A. Cisneros**

3:15 PHYS **90.** Exploring water penetration in soluble proteins and ion pumps. **Q. Cui**

3:50 PHYS **91.** Withdrawn.

4:25 PHYS **92.** Theoretical analysis and modeling of rhodopsin's unusual kinetics of thermal reactions and its role in dim-light vision. Y. Guo, S. Sekharan, J. Liu, V.S. Batista, J.C. Tully, **E.C. Yan**

Section F

Colorado Convention Center
Room 505

Modeling Excited States of Complex Systems

Complex Materials and Molecules

Cosponsored by COMP

B. G. Levine, S. A. Varganov, *Organizers*
S. W. Kilina, *Presiding*

1:30 PHYS **93.** Quantum simulation of coherent exciton dynamics in conjugated systems. **P.J. Rossky**

2:10 PHYS **94.** Electronic excitation of metal-organic frameworks. **H. Jaeger**

2:50 PHYS **95.** Auger relaxation of hot electrons in CdSe quantum dots using GFSH. **D. Trivedi**, L. Wang, O. Prezhdo

3:10 PHYS **96.** Nonlinear optical structural properties of room-temperature ionic liquids, calculated with the combined fragment molecular orbital and linear-response time-dependent density functional theory method (FMO/LR-TDDFT). **A.D. Findlater**, F. Zahariev, M.S. Gordon

3:30 Intermission.

3:50 PHYS **97.** Evolution of photoexcited states in extended molecular chromophores. **S. Tretiak**

4:30 PHYS **98.** Excited state dynamics at metal to semiconductor interfaces. **D. Kilin**

5:10 PHYS **99.** Excited states in large molecular systems by the combined quantum Monte Carlo/effective fragment molecular orbital method. **F. Zahariev**, A.D. Findlater, M.S. Gordon

5:30 PHYS **100.** Electronic structure study of CIGS solar cells by X-ray absorption spectroscopy: Experiment and theory. **C.P. Schwartz**, D. Nordlund, T. weng, K. Ramanathan, D. Sokaras, D. Prendergast, S. Christensen

Section G

Colorado Convention Center
Room 506

Probing Nano-Plasmonic Phenomena at the Single Molecule, Single Electron, & Single Photon Level

S. Link, D. J. Masiello, *Organizers*
K. A. Willets, *Organizer, Presiding*
J. P. Camden, *Presiding*

1:30 PHYS **101.** Quantum and molecular plasmonics. **P.J. Nordlander**

2:05 PHYS **102.** Single photon interactions with localized surface plasmons: Exploiting fano resonances to generate quantum beats. **N. Thakkar**, C. Cherqui, D.J. Masiello

2:25 PHYS **103.** Understanding heterogeneity in plasmonic metal oxide nanocrystals. **D.J. Milliron**, R. Johns, A. Agrawal, S.D. Lounis, D. Nordlund, H. Bechtel

3:00 PHYS **104.** Mid-infrared surface phonon polaritons in dolar Dielectrics: An alternative approach. **A.J. Giles**, J. Caldwell

3:20 PHYS **105.** Life and times of plasmonically-generated energetic electrons. **M. Moskovits**

3:55 PHYS **106.** Characterizing the generation of hot electrons by metal nanoparticles through their interaction with molecular-type electron acceptors. **A. Hoggard**, B. Foerster, D. Huang, W. Chang, S. Link

4:15 PHYS **107.** Towards nanophotonic and time-resolved spectroscopy of plasmonic systems. **I. Thomann**

Section H

Colorado Convention Center
Room 607

Design of Materials and Chemical Processes: The Genomic Approach

Gas Separation & Gas Storage: Experiments & Calculations

L. Gagliardi, B. Smit, *Organizers, Presiding*

1:30 PHYS **55.** Accurate first-principles force fields for high-throughput screening of gas uptake in metal-organic frameworks. J.G. McDaniel, S. Li, E. Tyllianakis, R. Snurr, **J.R. Schmidt**

2:00 PHYS **56.** First principles simulations in the study of metal-organic frameworks: From stability to activity. **N. Lopez**

2:30 PHYS **57.** Metal organic framework based catalyst for release of chemically stored nitric oxide. **R. Kumar**

3:00 PHYS **58.** Top-down generation and screening of metal-organic frameworks for gas storage and separation applications. D. Gomez-Gualdron, Y.J. Colon, Y. Chung, **R. Snurr**

3:30 Intermission.

3:50 PHYS **108.** Ab initio simulation of adsorption isotherms for gases and gas mixtures in porous media. **J. Sauer**

4:20 PHYS **109.** 2D crystalline zeolites, non-aluminosilicate molecular sieves, and metal organic frameworks. **M. Tsapatsis**

4:50 PHYS **110.** Developing a predictive, descriptor based approach for CO and NO adsorption to Fe, Co, Ni and Cu sites in zeolites. **F. Goeltl**, P. Mueller, I. Hermans, P. Sautet

Computational Design, Discovery and Optimization of Organic Semiconductor Materials

Sponsored by COMP, Cosponsored by PHYS

TECHNICAL PROGRAM

Electronic Structure Methods for Highly Polarizable Systems

Embedding: QM/QM and QM/MM

Sponsored by COMP, Cosponsored by PHYS

Quantum Chemistry

Methodology

Sponsored by COMP, Cosponsored by PHYS

MONDAY MORNING

Section A

Colorado Convention Center
Room 501

Atmospheric Chemistry: Transformations of Matter in the Troposphere

Water & Organic Aerosol

D. Cziczo, M. Freedman, *Organizers*
R. Washenfelder, Q. Zhang, *Presiding*

8:00 PHYS **111.** Hydration state of methylglyoxal at the air-water interface. G.L. Richmond, **S. Wren**, B.P. Gordon, N. Valley, L. McWilliams

8:40 PHYS **112.** Direct and quantitative measurement of the surface tension of airborne microdroplets. **B.R. Bzdek**, R.M. Power, J.P. Reid

9:00 PHYS **113.** Calculated equilibrium constants for formation of peroxy radical/water complexes to elucidate radical inititated particle formation. **R.B. Shirts**, S. Kumbhani, E. Burrell, J.C. Hansen

9:20 Intermission.

9:35 PHYS **114.** Liquid/vapor interface of aqueous solutions relevant to tropospheric chemistry. **J.C. Hemminger**

10:15 PHYS **115.** Single scattering albedo studies of brown carbon formation in evaporating droplets. **M. Zauscher**, M.A. Symons, D.O. Dehaan

10:35 PHYS **116.** Air-water interface: As Influenced by ions, lipids, and electric fields. **H.C. Allen**

11:00 PHYS **117.** Redistribution of black carbon in aerosol particles undergoing liquid-liquid phase separation. **S. Brunamonti, U. Krieger, C. Marcolli**, T. Peter

Section B

Colorado Convention Center
Room 502

Carbon in the Galaxy: The Formation of Complex Organics from the Outflow of Carbon Stars & Their Evolution

Organic Molecules in the Diffuse Interstellar Medium

L. J. Allamandola, T. J. Lee, *Organizers*
J. Cami, *Presiding*

8:00 PHYS **118.** Carbon bearing molecules in interstellar clouds. **J. Krelowski**

8:35 PHYS **119.** Molecular laboratory astrophysics: About molecular transients and molecule formation under interstellar conditions. **H. Linnartz**

9:10 PHYS **120.** Carbon in the galaxy. **E. Roueff**

9:45 Intermission.

10:15 PHYS **121.** Low temperature formaton of polycyclic aromatic hydrocarbons in the Interstellar medium via bimolecular neutral-neutral reactions. **R. Kaiser**

10:50 PHYS **122.** Angle-resolved PEPICO imaging of the dissociative ionization of methyl azide and methylenimine using a tabletop high harmonic generation light source. W.K. Peters, **D.E. Couch**, C.W. Hogle, D. Beltran, P. Towstik, D.M. Jonas, H. Kapteyn, M.M. Murnane

11:15 PHYS **123.** Electronic excited states of interstellar species: Quantum chemical prediction of spectroscopic signatures using quartic force fields. **W.J. Morgan,** R.C. Fortenberry

Section C

Colorado Convention Center
Room 503

Computational Chemical Dynamics: Advancing our Understanding of Chemical Processes in Gas-Phase, Biomolecular & Condensed-Phase Systems: A Symposium in Honor of Donald Truhlar

Enzyme Kinetics and Dynamics

Cosponsored by COMP

J. Gao, B. C. Garrett, B. Mennucci, *Organizers*
S. Hammes-Schiffer, *Presiding*

8:00 PHYS **124.** Tunneling and the role of barrier width in enzymatic C-H activation. **J.P. Klinman**

8:30 PHYS **125.** Theoretical studies of enzymatic reactions. **W. Thiel**

9:00 PHYS **126.** Role of dynamics in enzyme catalysis: Challenges in comparing calculations to measurements. **A. Kohen**

9:20 PHYS **127.** Quantum mechanical/molecular mechanical simulations of the hydride transfer reactions in quinone reductase 2. C.R. Reinhardt, **S. Bhattacharyay**

9:40 Intermission.

10:00 PHYS **128.** QM/MM excited state dynamics of complex systems. **U. Roethlisberger**

10:30 PHYS **129.** Understanding metalloenzyme catalysis with QM/MM free energy simulations. **Q. Cui**

11:00 PHYS **130.** Adaptive-partitioning QM/MM dynamics simulations of proton transfer. S. Pezeshki, **H. Lin**

11:20 PHYS **131.** Functional mode electron transfer theory. **H. Chen**

Section D

Colorado Convention Center
Room 504

Role of Membrane in Amyloid-Formation & the Pathogenicity of Amyloid Disease

α-Synuclein, the Parkinson's Protein

Cosponsored by COLL and COMP

J. C. Lee, J. E. Straub, *Organizers*
G. L. Millhauser, *Presiding*

8:00 PHYS **132.** Structure of the toxic core of α-synuclein, the amyloid associated with Parkinson's disease. **D. Eisenberg**, J.A. Rodriguez, M. Ivanova, M. Sawaya, D. Cascio, F. Reyes, D. Shi, E. Guenther, L. Johnson, J. Hattne, S. Sangwan, B. Nannega, A. Brewster, M. Messerschmidt, S. Boutet, N. Sauter, T. Gonen

8:40 PHYS **133.** NMR approaches to uncovering the molecular basis of inhibition of alpha-synuclein aggregation by beta synuclein. **J. Baum**, M. Janowska, G. Moriarty, M. Olson, N. Sikka

9:20 PHYS **134.** Examining the folding landscape of α-synuclein using time-resolved FRET. **S.K. Hess**, J.C. Lee

9:40 Intermission.

10:00 PHYS **135.** Misfolding and membrane interaction of amyloidogenic proteins. **R. Langen**

10:40 PHYS **136.** Aggregation mechanism of amyloidogenic proteins involved in neurodegenerative disorders. **C. Stultz**

11:20 PHYS **137.** Amyloidogenic proteins A-beta, alpha-synuclein and Tau interact with and disrupt membranes via different mechanisms and exhibit cell-type dependent toxicity. **H. Lashuel**

Section E

Colorado Convention Center
Room 507

Modeling Complex Biomolecules: From Structure to Dynamics & Function

Membrane Proteins

Cosponsored by COMP

A. E. Garcia, G. Hummer, *Organizers*
E. Tajkhorshid, *Presiding*

8:00 PHYS **138.** Large-scale computer simulations of lipids: Coarse-grained simulations of complex mixed bilayers. **D.P. Tieleman**

8:35 PHYS **139.** Membrane proteins: From structure refinement and remodeling to functional mechanisms. **H. Zhou**

9:10 PHYS **140.** Specific protein-lipid interactions stabilize an active state of the beta 2 adrenergic receptor. **C. Neale**, H.D. Herce, R. Pomès, A.E. Garcia

9:45 PHYS **141.** Dynamics of dopamine transporter: Molecular simulations and comparison with LeuT dynamics. M.H. Cheng, **I. Bahar**

10:20 PHYS **142.** Channel rhodopsin: Structure vs. function relationships from molecular dynamics simulations. S.W. Rick, **M. VanGordon**, S.L. Rempe

10:55 PHYS **143.** Assembly and mechanistic details of drug translocation in MexAB-OprM efflux pump. C.A. Lopez, J. Phillips, B. Alexandrov, **G. Gnanakaran**

Section F

Colorado Convention Center
Room 505

Modeling Excited States of Complex Systems

Excited States in Biology

Cosponsored by COMP

B. G. Levine, S. A. Varganov, *Organizers*
L. V. Slipchenko, *Presiding*

8:00 PHYS **144.** Excitonic states in natural light-harvesting systems. **B. Mennucci**

8:40 PHYS **145.** Electronic progression during the photoisomerization of microbial and vertebrate light-sensing rhodopsins. H. Luk, S. Gozem, F. Melaccio, S. Rinaldi, **M. Olivucci**

9:20 PHYS **146.** Theoretical study of the electron transfer in DNA repair process of the cyclobutane pyrimidine dimer lesion. **L. Joubert-Doriol**, T. Domratcheva, M. Olivucci, A.F. Izmaylov

9:40 Intermission.

10:00 PHYS **147.** Insights into the role of excimers/exciplexes in the photophysics and photochemistry of DNA. **S. Matsika**

10:40 PHYS **148.** Excited-state electron transfer in fluorescent proteins. **A. Krylov**

11:20 PHYS **149.** Charge-transfer dynamics of light-harvesting systems in complex solvated environments. **B.M. Wong**, M. Oviedo

11:40 PHYS **150.** Spectroscopic properties of a cholesteric liquid glass platinum acetylide. **T.M. Cooper**, A.R. Burke, D.M. Krein, R.F. Ziolo, J.E. Haley, D.J. Stewart, S.L. Long, A.E. Bell

Section G

Colorado Convention Center
Room 506

Probing Nano-Plasmonic Phenomena at the Single Molecule, Single Electron, & Single Photon Level

S. Link, K. A. Willets, *Organizers*
D. J. Masiello, *Organizer, Presiding*
I. Thomann, *Presiding*

8:00 PHYS **151.** Shape and surface control of plasmonic particles. **C.J. Murphy**

8:35 PHYS **152.** Plasmonic properties of coupled gold nanostructures. C. Liow, A. Li, **S. Li**

8:55 PHYS **153.** Mechanisms of on-colloid nanoparticle growth. **J. Millstone**, P. Straney, L. Marbella

9:30 PHYS **154.** Probing G_{M3} and G_{M1} contents of HIV-1 and ebola virus-like particles through plasmon coupling microscopy. **A. Feizpour**, C. Silva, H. Akiyama, C.M. Miller, S. Gummuluru, B.M. Reinhard

9:50 PHYS **155.** Surface plasmon polaritons in chemically synthesized nanostructures. **G.V. Hartland**, P. Johns, M. Devadas, K. Yu

10:25 PHYS **156.** Understanding the STEM/EELS magneto-optical responses of aromatic plasmon-supporting metal oligomers. **N. Bigelow**, C. Cherqui, A. Vaschillo, H. Goldwyn, D.J. Masiello

10:45 PHYS **157.** Plasmon/exciton and plasmon/photonic mode interaction. **G.C. Schatz**

Section H

Colorado Convention Center
Room 607

Design of Materials and Chemical Processes: The Genomic Approach

The Materials Genome and DataMining

L. Gagliardi, B. Smit, *Organizers, Presiding*

8:00 PHYS **158.** Materials project for accelerated materials design. **K. Persson**

8:30 PHYS **159.** Predictive materials discovery: Finding optimal zeolites for challenging separations and chemical conversions. **J.I. Siepmann**, P. Bai, M. Jeon, L. Ren, C. Knight, M.W. Deem, M. Tsapatsis

9:00 PHYS **160.** Recent applications of databases of crystal structures and experimental data for metal-organic framework materials. **D. Sholl**, X. Nie, T. Duerinck, K. Walton, D. Nazarian, J. Camp

9:30 PHYS **161.** Computational screening of MOFs with open metal sites for adsorption and catalysis applications. **K.D. Vogiatzis**, E. Haldoupis, J.I. Siepmann, L. Gagliardi

9:50 Intermission.

10:10 PHYS **162.** Material informatics in discovery of nanoporous materials for energy applications. **M. Haranczyk**

10:40 PHYS **163.** Prediction of high deliverable capacity metal-organic frameworks with an evolutionary algorithm. Y. Bao, R. Martin, C. Simon, M. Haranczyk, B. Smit, **M.W. Deem**

11:10 PHYS **164.** Materials genome in action: Finding a nanoporous material for methane storage. **C. Simon**, J. Kim, D. Gomez-Gualdron, J. Camp, Y. Chung, R. Martin, R. Mercado, M.W. Deem, D. Gunter, M. Haranczyk, D. Sholl, R. Snurr, B. Smit

11:30 PHYS **165.** Cheminformatics-inspired approaches for big materials data. **O. Isayev**, D. Fourches, E. Muratov, A. Tropsha

Molecular Mechanics

Force Field Development

Sponsored by COMP, Cosponsored by PHYS

WCC Rising Stars Awards Symposium

Sponsored by WCC, Cosponsored by BIOT, COLL, GEOC, INOR, ORGN, PHYS, PMSE and PROF

Computational Design, Discovery and Optimization of Organic Semiconductor Materials

Sponsored by COMP, Cosponsored by PHYS

Electronic Structure Methods for Highly Polarizable Systems

Correlation Methods & DFT

Sponsored by COMP, Cosponsored by PHYS

MONDAY AFTERNOON

Section A

Colorado Convention Center
Room 501

Atmospheric Chemistry: Transformations of Matter in the Troposphere

Aqueous Chemistry

D. Cziczo, M. Freedman, *Organizers*
D. O. Dehaan, M. D. Zauscher, *Presiding*

1:30 PHYS **166.** Aqueous-phase and organic-phase photochemistry of atmospheric organic compounds. **S.A. Nizkorodov**

2:10 PHYS **167.** Laboratory and field studies of brown carbon aerosol in the near-ultraviolet spectral region. **R. Washenfelder**, J. Flores, G. Adler, C. Brock, J. Lee, J. Laskin, A. Laskin, S.A. Nizkorodov, L. Segev, S.S. Brown, Y. Rudich

‡ *Cooperative Cosponsorship*

2:30 PHYS **168.** Formation and photochemical evolution of phenolic SOA in aqueous phase. **Q. Zhang**, L. Yu, J.D. Smith, C. Anastasio, A. Laskin, J. Laskin

2:55 PHYS **169.** Cloud and fog processing of atmospheric organic matter. **J.L. Collett**, A. Boris, M. Schurman, Y. Desyaterik

3:20 Intermission.

3:35 PHYS **170.** Aerosol organics: Formation and processing in the aqueous phase. **V. McNeill**

4:15 PHYS **171.** Multiphase atmospheric chemistry of pyruvic acid. **V. Vaida**, A. Monod, J. Doussin, A.E. Reed Harris, E. Griffith, J.A. Kroll, R.J. Rapf

4:40 PHYS **172.** Aqueous-phase aldehyde photooxidation in the presence of ammonium salts, amines, and SO_2: brown carbon formation. **D.O. Dehaan**, N.G. Jimenez, P.D. Wickremasinghe, K.D. Sharp

Section B

Colorado Convention Center
Room 502

Carbon in the Galaxy: The Formation of Complex Organics from the Outflow of Carbon Stars & Their Evolution

Organic Molecules in Dense Interstellar Clouds

L. J. Allamandola, T. J. Lee, *Organizers*
H. Linnartz, *Presiding*

1:30 PHYS **173.** Review of the molecular complexity of organic material in the gas-phase ISM. **S.N. Milam**

2:05 PHYS **174.** Global optimization and broadband analysis software for interstellar chemistry. S.L. Widicus Weaver, **L. Zou**, M. Rad, J. Sanders

2:40 PHYS **175.** Molecular line lists of carbon-containing molecules for exoplanets and other hot bodies. **J. Tennyson**

3:15 Intermission.

3:45 PHYS **176.** Observations of carbon in interstellar and circumstellar ices. **A. Boogert**

4:20 PHYS **177.** Reliable abundances of extra-terrestrial hydrocarbon ices: Interminable quest or end in sight? **R.L. Hudson**, P.A. Gerakines

4:45 PHYS **178.** Optical properties of titan hazeaAnalogs using photoacoustic and cavity ring-down spectroscopy. **M.S. Ugelow**, K.J. Zarzana, M.A. Tolbert

Section C

Colorado Convention Center
Room 503

Computational Chemical Dynamics: Advancing our Understanding of Chemical Processes in Gas-Phase, Biomolecular & Condensed-Phase Systems: A Symposium in Honor of Donald Truhlar

Catalysis

Cosponsored by COMP

J. Gao, B. C. Garrett, B. Mennucci, *Organizers*
C. T. Campbell, *Presiding*

1:30 PHYS **179.** Silica thin films: From crystals to glass in 2D. **H. Freund**

2:00 PHYS **180.** Doped metal clusters on oxides: Rationalization and design through the prism of chemical bonding. **A. Alexandrova**

2:30 PHYS **181.** Some recent developments in saddle point finding methods: Gradient squared minimization, solid state transitions, and temperature accelerated adaptive kinetic Monte Carlo. **G.A. Henkelman**

3:00 PHYS **182.** Catalysis with metal clusters anchored at the Zr6-based metal-organic framework NU-1000. **L. Gagliardi**, D.G. Truhlar, C.J. Cramer, J. Borycz, L. Fernandez, S. Tussupbayev

3:20 Intermission.

3:40 PHYS **183.** New approaches to simulating biological and molecular catalysts. **T.F. Miller**

4:10 PHYS **184.** Organometallic and organocatalytic reactions explored using the automated reaction route mapping method. **K. Morokuma**

4:40 PHYS **185.** Hydrazine decomposition in the gas phase and on an Iridium catalyst. **M.W. Schmidt**, M.S. Gordon

5:00 PHYS **186.** Density functional theory study of lithium ion battery anode materials: Ruthenium (IV) oxide, tin (IV) oxide, and tin (IV) sulfide. **B.R. Ramachandran**, A.S. Hassan, K. Moyer, T. Dixon, C.D. Wick

Section D

Colorado Convention Center
Room 504

Role of Membrane in Amyloid-Formation & the Pathogenicity of Amyloid Disease

Islet Amyloid Polypeptide (IAPP) at the Water/Lipid Interface

Cosponsored by COLL and COMP

J. C. Lee, J. E. Straub, *Organizers*
T. L. Head-Gordon, *Presiding*

1:30 PHYS **187.** Islet amyloid polypeptide: Membrane interactions and cytotoxicity. **D.P. Raleigh**

2:10 PHYS **188.** Aggregation and Orientation of amyloid proteins at lipid/water interfaces probed by chiral sum frequency generation spectroscopy. L. Fu, Z. Wang, D. Xiao, V.S. Batista, **E.C. Yan**

2:50 PHYS **189.** β-Sheet intermediate dictates the fiber formation kinetics of amylin from type 2 diabetes. **M.T. Zanni**

3:30 Intermission.

3:50 PHYS **190.** Islet amyloid and the shared molecular origins of membrane poration and cytotoxicity. **A. Miranker**

4:30 PHYS **191.** Exploring the free energy and conformational landscape of amyloidogenic peptides upon aggregation and amyloid formation. **R. Winter**

5:10 PHYS **192.** Protein folding and assembly on membrane-mimics in constant volume replica-exchange simulations. **Z.A. Levine, R.G. Mullen, J.E. Shea**

5:30 PHYS **193.** Structure of insulin at the air/water interface: monomers or dimers? **S. Mauri, T. Weidner**, H. Arnolds

Section E

Colorado Convention Center
Room 507

Modeling Complex Biomolecules: From Structure to Dynamics & Function

Molecular Machines

Cosponsored by COMP

A. E. Garcia, *Organizer*
G. Hummer, *Organizer, Presiding*

1:30 PHYS **194.** Modeling the function of molecular motors and other challenging biological systems. **A. Warshel**

2:05 PHYS **195.** Energy barriers and driving forces in tRNA translocation through the ribosome. **K. Grubmueller**, L.V. Bock, G.F. Schroder, I.I. Davydov, M.V. Rodnina, H. Stark, A.C. Vaiana, N. Fischer, C. Blau

2:40 PHYS **196.** Simulating conformational changes of the ribosome. **K. Sanbonmatsu**

3:15 PHYS **197.** Unraveling the mystery of ATP hydrolysis in actin filaments. **G.A. Voth**

3:50 PHYS **198.** Specificity, mechanism, and membrane organization of ATP synthases. **J. Faraldo-Gomez**

4:25 PHYS **199.** Visualizing complex functional motions of membrane transporters using advanced simulation and free energy techniques. **E. Tajkhorshid**

Section F

Colorado Convention Center
Room 505

Modeling Excited States of Complex Systems

Multiple Chromophores

Cosponsored by COMP

B. G. Levine, S. A. Varganov, *Organizers*
A. F. Izmaylov, *Presiding*

1:30 PHYS **200.** Ab initio exciton model for nonadiabatic dynamics of multichromophoric systems on GPUs. A. Sisto, D.R. Glowacki, **T.J. Martinez**

2:10 PHYS **201.** New electronic structure methods for describing excited states in multichromophore and other large systems. **J.M. Herbert**, X. Zhang, A.F. Morrison

2:50 PHYS **202.** Charge transfer-like excitations in solution: A critical assessment of TDDFT/continuum models. **C.A. Guido**, D. Jacquemin, C. Adamo, B. Mennucci

3:10 PHYS **203.** Modeling protein - chromophore electrostatic interactions with multiple electronic states: Diabatic population matrix approach. J.W. Park, **Y.M. Rhee**

3:30 Intermission.

3:50 PHYS **204.** Vibronic interactions in bi- and multi-chromophores. **L.V. Slipchenko**

4:30 PHYS **205.** Accurate simulation of exciton dynamics for hundreds to tens of thousands of chromophores: Theoretical methods and acceleration by general-purpose graphics processing units (GPGPU). **A. Aspuru-Guzik**

5:10 PHYS **206.** Photoexcited energy transfer in a weakly coupled dimer. L. Alfonso Hernandez, **T. Nelson**, S. Tretiak, S. Fernandez-Alberti

5:30 PHYS **207.** Theoretical investigation of singlet fission in quinoidal bithiophenes. **A. Chien**, A. Molina, T.G. Goodson, P.M. Zimmerman

Section G

Colorado Convention Center
Room 506

Probing Nano-Plasmonic Phenomena at the Single Molecule, Single Electron, & Single Photon Level

S. Link, K. A. Willets, *Organizers*
D. J. Masiello, *Organizer, Presiding*
P. K. Jain, *Presiding*

1:30 PHYS **208.** Mechanistic study of serum albumin interaction with therapeutic nanoparticles. **C.F. Landes**, S. Dominguez-Medina, L. Kisley, S. Link

2:05 PHYS **209.** Biological targeting of plasmonic nanoparticles improves cellular imaging via the enhanced scattering in the aggregates formed. **M. Aioub**, B. Kang, M. Mackey, M.A. El-Sayed

2:25 PHYS **210.** Probing single metal-semiconductor heterostructures for visible light photocatalysis. **N. Fang**, B. Dong, F. Zhao

3:00 PHYS **211.** Triplet-state mediated super-resolution imaging of fluorescently-labeled gold nanorods. **K. Blythe**, K.A. Willets

3:20 PHYS **212.** Plasmon-enhanced fluorescent protein emission: A new paradigm for improved single-molecule bio-imaging. **J.S. Biteen**

3:55 PHYS **213.** Superstudies of plasmonically mediated emission: Beyond the Gaussian point-spread function. **E.J. Titus**, K.A. Willets

4:15 PHYS **214.** Energy conversion within a single nanocavity structure. **T.W. Odom**

Section H

Colorado Convention Center
Room 607

Design of Materials and Chemical Processes: The Genomic Approach

Gas Separation & Gas Storage: Experiments & Calculations

L. Gagliardi, B. Smit, *Organizers, Presiding*

1:30 PHYS **215.** Experimental and theoretical approach to the study of CO_2 adsorption in an extensive family of metal-organic frameworks. **W.L. Queen**, E.D. Bloch, J.S. Lee, J.D. Howe, J.A. Mason, M.I. Gonzalez, M.R. Hudson, K. Lee, S.J. Teat, J. Neaton, B. Smit, J.R. Long, C.M. Brown

2:00 PHYS **216.** Engineering metal organic framework materials for optimum methane storage. **T. Yildirim**

2:30 PHYS **217.** Computational screening of MOFs for gas separations. **S. Keskin**

3:00 PHYS **218.** Parasitic energy: A potential building block for the prediction of CCS materials. **J. Huck**, L. Joos, R. Mercado, L. Lin, A. Berger, A. Bhown, K.U. Reuter, B. Smit

3:20 Intermission.

3:40 PHYS **221.** Small molecule adsorption in metal organic frameworks with open meal sites. **B. Vlaisavljevich**, R. Mercado, L. Lin, K. Lee, J. Huck, B. Smit

4:00 PHYS **220.** Robust metal-organic frameworks: rational design and gas storage. **D. Feng**, H. Zhou

4:30 PHYS **219.** Gas separations in metal-organic frameworks. T.M. McDonald, E.D. Bloch, Z.R. Herm, J.A. Mason, B.M. Wiers, M.T. Kapelewski, M.I. Gonzalez, J. Oktawiec, G. Barin, D. Gygi, W. Queen, **J.R. Long**

WCC Rising Stars Awards Symposium

Sponsored by WCC, Cosponsored by BIOT, COLL, GEOC, INOR, ORGN, PHYS, PMSE and PROF

ACS Award for Computers in Chemical and Pharmaceutical Research: Symposium in Honor of David A. Case

Sponsored by COMP, Cosponsored by PHYS

Electronic Structure Methods for Highly Polarizable Systems

Excitons

Sponsored by COMP, Cosponsored by PHYS

Quantum Chemistry

Methodology

Sponsored by COMP, Cosponsored by PHYS

MONDAY EVENING

Section A

Colorado Convention Center
Halls C/D

Sci-Mix

E.L. Sibert, Organizer

8:00 - 10:00

32, 43, 88, 113, 175, 196, 205, 212. See previous listings.

PHYS**222.** Discovery and Innovation of inorganic graphene analogs by computations. **Z. Chen**

286, 316, 324, 376, 405, 409, 463, 483, 519, 532, 557, 580. See subsequent listings.

TUESDAY MORNING

Section B

Colorado Convention Center
Room 607

PHYS Award Symposium

E. L. Sibert, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 PHYS **223. Award Address** (Peter Debye Award in Physical Chemistry sponsored by E. I. du Pont de Nemours & Co.). Single molecule biophysical chemistry: Life at the single molecule level. **S. Xie**

TECHNICAL PROGRAM

8:35 PHYS **224. Award Address** (Joel Henry Hildebrand Award in the Theoretical and Experimental Chemistry of Liquids sponsored by ExxonMobil Research and Engineering). Dynamics of polar solvation. **M. Maroncelli**

9:05 PHYS **225. Award Address** (Francis P. Garvan–John M. Olin Medal sponsored by the Francis P. Garvan–John M. Olin Medal Endowment). Theoretical development and modeling across the periodic table: Toward accurate and inaccurate energetic prediction. **A.K. Wilson**

9:35 PHYS **226. Award Address** (ACS Award in Theoretical Chemistry sponsored by the ACS). Fragmentation: A route to accurate calculations on large molecular systems. **M.S. Gordon**

10:05 PHYS **227. Address Award** (ACS Award in Pure Chemistry sponsored by the Alpha Chi Sigma Fraternity and the Alpha Chi Sigma Educational Foundation). Bringing bioelectricity to light. **A.E. Cohen**

10:35 Intermission.

10:55 PHYS **228. Award Address** (Ahmed Zewail Award in Ultrafast Science and Technology sponsored by the Ahmed Zewail Endowment Fund established by Newport). Multidimensional electronic and vibrational spectroscopy of molecules using attosecond X-ray pulses and quantum light. **S. Mukamel**

11:25 PHYS **229. Award Address** (E. Bright Wilson Award in Spectroscopy sponsored by the ACS Division of Physical Chemistry). Mapping atomic motions with ultrabright electrons: The chemists' gedanken experiment enters the lab frame. **R. Miller**

ACS Award for Computers in Chemical and Pharmaceutical Research: Symposium in Honor of David A. Case

Sponsored by COMP, Cosponsored by PHYS

TUESDAY AFTERNOON

Section A

Colorado Convention Center

Room 501

Atmospheric Chemistry: Transformations of Matter in the Troposphere

Organic Aerosol

D. Cziczo, M. Freedman, *Organizers*

N. Riemer, J. Surratt, *Presiding*

1:30 PHYS **230.** Sources, properties, aging, and anthropogenic influences on OA and SOA over the Southeast US and the Amazon during SOAS, DC3, SEAC4RS, and GoAmazon. **J.L. Jimenez**

2:10 PHYS **231.** Isoprene-derived SOA formation across mulitiple sites in the southeastern U.S.: Implications for air quality and human health. **J.D. Surratt, S. Budisulistiorini, W. Rattanavaraha,** Y. Lin, X. Li, M. Arashiro, A. Gold, Z. Zhang, S. Shaw, P. Croteau, M. Canagaratna, E. Knipping, S. Bairai, R.L. Tanner, M. Riva, T.P. Riedel, K. Chu

2:35 PHYS **232.** Gas-phase vs. aqueous-phase aging of secondary organic aerosol. **J.H. Kroll**, J. Hunter, K. Daumit, A.J. Carrasquillo

3:00 PHYS **233.** Influence of particle phase and viscosity on the heterogeneous OH-initiated oxidation of organic aerosol. **J.F. Davies**, K.R. Wilson

3:20 Intermission.

3:35 PHYS **234.** On the surface chemistry of secondary organic aerosol particles. **F. Geiger**

4:00 PHYS **235.** LIfetime of photosensizer triplet states in model troposheric aerosol. **E. Woods**, M. Barthold, J. Wan, M. Tigue

4:20 PHYS **236.** Organic aerosol composition and aging in the atmosphere: How to fit laboratory experiments, field data, and modeling together. **C.L. Heald**, Q. Chen

4:45 PHYS **237.** On the connection of organic aerosol ageing to viscosity. **F.A. Houle**, W. Hinsberg, K.R. Wilson

5:05 PHYS **238.** Oxidation flow reactors for the study of atmospheric chemistry systematically examined by modeling. **Z. Peng**, D.A. Day, A.M. Ortega, W. Hu, B.B. Palm, R. Li, K. Tsigaridis, J.A. de Gouw, W.H. Brune, J.L. Jimenez

Section B

Colorado Convention Center

Room 607

Ahmed Zewail Prize in Molecular Sciences

R. van Daalen, *Organizer*

D. C. Clary, *Presiding*

2:00 Introductory Remarks.

2:10 PHYS **239.** Chemical adventures using the unified principles of homogeneous and heterogeneous catalysis. **J.M. Thomas**

3:00 PHYS **240.** 4D electron microscopy: Developments and applications. **A.H. Zewail**

3:50 Intermission.

4:10 PHYS **241.** Catalytic chemistry: a subtle blend of voids and single sites. **M. Che**

4:45 PHYS **242.** Solution metallic catalysis on the nanoscale. **M.A. El-Sayed**

5:20 PHYS **243.** From single sites to nanostructured assemblies: Designing tools for high-precision chemical transformations. **T. Maschmeyer**

5:55 Concluding Remarks.

Section C

Colorado Convention Center

Room 503

Physical Electrochemistry of Electrocatalytic Processes

Electrocatalysis of O2

A. Co, D. A. Scherson, *Organizers*

J. M. Feliu, U. S. Ozkan, *Presiding*

1:30 Introductory Remarks.

1:35 PHYS **244.** Bi adatoms at the surface of Pt single crystals. **J.M. Feliu**

2:15 PHYS **245.** Impurity effects on the oxygen reduction reaction (ORR). A. Jacob Jebaraj, N. Georgescu, **D. Scherson**

2:35 PHYS **246.** Effect of nitrogen functionalization on stability and performance of carbon-supported PtRu electrocatalysts in acid and alkaline media. **S. Pylypenko**, P. Joghee, K. Wood, A.R. Corpuz, J. Christ, G. Bender, R. O'Hayre

2:55 PHYS **247.** Galvanic displacement of Pt on nanoporous copper: An alternative synthetic route for obtaining robust and reliable oxygen reduction and alcohol oxidation catalysts. E. Coleman, H. Choi, K. Walz, **A. Co**

3:15 Intermission.

3:35 PHYS **248.** Tuning of perovskite oxides electrocatalytic activity for water oxidation and oxygen reduction. **K.J. Stevenson**, T. Mefford, W. Hardin, K.P. Johnston

4:15 PHYS **249.** Development of oxide-based materials for oxygen reduction and oxygen evolution reactions. **P.B. Atanassov**, A. Serov, I. Matanovic, A. Roy, N. Andersen

4:55 PHYS **250.** Theoretical investigation of water oxidation processes on small pure and Ca-doped MnO_2 complexes. **K. Weerawardene**, C.M. Aikens

Section D

Colorado Convention Center

Room 504

Role of Membrane in Amyloid-Formation & the Pathogenicity of Amyloid Disease

Prions and Beyond

Cosponsored by COLL and COMP

J. C. Lee, J. E. Straub, *Organizers*

D. P. Raleigh, *Presiding*

1:30 PHYS **251.** Surprising new structure for the cellular prion protein, and how this structure may influence membrane processes and prion disease. **G.L. Millhauser**

2:10 PHYS **252.** Influence of induced polarization on amyloid peptide misfolding in different solution environment. **J.A. Lemkul**

2:50 PHYS **253.** Role of cofactor molecules in encoding mammalian prion infectivity. **S. Supattapone**

3:30 Intermission.

3:50 PHYS **254.** Curli: Functional bacterial amyloid fibers. **C. Reichhardt**, D.M. Rice, J. Uang, L. Cegelski

4:10 PHYS **255.** Membrane microdomain composition may temporally modulate or determine protein function. H. Jang, A.L. Gillman, J. Lee, S. Ramachandran, F. Teran Arce, B. Kagan, R. Lal, **R. Nussinov**

4:50 PHYS **256.** What can theory and computations teach us about protein aggregation? **D. Thirumalai**

5:30 Closing Remarks.

Section F

Colorado Convention Center

Room 505

Modeling Excited States of Complex Systems

Electronic Structure

Cosponsored by COMP

B. G. Levine, S. A. Varganov, *Organizers*

K. A. Lopata, *Presiding*

1:30 PHYS **257.** Excited electronic states: Solvent effects and dynamics. **M.S. Gordon**, F. Zahariev, K. Keipert, Y. Harabuchi

2:10 PHYS **258.** Relativistic variational density functional theory of electronic excited states. **F.A. Evangelista**, W.D. Derricotte, P. Verma

2:50 PHYS **259.** Photoelectron spectra and photoelectron angular distributions from ab initio electronic structure methods. **S. Gozem**, A. Krylov

3:10 Intermission.

3:30 PHYS **260.** Potential energy surfaces for excited electronic states. **R. Dawes**

4:10 PHYS **261.** New developments in complete active space spin-flip methods for ground and excited states of large molecules with strong electron correlations. N. Mayhall, **M.P. Head-Gordon**

4:50 PHYS **262.** Time-resolved spectroscopy: A challenge for time-dependent density functional theory. **K. Luo**, J.I. Fuks, E. Sandoval, N. Maitra

5:10 PHYS **263.** Capturing geometric phase effects by mixed quantum-classical methods. **R. Gherib**, I.G. Ryabinkin, A.F. Izmaylov

ACS Award for Computers in Chemical and Pharmaceutical Research: Symposium in Honor of David A. Case

Sponsored by COMP, Cosponsored by PHYS

Quantum Chemistry

Applications

Sponsored by COMP, Cosponsored by PHYS

WEDNESDAY MORNING

Section A

Colorado Convention Center

Room 501

Atmospheric Chemistry: Transformations of Matter in the Troposphere

Heterogeneous Chemistry, Sea Spray, Mineral Dust, and Black Carbon

D. Cziczo, M. Freedman, *Organizers*

J. G. Navea, E. Woods, *Presiding*

8:00 PHYS **264.** Water uptake and heterogeneous chemistry of model and authentic sea spray aerosol particles. **V.H. Grassian**

8:40 PHYS **265.** Transformations of nitrogen oxides at the troposphere-soil interface. **J.D. Raff**

9:05 PHYS **266.** Optical properties of mineral dust components and mixtures. **D. Veghte**, J. Moore, L. Jensen, M. Freedman

9:25 Intermission.

9:40 PHYS **267.** Determination of near UV absorption crossSections of surface-adsorbed H_2O and heterogeneous nucleation of H_2O on fused silica surfaces. **L. Zhu**

10:00 PHYS **268.** From the particle scale to the global scale: Quantifying black carbon climate impacts using a stochastic particle-resolved model. **N. Riemer**

10:25 PHYS **269.** Comparative photochemistry of nitric acid chemisorbed on different components of tropospheric particulate matter. **J.G. Navea**

10:45 PHYS **270.** Probing the impacts of aerosol sources on cloud microphysics and precipitation through in situ measurements of aerosol chemical mixing state. **K.A. Prather**

Section B

Colorado Convention Center

Room 502

Carbon in the Galaxy: The Formation of Complex Organics from the Outflow of Carbon Stars & Their Evolution

Organic Molecules in Dense Interstellar Clouds

L. J. Allamandola, T. J. Lee, *Organizers*

S. N. Milam, *Presiding*

8:00 PHYS **271.** Organic molecules in ices and their release Into the gas phase. **E. Fayolle**, K. Oberg, R.T. Garrod, E.F. van Dishoeck, M. Rajappan, M. Bertin, C. Romanzin, J. Fillion

8:35 PHYS **272.** Ice chemistry in interstellar dense molecular clouds, protostellar disks, and comet. **S.A. Sandford**

9:10 PHYS **273.** Like a fly and the fire — polycyclic aromatic hydrocarbons (PAHs) in icy environments: A historical perspective. **M.S. Gudipati**

9:45 Intermission.

10:15 PHYS **274.** Theoretical studies of interstellar ice chemistry involving polycyclic aromatic hydrocarbons and other compounds. **D.E. Woon**

10:50 PHYS **275.** Formation of aromatic heterocycles from the UV-photoirradiation of aromatic hydrocarbons in ices. **C.K. Materese**, M. Nuevo, S.A. Sandford

11:15 PHYS **276.** Infrared spectroscopic properties of polycyclic aromatic nitrogen heterocycles (PANHs): The acridine series. **A.L. Mattioda**, J. Bregman, C. Bauschlicher, A. Ricca, D. Hudgins, L.J. Allamandola

Section C

Colorado Convention Center

Room 503

Computational Chemical Dynamics: Advancing our Understanding of Chemical Processes in Gas-Phase, Biomolecular & Condensed-Phase Systems: A Symposium in Honor of Donald Truhlar

Properties and Processes in Solvated Systems

Cosponsored by COMP

J. Gao, B. C. Garrett, *Organizers*

B. Mennucci, *Organizer, Presiding*

8:00 PHYS **277.** 25 years of SM*x* models: Quantum and classical continuum solvation. **C.J. Cramer**, D.G. Truhlar

8:30 PHYS **278.** Protein aggregation, collapse, and disorder: Model systems. **B.M. Pettitt**, D. Karandur

9:00 PHYS **279.** BioEFP: Effective fragment potential method for biological systems. **L.V. Slipchenko**

9:20 PHYS **280.** Role of solvent structure on the rate of ion-pairing. **M.D. Baer,** C.J. Mundy, G.K. Schenter

9:40 Intermission.

10:00 PHYS **281.** Quantum-classical path integral: A rigorous methodology. **N. Makri**

10:30 PHYS **282.** Structure, properties, excited states and reactivity of complex systems in solution: Putting together the pieces. **G. Scalmani**, M.J. Frisch

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11:00 PHYS **283.** How reliable are calculations of absorption spectra of solvated molecules with CC theory and PCM? **M. Caricato**

11:20 PHYS **284.** Continuum solvation calculations of solvatochromic shifts: Recent advances and perspectives. **A.V. Marenich**, C.J. Cramer, D.G. Truhlar, G. Scalmani, M.J. Frisch

Section D

Colorado Convention Center
Room 504

Physical Electrochemistry of Electrocatalytic Processes

Electrochemical Formation of Semiconductors

D. A. Scherson, *Organizer*
A. Co, *Organizer, Presiding*
S. Maldonado, *Presiding*

8:00 PHYS **285.** Investigations into the electrochemical formation of germanene. **J.L. Stickney**, M. Ledina, J. Jung

8:40 PHYS **286.** Electrocatalytic crystallization of covalent inorganic semiconductors. **S. Maldonado**

Section D

Colorado Convention Center
Room 504

Physical Electrochemistry of Electrocatalytic Processes

Electrocatalysis of H2O and H2

A. Co, *Organizer*
D. A. Scherson, *Organizer, Presiding*
S. Maldonado, *Presiding*

10:00 PHYS **287.** Withdrawn.

10:40 PHYS **288.** Graphene oxide-promoted hydrogen and oxygen evolution. **N. Wu**

11:00 PHYS **289.** Electrocatalytic hydrogen production performed by model protein scaffolds. **H.S. Shafaat**, J.W. Slater, A.C. Manesis, S.L. Cirino, H.A. Monaco

11:20 PHYS **290.** Electrocatalytic water oxidation by iminium ions. **K. Glusac**

11:40 PHYS **291.** Electrocatalytic water oxidation on model cobalt oxide dimer and cubane complexes. **A. Fernando**, C.M. Aikens

Section E

Colorado Convention Center
Room 507

Modeling Complex Biomolecules: From Structure to Dynamics & Function

Modeling of Macromolecular Structure and Function

Cosponsored by COMP

A. E. Garcia, G. Hummer, *Organizers*
M. Chu-Moyer, *Presiding*

8:00 PHYS **292.** Integrative structural biology. **A. Sali**

8:35 PHYS **293.** Unveiling the function of macromolecular assemblies using integrative dynamic modeling. **M. Dal Peraro**

9:10 PHYS **294.** Introducing molecular flexibility in Monte Carlo simulations of many-protein systems. V. Prytkova, M. Heyden, J.A. Freites, **D.J. Tobias**

9:45 PHYS **295.** Building toy models of proteins using co-evolutionary information. **R.R. Cheng**, M. Raghunathan, J.N. Onuchic

10:20 PHYS **296.** Atomistic and coarse-grained simulations of histones, Nuclesomes and DNA. **G. Papoian**, D. Winogradoff, H. Zhao, I. Echeverria, Y. Dalal

10:55 PHYS **297.** Relative resolution: A hybrid strategy for molecular modeling. **A. Chaimovich**, K. Kremer, C. Peter

11:30 PHYS **298.** Beyond Hofmeister: Interactions between ions and proteins in water. **P. Jungwirth**

Section F

Colorado Convention Center
Room 505

Modeling Excited States of Complex Systems

Electronic Structure

Cosponsored by COMP

B. G. Levine, S. A. Varganov, *Organizers*
F. A. Evangelista, *Presiding*

8:00 PHYS **299.** Understanding photochemistry and photoelectron spectra with highly correlated electronic structure methods based on coupled-cluster theory. **P. Piecuch**, J.A. Hansen, N.P. Bauman

8:40 PHYS **300.** Electronic structure methods for high-energy excited states. **X. Li, P. Lestrange**, D.B. Williams-Young, J.J. Goings

9:20 PHYS **301.** Linear response time-dependent complex generalized Hartree-Fock for frustrated spin systems. **J.J. Goings**, D.B. Williams-Young, F. Ding, M.J. Frisch, X. Li

9:40 PHYS **302.** Graphical processing unit acceleration of "two-step" complete active space configuration interaction (CASCI) methods. **B. Fales**, B. Levine

10:00 Intermission.

10:20 PHYS **303.** Above-ionization excited states with non-Hermitian time-dependent density functional theory. **K.A. Lopata**

11:00 PHYS **304.** Caution when using real-time TDDFT: Two-electron Rabi oscillations and peak-shifting. **C. Isborn**, M. Provorse, B. Habenicht

11:40 PHYS **305.** Charge transfer and other non-linear electron dynamics: the problem of detuning in TDDFT. **J.I. Fuks**, K. Luo, E. Sandoval, N. Maitra

12:00 PHYS **306.** Experimental perspective on the electronic structure and dynamics of higher-lying electronic states. **C.G. Elles**, C.L. Ward, A.L. Houk, T.J. Quincy

Section G

Colorado Convention Center
Room 506

Probing Nano-Plasmonic Phenomena at the Single Molecule, Single Electron, & Single Photon Level

S. Link, K. A. Willets, *Organizers*
D. J. Masiello, *Organizer, Presiding*
J. S. Biteen, *Presiding*

8:30 PHYS **307.** Probing the mechanistic of charge transfer from optically excited plasmonic metal nanoparticles to adsorbates leading to chemical transformations. **S. Linic**

9:05 PHYS **308.** Electrochemistry on plasmonic nanoparticle electrodes. **A. Wilson**, K.A. Willets

9:25 PHYS **309.** Collective behavior in the solid-state elucidated by plasmonic spectroscopy. **P.K. Jain**

10:00 PHYS **310.** Single-particle absorption spectroscopy of plasmonic nanostructures. **M. Yorulmaz**, S. Nizzero, W. Chang, L. Wang, S. Link

10:20 PHYS **311.** Atomistic simulations of surface-enhanced spectroscopies. **L. Jensen**

10:55 PHYS **312.** Design and optimization of plasmonic crystals for surface enhanced Raman spectroscopy using the finite-difference time-domain method. **R. Petit**, J.M. Montgomery

11:15 PHYS **313.** Electron microscopy and spectroscopy of plasmonic alloys. **E. Ringe**, S.M. Collins, C.J. DeSantis, S.E. Skrabalak, P.A. Midgley

Section H

Colorado Convention Center
Room 607

Design of Materials and Chemical Processes: The Genomic Approach

Catalysis and Materials for Catalysis: Experiments & Calculations

L. Gagliardi, B. Smit, *Organizers, Presiding*

8:00 PHYS **314.** Global energy and emissions reduction potential of new materials development. **C. Tway**, E.G. Rightor, J. Liu, C. Han, M. McAdon, J. Goss, K. Andrews

8:30 PHYS **315.** Thermodynamics and kinetics of elementary reaction steps on late transition metal catalysts, and using them to search for better catalysts. **C.T. Campbell**

9:00 PHYS **316.** Tailored mesoscale gold alloy materials for energy- and resource-efficient catalysis. **M.L. Personick**, B. Zugic, C.M. Friend

9:20 Intermission.

9:40 PHYS **317.** Impact of location and concentration of acid sites in zeolites for acid catalyzed reactions in condensed phase. **J.A. Lercher**

10:10 PHYS **318.** Harnessing polymorphism for the rational design of new nanoporous materials: assessing mechanical, thermal stability, and experimental feasibility. F. Trousselet, L. Bouessel du Bourg, **F. Coudert**

10:30 PHYS **319.** Material descriptor of oxygen vacancy formation energies in wide band gap oxides. **A. Deml, A. Holder**, R. O'Hayre, C. Musgrave, V. Stevanovic

Quantum Chemistry

Quantum Dynamics & Monte Carlo Simulations

Sponsored by COMP, Cosponsored by PHYS

Computational Chemistry in the Undergraduate Curriculum: What is Working and How Do We Assess It?

Sponsored by CHED, Cosponsored by PHYS

WEDNESDAY AFTERNOON

Section A

Colorado Convention Center
Room 501

Atmospheric Chemistry: Transformations of Matter in the Troposphere

Gas Phase Atmospheric Chemistry

D. Cziczo, M. Freedman, *Organizers*
K. T. Kuwata, C. Womack, *Presiding*

1:30 PHYS **320.** Photochemical and multiphase sources of isoprene derived secondary organic aerosol. **J.A. Thornton**, B. Lee, C. Gaston, E. D'Ambro, F. Lopez-Hilfiker, J. Liu, J. Shilling, C. Mohr, T.P. Riedel, Z. Zhang, A. Gold, J. Surratt, W. Hu, D. Day, P. Campuzano-Jost, B. Palm, J.L. Jimenez, N. Ng, L. Xu

2:10 PHYS **321.** Atmospheric chemistry in the southeast U.S. **J. de Gouw, C. Warneke, M. Trainer**

2:35 PHYS **322.** Uncertainties in global atmospheric composition due to uncertainties in inorganic and organic rate constants. **M.J. Evans**, B. Newsome

3:00 Intermission.

3:15 PHYS **323.** Relative abundances of gas phase amines and ammonia in the ambient atmosphere. **J. Murphy**, T.C. Vandenboer, G. Wentworth, M. Markovic, P. Gregoire

3:40 PHYS **324.** Probing the composition of atmospheric interfaces through measurement of trace gas reactive uptake and product yields. **T.H. Bertram**, O.S. Ryder, N. Campbell

4:05 PHYS **325.** Heterogeneous chemistry of nitrogen oxides: Results from recent field studies. **S.S. Brown**

Section B

Colorado Convention Center
Room 502

Carbon in the Galaxy: The Formation of Complex Organics from the Outflow of Carbon Stars & Their Evolution

Organic Molecules in Dense Clouds and Star and Planet Forming Regions

L. J. Allamandola, T. J. Lee, *Organizers*
E. Peeters, *Presiding*

1:30 PHYS **326.** Complex organic molecules in star-forming regions: Sweet results from ALMA. **E.F. van Dishoeck**

2:05 PHYS **327.** Polycyclic aromatic hydrocarbons as catalysts for interstellar molecular hydrogen formation. **L. Hornekaer**

2:40 PHYS **328.** Modeling grain surface chemistry in dense molecular clouds. **H. Cuppen**, L. Karssemeijer

3:15 Intermission.

3:45 PHYS **329.** Formation of complex organic molecules in protoplanetary disks. **T. Millar**

4:20 PHYS **330.** Time-domain terahertz spectroscopy of polycyclic aromatic hydrocarbons. **M.A. Allodi**, P. Carroll, S. Ioppolo, B.A. McGuire, G.A. Blake

4:45 PHYS **331.** Tackling the theoretical anharmonic infrared spectra of polycyclic aromatic hydrocarbons. **C. Mackie**, A. Candian, X. Huang, T.J. Lee, A. Tielens

Section C

Colorado Convention Center
Room 503

Computational Chemical Dynamics: Advancing our Understanding of Chemical Processes in Gas-Phase, Biomolecular & Condensed-Phase Systems: A Symposium in Honor of Donald Truhlar

Nonadiabatic Dynamics

Cosponsored by COMP

J. Gao, B. C. Garrett, B. Mennucci, *Organizers*
X. Li, *Presiding*

1:30 PHYS **332.** Beyond the Born-Oppenheimer approximation: Construction of accurate multicomponent wave function using explicitly-correlated and projection-based methods. **A. Chakraborty**

2:00 PHYS **333.** Directly correlating electronic and vibrational motions with multidimensional coherent spectroscopies. **M.H. Khalil**

2:30 PHYS **334.** Approximate time-dependent diabatic states computed using a measure driven tessallation technique for use in on-the-fly quantum dynamics methods. **S.S. Iyengar**

3:00 PHYS **335.** Avoiding the Born-Oppenheimer separation between electrons and protons in wavefunction and density functional theory calculations. **S. Hammes-Schiffer**

3:20 Intermission.

3:40 PHYS **336.** Surface hopping and spectroscopy. **J.E. Subotnik, A.S. Petit**

4:10 PHYS **337.** Novel approaches to nonadiabatic molecular dynamics. **O.V. Prezhdo**

4:40 PHYS **338.** Time-dependent electronic and nuclear potentials that exactly capture electron-ion coupling. **N. Maitra**

5:00 PHYS **339.** Time-derivative coupling scheme for accurate electronic state transition probabilities in nonadiabatic molecular dynamics. **G. Meek, B. Levine**

Section D

Colorado Convention Center
Room 504

Physical Electrochemistry of Electrocatalytic Processes

In Situ Characterization

A. Co, D. A. Scherson, *Organizers*
C. L. Korzeniewski, D. Scherson, *Presiding*

1:30 PHYS **340.** Vibrational spectroscopy and 2D correlation analysis applied to probe structure in ionomer membrane materials. **C.L. Korzeniewski**, T. Zhang

2:10 PHYS **341.** Operando X-ray studies of electrocatalysis for energy conversion. **D. Friebel**

2:50 Intermission.

3:10 PHYS **342.** Irrelevance of CO poisoning in methanol oxidation on PtRu electrocatalysts: A re-visit of the bifunctional mechanism. **Y. Tong**

3:50 PHYS **343.** In operando optical studies of solid oxide fuel cells operating with biogas: heterogeneous surface chemistry vs. electrochemical oxidation. **R.A. Walker**, J. Kirtley, J. Owrutsky, D.A. Steinhurst

Section E

Colorado Convention Center
Room 507

Modeling Complex Biomolecules: From Structure to Dynamics & Function

Folding and Aggregation

Cosponsored by COMP

A. E. Garcia, G. Hummer, *Organizers*
R. Nussinov, *Presiding*

1:30 PHYS **344.** Accurate atomistic simulations of intrinsically disordered proteins. **R.B. Best**, W. Zheng, J. Mittal

2:05 PHYS **345.** Regulation and aggregation of intrinsically disordered peptides. **J.E. Shea**

2:40 PHYS **346.** Multiscale and multiresolution simulations of aggregation in polyglutamine containing block copolymers. **R.V. Pappu**

3:15 PHYS **347.** Spontaneous formation of oligomers and fibrils in large scale molecular dynamics simulations of peptides. **C.K. Hall**, M. Cheon, D.C. Latshaw, I. Chang

3:50 PHYS **348.** Alzheimer's disease: Aggregation of WT and protective Aβ peptides, free or in the presence of inhibitors and under shear flow by all-atom and coarse-grained simulations. J. Nasica-Labouze, P. Nguyen, B. Tarus, F. Sterpone, M. Chiricotto, O. Berthoumieu, P. Faller, A. Doig, S. Melchionna, **P. Derreumaux**

4:25 PHYS **349.** Protein folding and recognition in the cell — an in silico approach. **M.S. Cheung**

Section F

Colorado Convention Center
Room 505

Modeling Excited States of Complex Systems

Electronic Structure

Cosponsored by COMP

B. G. Levine, S. A. Varganov, *Organizers*
J. I. Fuks, *Presiding*

1:30 PHYS **350.** Modeling excited states with multireference quantum chemical methods. **L. Gagliardi**, R. Carlson, D.G. Truhlar, K. Vogiatzis

2:10 PHYS **351.** Single- and multireference quantum chemical methods for nonadiabatic molecular dynamics. **H. Lischka**, M. Barbatti

2:50 PHYS **352.** Low valency in rare earth diatomics. **G. Schoendorff**, A.K. Wilson

3:10 Intermission.

3:30 PHYS **353.** Active space decomposition. **T. Shiozaki**

4:10 PHYS **354.** Representation of adiabatic potential energy surfaces coupled by conical intersections and their use in describing nonadiabatic processes. **D.R. Yarkony**, X. Zhu, J. Dillon, C. Malbon

4:50 PHYS **355.** Electronic structure of diatomic rare earth species. **C. South**, G. Schoendorff, A.K. Wilson

5:10 PHYS **356.** Size-inconsistency effects in transition moments for quasi-degenerate variational perturbation theory and averaged coupled-pair functional theory. **K. Dwelle**, R.J. Cave

Section G

Colorado Convention Center
Room 506

Probing Nano-Plasmonic Phenomena at the Single Molecule, Single Electron, & Single Photon Level

D. J. Masiello, K. A. Willets, *Organizers*
S. Link, *Organizer, Presiding*
R. R. Frontiera, *Presiding*

1:30 PHYS **357.** Raman scattering in time and frequency on a nantenna and its molecular load. **V.A. Apkarian**

2:05 PHYS **358.** Photoluminescence quantum yield of strongly coupled gold plasmonic molecule. **D. Huang**, C. Byers, L. Wang, A. Hoggard, B. Hoener, W. Chang, C.F. Landes, S. Link

2:25 PHYS **359.** Plasmons and intraband transitions. **P. Guyot-Sionnest**

3:00 PHYS **360.** Electron dynamics in gold nanoparticles under strong laser fields. **J. Powell**, A. Rudenko, C.M. Sorensen

3:20 PHYS **361.** Controlling and probing spatially dependent plasmonic field effect and charge transfer dynamics using single quantum dot modified AFM tips. **T. Lian**

3:55 PHYS **362.** Strong coupling between individual plasmonic metal nanostructures and quantum dots. **M. Pelton**

Section H

Colorado Convention Center
Room 607

Design of Materials and Chemical Processes: The Genomic Approach

Catalysis and Materials for Catalysis: Experiments & Calculations

L. Gagliardi, B. Smit, *Organizers, Presiding*

1:30 PHYS **363.** Computational design of highly selective transition metal catalysts encapsulated by metal-organic frameworks for butane oxidation to 1-butanol. S. Dix, **R. Getman**

2:00 PHYS **364.** Metal–organic frameworks as highly functional catalytic arrays. **O.K. Farha**

2:30 PHYS **365.** Metal-organic framework materials for solar energy applications. **W. Lin**

3:00 PHYS **366.** Performance descriptors for the design of solar energy materials. **A. Walsh**

3:20 Intermission.

3:40 PHYS **367.** Withdrawn.

4:10 PHYS **368.** In silico prediction of emergent catalysts. **D.G. Vlachos**

4:40 PHYS **369.** Impact of MOF topology upon solvent organization, dynamics, and solution phase stability. **A.E. Clark**, W. Queen, X. Yang

Quantum Chemistry

Applications

Sponsored by COMP; Cosponsored by PHYS

Computational Chemistry in the Undergraduate Curriculum: What is Working and How Do We Assess It?

Sponsored by CHED, Cosponsored by PHYS

WEDNESDAY EVENING

Section G

Colorado Convention Center
Hall C

Physical Chemistry Poster Session

E. L. Sibert, *Organizer*

6:30 - 9:30

PHYS **370.** Quantum numerical control for particles at matter surface. **Q. Wang**

PHYS **371.** Scaled quantum mechanical scale factors for vibrational calculations using alternate polarized and augmented basis sets with the B3LYP density functional calculation model. **W.B. Collier**, C.R. Legler, N.R. Brown, R.A. Dunbar, M.D. Harness, K. Nguyen, O.O. Oyewole

PHYS **372.** Calculating the infrared spectra of the eigenion using anharmonic vibrational theory. **B. Thomsen**, K. Yagi, Y. Sugita

PHYS **373.** Theory and efficient computation of vibrational difference spectra. **T. Joutsuka**, A. Morita

PHYS **374.** Diabatic states of a delta function model. **T. Middlemas**, R.J. Cave

PHYS **375.** Lifetimes of vibrational states of XY ions (X=Li, Na; Y=Be, Mg) calculated using the CCSDT potential energy and dipole moment curves. **D.K. Barnes**, D. Fedorov, S.A. Varganov

PHYS **376.** Probing vibrational-electronic interactions of a sensitizing dye at the TiO_2 surface using heterodyne detected doubly resonant sum-frequency generation spectroscopy. **C.C. Rich**, M. Mattson, A.T. Krummel

PHYS **377.** Time-resolved infrared spectrocopy of [FeFe]-hydrogenase model compounds. **R. Meyer**, A. Zhandosova, E.J. Heilweil, C.J. Stromberg

PHYS **378.** Statistically weight averaged vibrational spectrum over molecular fragments for studying the amide I vibration of sphingomyelin bilayer. **K. Yagi**, P. Li, K. Shirota, T. Kobayashi, Y. Sugita

PHYS **379.** Structural and energetic properties of lanthanide trihalides via DFT and ab initio approaches. **R.J. Weber**, G. Schoendorff, A.K. Wilson

PHYS **380.** Ferrocene - ozone reactions: A matrix-isolation and DFT study. **R.W. Kugel**, L. Pinelo, B.S. Ault

PHYS **381.** Mechanistic investigations of siderophore complexation via density functional theory. M.F. Skaro, M.S. Hughey, **J.L. Sonnenberg**

PHYS **382.** Theoretical phase diagram for Fe_3O_4 (111) surfaces using a DFT + *U*(Fe) approach. **X. Huang**, S. Ramadugu, S.E. Mason

PHYS **383.** DFT and ab initio composite method investigations of oxygen fluorides and related hydrides. **Z.H. Alsunaidi**, A.K. Wilson

PHYS **384.** Effect of choline chloride on secondary structure conformation for two small peptides: A circular dichroism study. **M. Giordano**, M. Vermeuel, P. Gupta, D. Léon, M.R. Bunagan

PHYS **385.** Deconstructing solvent organization in confined nanoporous materials: Implications for separation. **C. Wang**, A.E. Clark

PHYS **386.** Crystallographic characterization of three furan-substituted benzimidazoles and calculation of C-H/π and π/π interaction energies. D.K. Geiger, **C. Geiger**

PHYS **387.** Quantum electronic kinetics from an atom-centered bath model. **T. Nguyen**, S. Blau, T. Markovich, J. Parkhill

PHYS **388.** Impact of resonance stabilization on H-atom shift isomerization and ring closure reactions. **K. Wang**, S. Villano, A.M. Dean

PHYS **389.** Sodium dodecyl sulfate monomers induce XAO peptide polyproline II to ⊠-helix transition. **Z. Hong,** D. Krishnan Achary, S.A. Asher

PHYS **390.** Multishells vs. gradient-alloyed shells on core quantum dots: Ensemble and single particle optical properties. **P. Bajwa**, F. Gao, B.O. Omogo, C.D. Heyes

PHYS **391.** Physicochemical investigation of ionic liquid mixtures. **M.T. Clough**, J. Gräsvik, P. Hunt, H. Niedermeyer, T. Welton

PHYS **392.** Antibunching in small clusters of quantum dots. **J.Q. Geisenhoff**, K.J. Whitcomb, D. Ryan, M.P. Gelfand, A.K. Van Orden

PHYS **393.** Modification method of natural zeolite by ultrasonic and sodium chloride. **W. Qun**, Y. Zhichao, G. Mingkun, X. He, C. Bin, C. Shuang

PHYS **394.** Understanding nanoconfined hydrogen: first ever quantum free-energy profiles of diffusion of hydrogen and the importance of condensed phase environment in sII clathrate hydrate. **A. Powers**, O. Marsalek, L. Ulivi, M.E. Tuckerman, Z. Bacic

PHYS **395.** Solution dynamics of group 8 metal pentacarbonyls in fluorinated benzene solvents. **C.P. Baryiames,** A. Devanny, C. Laperle

PHYS **396.** Solution dynamics of osmium pentacarbonyl in alcohol solvents. **C. Laperle, A. Devanny**

PHYS **397.** Surface thermodynamics and vesicle formation of decanoic acid. **B. Kessenich**, R. Rapf, R.J. Perkins, V. Vaida

PHYS **398.** Molecular dynamics simulation of ion transports through liquid-liquid interface. **N. Kikkawa**, A. Morita, L. Wang

PHYS **399.** Raman spectroscopic study of graphene photochlorination dynamics in the gas phase and in solution. **K.Z. Rinaldi**, N. Patel, S. Ramrattan, A. Crowther

PHYS **400.** Decomposing hydrogen bond dynamics into multiscale components: Understanding the hydrophobic effect. **T. Zhou**, A.E. Clark

PHYS **401.** Diabatic electronic population matrix and its utilization in simulating electronically excited state dynamics. **J. Park**, Y.M. Rhee

PHYS **402.** Decoherence in nonadiabatic dynamics from an approximate mixed quantum-classical Poisson bracket mapping equation formalism. **H. Kim,** Y.M. Rhee

PHYS **403.** Interdomain dynamics of chloroplast signal recognition particle proteins studied by time-resolved single-molecule FRET. **D. Baucom**, F. Gao, P. Patel, A. Kight, R. Goforth, R. Henry, C. Heyes

PHYS **404.** Molecular dynamics to study energy transduction in the ATP powered translocation of PcrA along DNA. **R.B. Davidson**, M. McCullagh

PHYS **405.** Two-photon spectroscopy, dynamics, and quantum yields of a photochromic molecular switch. **A.L. Houk**, C.G. Elles

PHYS **406.** Global potential energy surfaces of O_4 and dynamics of high-energy O_2-O_2 collision-induced energy transfer and dissociation. **Y. Paukku**, Z. Varga, W. Lin, R. Meana-Pañeda, J. Bender, G.V. Candler, D.G. Truhlar

PHYS **407.** Time-dependent excited-state molecular dynamics of photofragmentation of gas-phase tris(isopropylcyclopentadienyl) lanthanum complexes. **Y. Han**, Q. Meng, P.S. May, M.T. Berry, D. Kilin

PHYS **408.** Structural characterization of supported noble metal nanocatalyst from atomistic simulations. **S. Xiong**, R. Diwan, Y. Li

PHYS **409.** Investigating the efficient conversion of unsaturated acids to olefins over acid catalysts. **T.J. Evans**, J.M. Clark, C. Mukarakate, M.M. Yung, M.R. Nimlos, D.J. Robichaud

PHYS **410.** First principles treatment of photoluminescence linewidth in semiconductors. **D.J. Vogel**, D. Kilin

PHYS **411.** Investigating the best type of gold and platinum bimetallic nanoparticle catalyst for alcohol oxidation reactions. A. Earle, **J.M. Petroski**

PHYS **412.** Laser-assisted nickel liquid phase deposition on surface of dielectrics and semiconductors. **E. Khairullina**, S. Araslanova, S. Safonov

PHYS **413.** Reaction kinetics of NO and NO_2 with pyrite. **H.M. Bevsek**

PHYS **414.** Probing the mechanism of DNA duplex formation in sequences with consecutive versus alternating purines and pyrimidines using stopped flow kinetics experiments. **S.P. Carney**, R. Stratil, A. Deckert

PHYS **415.** Monitoring internal temperatures and kinetics in nitrogen- and oxygen-containing plasma systems. **E. Sutor**, J. Blechle, E.R. Fisher

PHYS **416.** Effects of organic matter on polycyclic aromatic hydrocarbon photolysis kinetics in ice and at ice surfaces. **P. Malley**, T. Kahan

PHYS **417.** Dissociation processes of deprotonated nucleobases: Astrobiological implications. **C.A. Cole**, Z. Wang, T.P. Snow, V.M. Bierbaum

PHYS **418.** Carbon chains in low-mass young stellar objects. **O.H. Wilkins**, D.M. Graninger, K. Oberg

‡ *Cooperative Cosponsorship*

PHYS **419.** Formation mechanism of interstellar PANH cations: Experimental and computational studies. **Z. Wang**, V.M. Bierbaum, C.A. Cole, T.P. Snow

PHYS **420.** Spectral characteristics and lightfastness of fluorescent dyes absorbed on nanoparticles of aerosil dispersed in polymer matrix. **N. Barashkov, S. Sheshenia, T. Sakhno**, V. Granchak, S. Kuchmii, I. Irgibayeva

PHYS **421.** Investigation of two alternative methods of introducing fluorescent dyes in the Au nanoparticles-polysiloxane composites. **N. Barashkov**, I. Irgibayeva, A. Aldongarov, A. Mantel, A. Ishchenko, T. Sakhno

PHYS **422.** Electron and nuclear dynamics in gold and silver nanoparticles. **R.D. Senanayake**, C.M. Aikens

PHYS **423.** Electrochemical fabrication of CdSe/TiO_2 nanotubes for photoelectrocatalytical water splitting application. **F. de Souza Lucas**, M. Sant'anna, R.G. Freitas, L.H. Mascaro, E.C. Pereira

PHYS **424.** Pseudo-direct bandgap transitions in silicon nanocrystals: Effect on optoelectronics and thermoelectrics. V. Singh, Y. Yu, **Q. Sun**, B. Korgel, P. Nagpal

PHYS **425.** Work function modification of various electrodes by deposition of carbon nanotubes via aerosol jet printing. **C.A. Jordan**, R.S. Aga, E. Kreit, C.M. Bartsch, E.M. Heckman, R.S. Aga

PHYS **426.** Temperature dependent solubility of gold nanoparticle suspensions. **J. Powell**, K. Bayliff, E. Herman, C.M. Sorensen

PHYS **427.** Doping of wide-bandgap titanium-dioxide nanotubes: Optical, electronic and magnetic properties. **Y. Ding**, Y. Alivov, V. Singh, P. Nagpal

PHYS **428.** Computational studies of pathways toward the growth of small boron and boron-carbon nanomaterials. **D.C. Woods**, A.L. Dibble, J.R. Rocha

PHYS **429.** Withdrawn.

PHYS **430.** Quantitative SERS-based detection using Ag–Fe3O4 nanocomposites with an internal reference. **P.B. Joshi., Y. Zhou**, T. Ozkaya, P. Zhang

PHYS **431.** Singlet oxygen generation under NIR and light visible light excitation of Chlorin e6 on the surface of fluorescent polymer coated $NaYF_4$ upconversion nanoparticles. **P.B. Joshi**, P. Zhang

PHYS **432.** Novel approach to modeling the absorption spectra and colloidal stability of few- and single-chirality single walled carbon nanotubes. **K.C. Tvrdy**, K. Prescott, K. Rosenthal

PHYS **433.** Withdrawn.

PHYS **434.** Preparation of metal oxide substrates for surface-enhanced Raman scattering. B. Li, C. Weng, C. Yang, C. Lin, **S. Lee**

PHYS **435.** Spin-forbidden transitions between electronic states of the active site of rubredoxin. **G. dePolo**, D. Kaliakin, S.A. Varganov

PHYS **436.** Charge transfer complexes and photochemistry of ozone with n-butylferrocene and ferrocene: A UV-Vis matrix isolation study. **L. Pinelo**, R. Kugel, B.S. Ault

PHYS **437.** Engineering long range ferromagnetism in 2D transition metal dichalcogenide WSe_2. **C. Gil**, A. Pham, S. Li

PHYS **438.** Structure and bonding of metal complexes containing possible hepatitis C inhibitors. **R.M. Drazenovic**, D.N. Ward, P.J. Smith, J.L. Sonnenberg

PHYS **439.** Interaction of niobium-containing chloride melts with niobium metal. M.V. Chernyshov, **I.B. Polovov**, V.A. Volkovich, O.I. Rebrin

PHYS **440.** Organic nanowire waveguide exciton-polariton nanolaser and its photonic application. **Q. Liao**

PHYS **441.** Triplet states of pyrazine. **R. Bendiak**, R.J. Cave

PHYS **442.** Effect of reaction environment on atmospheric photochemistry of pyruvic acid. **A.E. Reed Harris**, B. Ervens, R.K. Shoemaker, J.A. Kroll, R.J. Rapf, E.C. Griffith, A. Monod, J. Doussin, V. Vaida

PHYS **443.** Kirkwood-Buff derived force field for esters. **G. Pallewela**, P.E. Smith

PHYS **444.** Stabilization of a Cl—Cl– anion pair in the gas phase: Ab initio microsolvation study. **A.S. Ivanov, G. Frenking**, A.I. Boldyrev

PHYS **445.** Detecting organic nitrates using thermal dissociation cavity ringdown spectrometry. **N. Keehan**, B. Ayres, J.L. Fry

PHYS **446.** Rotational and hyperfine analysis of the E2$\Pi_{1/2}$ state of TaO. **T.D. Varberg**, C.R. Christopher, S.Y. Lee, F.B. Gwandu, A.J. Matsumoto, B.J. Knurr, T.K. Mahle, Z.W. Morrow

PHYS **447.** Metal-mediated proton transfer in maleic acid and implications for enzyme catalysis. **M.T. Ruggiero**, T.M. Korter

PHYS **448.** Combined photoelectron spectroscopy and ab initio studies of pure, carbon-doped, and transition-metal-doped boron clusters. **I.A. Popov**, W. Li, Z.A. Piazza, R. Pal, V.F. Popov, K.V. Bozhenko, I.Černušák, X.C. Zeng, A.I. Boldyrev, L. Wang

PHYS **449.** Raman spectra of EDAB and Its analogs in various solvents. **S. Farmer, M.L. Fetterolf**, G. Rowe

PHYS **450.** QM/MM simulations reveal the involvement of excimers in the photophysics of adenine based oligonucleotides. **V.A. Spata**, S. Matsika

PHYS **451.** TiO_2 mediated photooxidation of squalene: A kinetic and mechanistic study. **M.L. Kaak**, J.A. Ganske

PHYS **452.** Is ketene an intermediate in the addition of imines to azlactone to form a β-lactam? **C. Kordes**, P. Willoughby, J. Scanlon

PHYS **453.** Aerosol formation initiated by nucleation of radical- water complexes. **E. Burrell**, S. Kumbhani, R.B. Shirts, J.C. Hansen, L. Hansen

PHYS **454.** Drinking water disinfection by a low-voltage pulsed electric field device. P. Hung, **Y. LI,** O. LEE, K. LAM, S. Kwan, J. Kwan, K.L. Yeung

PHYS **455.** Experimental and computational investigation of the dissociation pathways of first generation protonated nitrile-terminated PPI dendrimer. **W.D. Price**

PHYS **456.** Photophysical properties and electronic structure of strongly coupled hydroporphyrin dyads with extended near-infrared absorption. **H. Kang**, N.N. Esemoto, J.R. Diers, D.M. Niedzwiedzki, J.A. Greco, J. Akhigbe, Z. Yu, C. Pancholi, G.V. Bhagavathy, J.K. Nguyen, R.R. Birge, C.R. Kirmaier, D.F. Bocian, M. Ptaszek, D. Holten

PHYS **457.** Investigation of the hygroscopicity of glycine and lysine aerosols and their mixtures with Na_2SO_4. **J.P. Darr**, P. Morales, S. Gottuso, A. Johnson

PHYS **458.** Docking studies of binding of *Plasmodium falciparum* plasmepsin II to normal and sickle hemoglobin. **S.C. Marguet**, V.F. Waingeh

PHYS **459.** Correlation consistent composite approach (ccCA): Application to organics and beyond. **A. Morris**, A. Wilson

PHYS **460.** Charge-transfer in fullerene: Molecular cluster co-crystals. **N. Patel**, K.Z. Rinaldi, E. O'Brien, X. Roy, A. Crowther

PHYS **461.** Raman spectroscopic study of solvent-mediated electron-transfer chemical doping of graphene. **J. Karten**, B. Janicek, A. Crowther

PHYS **462.** Rapid scan electron paramagnetic resonance improves sensitivity relative to conventional methods. **G.R. Eaton**, S. Eaton, M. Tseytlin, R. Quine, G. Rinard, D. Mitchell, J. Biller, Z. Yu, Y. Shi

PHYS **463.** Photon and water mediated sulfur oxide and acid chemistry in planetary atmospheres. **J.A. Kroll**, V. Vaida

PHYS **464.** Theoretical analysis on the methods to derive surface molecular orientation by sum frequency generation spectroscopy. **A. Morita**, T. Ishihara, K. Saito, T. Ishiyama, L. Wang

PHYS **465.** Thermodynamics of uranium in gallium-aluminum based liquid alloys. **V.A. Volkovich**, D.S. Maltsev, L.F. Yamshchikov, I.B. Polovov, A.G. Osipenko

PHYS **466.** Thermodynamic modeling and experimental verification of f-elements separation employing Ga-Sn eutectic alloys. S.Y. Melchakov, D.S. Maltsev, **V.A. Volkovich**, L.F. Yamshchikov, D.G. Lisienko, M.A. Rusakov

PHYS **467.** Thermodynamic properties of lanthanum in alloys based on gallium-aluminum eutectic mixture. A.V. Shchetinskiy, A.S. Dedyukhin, **V.A. Volkovich**, L.F. Yamshchikov, A.G. Osipenko

PHYS **468.** Characterization of aqueous metal-pyrazole complexes. **A.K. Huff**, G. Turcios, S. Miller

PHYS **469.** Photodissociation of cis- and trans-CH_3ONO: Is conformation destiny? **J. Lantis**, M. Birndorf, J.A. Bartz

PHYS **470.** Photodissociation of t-butyl nitrite: Steric influences on vector correlations. **M. Birndorf**, J. Lantis, J.A. Bartz

PHYS **471.** Effects of large water box on anatase thin film surface: A computational analysis on changing electronic properties. **S.J. Jensen**, D. Kilin

PHYS **472.** Influence of various solvents on the physical properties of materials for organic electronic devices. **A. Foote**, R. Aga, E. Niwemukiza

PHYS **473.** BOMD study of M+(tryptamine)$(H_2O)_n$ cluster ions. P.E. Hoerner, **J. Beck**, M.P. Gaigeot

PHYS **474.** Spectroscopic study of the effects of local environment and deuteration on the structure of trimethylamine N-oxide (TMAO). **L. McNamara**, D.N. Reinemann, H.U. Valle, J.C. Prather, P.L. Reves, D.H. Magers, T.K. Hollis, G.S. Tschumper, N. Hammer

PHYS **475.** Thermal decomposition of iron dithiocarbamates. J.C. Becca, **J.F. Fuller**

PHYS **476.** Enzymatic activation of nitric oxide. **J.C. Pearson**, A.K. Wilson

PHYS **477.** Characterizing novel solid-state reaction intermediates using advanced in situ X-ray diffraction techniques. **C. Benson**, J. Cox, I. Walton, J.B. Benedict

PHYS **478.** Withdrawn.

PHYS **479.** Withdrawn.

PHYS **480.** Spectroscopic characterization of free-base bis(arylethynyl)porphyrins bearing *p*-hydroxyphenyl substituents. **K.K. Evens**, K.E. Splan

PHYS **481.** Fingerprinting molecular structure via photoinization out of Rydberg states and microwave Rayleigh scattering. **R.D. Oster**, S. Purohit, S. Atkins, F. Rudakov

PHYS **482.** Impact of basis set completeness on computed dissociation energies of transition metal complexes. **J. Plascencia**, A.K. Wilson

PHYS **483.** On the B800-850 LH2 antenna complex of the purple sulfur bacterium *Allochromatium vinosum*. **A. Kell**, M. Jassas, K. Hacking, R.J. Cogdell, R. Jankowiak

PHYS **484.** Comments on the optical lineshape function: Application to transient hole burned spectra of bacterial reaction centers. **A. Kell**, M. Reppert, T.O. Pruitt, D. Sanchez, R. Jankowiak

PHYS **485.** Critical assessment of the low-temperature optical spectra of the CP47 antenna protein complex of Photosystem II: Revised structural assignments. **J. Chen**, A. Kell, T. Reinot, M. Jassas, R. Jankowiak

PHYS **486.** Heat capacity of oxygen atoms at high temperatures. **L. Biolsi**

PHYS **487.** Membrane catalyzed aggregation of amylin using 2D IR spectroscopy. **K. Rich**, M.T. Zanni

PHYS **488.** Ab initio approaches for accurate predictions of lanthanide thermochemistry. **C.C. Peterson**, A.K. Wilson

PHYS **489.** Evaluation of charge density analysis methods. **C.C. Jeffrey, M.J. Carlson, A.K. Wilson**

PHYS **490.** Electron transfer rate modulation in a compact Re(I) donor-acceptor complex. **Y. Yue**, T. Grusenmeyer, M. Zheng, P. Zhang, R.H. Schmehl, D.N. Beratan, I.V. Rubtsov

PHYS **491.** Study of low temperature oxidation reactions of 2-methylfuran using synchrotron photoionization mass spectrometry. **A.R. Smith**, G. Meloni

PHYS **492.** Gas-phase acidities of nitrated azole species from the extended kinetic method. **C.M. Nichols**, W. Old, W.C. Lineberger, V.M. Bierbaum

PHYS **493.** Modeling stopped-flow data for nucleic acid duplex formation reactions. **A. Deckert**, J. Sikora, B. Rauzan

PHYS **494.** DSC and rheological study of supercooled ethylene glycol-water mixture. **S. Kim**, R. Fore, E. Kook, B.H. Milosavljevic

PHYS **495.** Using kinetic models to understand H atom reactions in solid parahydrogen. **F.M. Mutunga**, D.T. Anderson

PHYS **496.** Evaluation of a novel nontraditional processing aid for the pulp and paper industry. **C. Kirwan**, R. Hamm, B. Wilson, L. Bava

PHYS **497.** Template and model sets of protein structures. **I. Anishchanka**, P. Kundrotas, A. Tuzikov, I. Vakser

PHYS **498.** Overcoming costly sampling simulations using non-Boltzmann Bennet's acceptance ratio method to generate potentials of mean force. P.S. Hudson, **F.L. Kearns**, S. Boresch, H.L. Woodcock

PHYS **499.** Development of bacteriochlorophyll a potential energy surface by quantum chemical calculations. **C. Kim**, Y.M. Rhee

PHYS **500.** Environmental effect on excited energy transfer in photosynthetic light harvesting complex: Comparing Poisson bracket mapping equation and reduced hierarchical equation of motion. **W. Lee**

PHYS **501.** Evaluation of defoamer chemistries for brown stock washing. **R. Hamm**, C. Kirwan, B. Wilson, L. Bava

PHYS **502.** DsDNA-assisted dissolution of tungsten (IV) disulfide in aqueous solution. **M. Simmons,** X. Xu, W. Zhao

PHYS **503.** Computational study of the reduction by 2-propanol of acetophenone in supercritical 2-propanol. **D.B. Lawson**

PHYS **504.** Electron transmission in molecular electronics: A computational study. **B. Topham**

PHYS **505.** Effect of substitution on the rate of benzyloxyl radical generation through a 1,2-Hydrogen atom shift: A computational study. **D.J. Van Hoomissen**, S. Vyas

PHYS **506.** Computational studies of inhibitor binding to human immunodeficiency virus, Type 2 (HIV-2) protease. **R. Summay**, V.F. Waingeh

PHYS **507.** Solid phase microextraction with polystyrene- poly(dimethylsiloxane) block copolymers. **A. Schlaus**

PHYS **508.** Mixed polarization vibrational sum frequency generation spectra of organic semiconducting thin films. **P.M. Kearns**, A.M. Massari

PHYS **509.** Stochastic approach to reaction diffusion modeling of the fragmentation processes during heterogeneous oxidation of organic aerosol. **A.A. Wiegel**, K.R. Wilson, W. Hinsberg, F.A. Houle

PHYS **510.** Characterization of a real-time tfor isoprene epoxydiols-derived secondary organic aerosol (IEPOX-SOA) from aerosol mass spectrometer measurements. **W. Hu**, P. Campuzano-Jost, B. Palm, D. Day, A. Ortega, P. Hayes, Q. Chen, M. Kuwata, Y. Liu, S. Simoes de Sa, S.T. Martin, M. Hu, S. Budisulistiorini, J. Surratt, K. Docherty, G. Isaacman, A. Goldstein, J. Clair, J.D. Crounse, P. Wennberg, J. Jimenez

PHYS **511.** Water vapor enhancement of peroxy radical reactions. **S. Kumbhani**, T. Cline, M. Killian, J. Clark, L. Hansen, R.B. Shirts, D. Robichaud, J.C. Hansen

PHYS **512.** Kinetics of acid-catalyzed dehydration of aerosol cyclic hemiacetals formed from the OH radical-initiated reaction of *n*-pentadecane. **A.P. Ranney**, P. Ziemann

PHYS **513.** Heterogeneous oxidation of liquid and solid alkanes by OH in the presence and absence of NO or SO_2. **N.K. Richards-Henderson**, M.D. Ward, A. Goldstein, K.R. Wilson

PHYS **514.** Investigating index of refraction trends in ammonium sulfate and glyoxal reactions. **M. Symons**, M.D. Zauscher, M.M. Galloway, D.O. Dehaan

PHYS **515.** Determination of N-containing conjugated brown carbon products In glycolaldehyde, methylamine, and glycine reaction mixtures. **T. Kress**

PHYS **516.** Measurements of in-situ SOA formation and chemistry using an oxidation flow reactor. **B.B. Palm**, P. Campuzano-Jost, D. Day, W. Hu, A.M. Ortega, S.S. de Sá, R. Seco, J. Park, A. Guenther, S. Kim, J. Brito, F. Wurm, P. Artaxo, R. Thalman, J. Wang, L. Kaser, W. Jud, T. Karl, A. Hansel, J. Fry, S.S. Brown, D. Draper, K.J. Zarzana, W.P. Dubé, N. Wagner, L. Hacker, A. Kiendler-Scharr, L. Yee, G. Isaacman, A. Goldstein, R. Souza, A. Manzi, O. Vega, J. Tota, M. Newburn, M. Alexander, S.T. Martin, W. Brune, J.L. Jimenez

PHYS **517.** SOA derived from isoprene epoxydiols: Insights into formation, aging and distribution over the continental US from the DC3 and SEAC4RS campaigns. **P. Campuzano Jost**, B.B. Palm, D. Day, W. Hu, A.M. Ortega, J. Jimenez, J. Liao, K.D. Froyd, I. Pollack, J. Peischl, T.B. Ryerson, J. Clair, J.D. Crounse, P. Wennberg, T. Mikoviny, A. Wisthaler, L. Ziemba, B.E. Anderson

PHYS **518.** Depositional ice nucleation on NX illite and mixtures of NX lilite with organic acids. **K.M. Primm, M. Tolbert**, G. Schill

PHYS **519.** Does the reaction of HO_2 with NO produce $HONO_2$ and HOONO? **L.A. Mertens**, H.M. Allen, M. Okumura, S.P. Sander

PHYS **520.** Gas/particle partitioning of organic acids during the southern oxidant and aerosol study (SOAS): Measurements and modeling. **S. Thompson**, L. Yatavelli, H. Stark, J. Kimmel, W. Hu, B.B. Palm, P. Campuzano-Jost, D. Day, G. Isaacman, A. Goldstein, R. Holzinger, A. Khan, F. Lopez-Hilfiker, C. Mohr, J.A. Thornton, J.T. Jayne, D.R. Worsnop, J.L. Jimenez

PHYS **521.** Reactions of resonantly-stabilized free radicals that impact molecular weight growth kinetics. **K. Wang**, S. Villano, A.M. Dean

PHYS **522.** Hydration of Krypton in dilute and concentrated solutions. **M. Chaudhari**, S.L. Rempe, D. Sabo, L.R. Pratt

PHYS **523.** Theoretical and experimental studies on the radical-radical reaction: $NO_2 + N_2H_3$. **G.L. Vaghjiani**, H. Sun, S.D. Chambreau, A. Schenk, C.K. Law

PHYS **524.** Estimation of quantum effects in atomic solids using quantum trajectory dynamics with dissipation. **B. Gu**, V. Rassolov, S. Garashchuk

PHYS **525.** Characterizing the effects of noncovalent interactions on hydrated azabenzene clusters: Charge localization and charge transfer. **J.T. Kelly**, K.H. Bowen, G.S. Tschumper, N. Hammer

PHYS **526.** Intrinsic bonding patterns via localized orbitals. **J. Duchimaza**, A. West, M.W. Schmidt, M.S. Gordon, K. Ruedenberg

PHYS **527.** Origins of long timescales in solvation dynamics of nanoconfined liquids. **J. Harvey**, W. Thompson

PHYS **528.** Magnetic stability and relaxation in single-molecule magnets: Insights from new stochastic theories. **D. Packwood**, K. Reaves, F. Federici Canova, I. Hamada, H. Katzgraber, W. Teizer

PHYS **529.** Multireference diagnostic criteria for 4d transition-metal-containing molecules. **J. Wang**, S. Manivasagam, A.K. Wilson

PHYS **530.** In search of an intrinsic chemical bond. **A. Morgenstern**, T. Wilson, T. Jones, J. Miorelli, M. Eberhart

PHYS **531.** Density functional theory study of the reduction of substituted quinones by lumiflavin. **E. Song**, C.R. Reinhardt, S. Bhattacharyay

PHYS **532.** First-principles interpretation of ultrafast time-resolved core-level spectroscopies investigating photo-induced charge transfer. **S. Pemmaraju**, S. Neppl, K. Siefermann, D. Prendergast, O. Gessner

PHYS **533.** Hydrocarbon structure impacts on the fumarate addition mechanism: Perspectives on the biodegradation susceptibility of fuels from electronic structure calculations. **V.S. Bharadwaj**, S. Vyas, S. Villano, C.M. Maupin, A.M. Dean

PHYS **534.** Intramolecular oxygen bond rearrangement reactions studied with density functional theory: Thermodynamics vs. kinetics. **F.X. Vazquez**

PHYS **535.** Creating transferrable multiscale models from all-atom data. **M. McCullagh**

PHYS **536.** Molecular polarizability as a descriptor of molecular conductance. **S. K. S. Mazinani**, R. Vatan, T. Pilarisetty, J.L. Palma, V. Mujica

PHYS **537.** Modeling electron transfer through hydrogen bonding. **M. Wimmer**, R. Vatan, T. Pilarisetty, V. Mujica, J.L. Palma

PHYS **538.** Raft environments assist the aggregation of the transmembrane region of Amyloid Precursor Protein. **N. Miyashita**, F. Ogushi, Y. Sugita

PHYS **539.** Influence of sequence and lipid type on membrane perturbation by human and rat amyloid β-peptide (1-42). **A. Brown**, D.R. Bevan

PHYS **540.** Light chain internalizes into human cardiomyocytes in a Dynamin-independent way. Amyloid fibrils recruit soluble protein in media and accelerate its internalization. **M. Marin-Argany**, M. Ramirez-Alvarado

PHYS **541.** Revisiting Thioflavin T as fibrilization sensor: What is actually probed? **J. Breffke**, M. Maroncelli

PHYS **542.** Contributions of collision-induced dissociation to collision crossSections measured using the crossSectional areas by Fourier transform ion cyclotron resonance (CRAFTI) approach. **C. Harper**, D.V. Dearden

PHYS **543.** Theoretical study of the two-photon circular dichroism of molecular structures simulating aromatic amino acids residues in proteins with secondary structures. **Y.K. Vesga Prada**, M. Higgs, C. Diaz, F. Hernandez

PHYS **544.** Analyzing small DNA constructs via chromophore model within the point dipole approximation. **P.G. Romano**

PHYS **545.** Octa-coordination and the hydrated Ba^{2+}(aq) ion. M. Chaudhari, **S.L. Rempe,** M. Soniat

PHYS **546.** Inferring latent states and force estimates via hierarchical Dirichlet process modeling in single particle tracking experiments. **C.P. Calderon**

PHYS **547.** Structure-activity and conformational-activity relationships of inhibitor of κB kinase-β. **M. Jones**, A.K. Wilson

PHYS **548.** New insight into the FMO antenna protein: Hole burning and modeling study. **A. Kell**, K. Acharya, M. Jassas, T. Reinot, J. Tang, R. Jankowiak

PHYS **549.** Computational study of folding thermodynamics and mechanism of Trp-cage mutants with RSFF2. **C. Zhou,** F. Jiang, Y. Wu

PHYS **550.** Engineering Aspects of Titania Nanotube Synthesis. **S.A. Ferdousi**, K.L. Yeung

PHYS **551.** Natural boundary condition for hydrodynamic transport is the slip boundary condition for all molecule sizes and all solvents. **S.R. Aragon**

PHYS **552.** Docking of protein models. **P. Kundrotas**, I. Anishchenko, A. Tuzikov, I. Vakser

PHYS **553.** Solvent effects on azobenzene photodynamics with spin-flip time-dependent density functional theory and effective fragment potential methods. **K. Keipert**, Y. Harabuchi, M.S. Gordon

PHYS **554.** Controlling the reactivity of large molecules by remote protonation of a side-group. J. Ditkovich, D. Pines, **E. Pines**

PHYS **555.** Bond energy orbitals: The concept and some applications. E.A. Boudreaux

THURSDAY MORNING

Section A

Colorado Convention Center
Room 501

Atmospheric Chemistry: Transformations of Matter in the Troposphere

Gas Phase Atmospheric Chemistry

D. Cziczo, M. Freedman, *Organizers*
T. H. Bertram, J. Murphy, *Presiding*

8:00 PHYS **556.** Reactions of atmospheric peroxy radicals studied by synchrotron VUV multiplexed photoionization mass spectrometry. L.G. Dodson, L. Shen, J. Savee, D.L. Osborn, N.C. Eddingsaas, S.P. Sander, C.A. Taatjes, F.J. Grieman, **M. Okumura**

8:40 PHYS **557.** Observation of the simplest criegee intermediate, CH_2OO, in the gas-phase ozonolysis of ethylene. **C. Womack**, M. Martin-Drumel, R. Field, M. McCarthy

9:00 PHYS **558.** Comprehensive theoretical mechanism for the Criegee intermediate-sulfur dioxide reaction. **K.T. Kuwata**, E.J. Guinn, M.R. Hermes, J.A. Fernandez

9:20 Intermission.

9:35 PHYS **559.** Ozone repsonses to climate change and NO_x reductions. **R.C. Cohen**

10:15 PHYS **560.** New 'bond and photons' paradigm for the tropospheric ozone budget. **P.M. Edwards**, M.J. Evans

10:35 PHYS **561.** How does nighttime oxidation of biogenic VOCs impact daytime ozone? **J. Mao**, J. Li, L. Horowitz, V. Naik, F. Paulot, M. Lin, I. Pollack, T.B. Ryerson, P.M. Edwards, K. Min, S.S. Brown, M. Graus, C. Warneke, J. Gilman, B. Lerner, A. Neuman, J.B. Nowak, P. Veres, J. Roberts, F. Lope-Hilfiker, B. Lee, J.A. Thornton, J. Kaiser, F. Keutsch, G.M. Wolfe, T.F. Hanisco, K. Wells, D. Millet, B. Henderson, K. Aikin, J. de Gouw

11:00 PHYS **562.** Novel method to estimate and evaluate OH rate constants for atmospherically relevant VOCs. **R.T. Lidster**, J.F. Hamilton, A.C. Lewis, M.J. Evans, A.R. Rickard, D.E. Heard, L.K. Whalley, D.R. Cryer, J.C. Young

11:20 Concluding Remarks.

Section B

Colorado Convention Center
Room 502

Carbon in the Galaxy: The Formation of Complex Organics from the Outflow of Carbon Stars & Their Evolution

PAH-Related Processes

L. J. Allamandola, T. J. Lee, *Organizers*
H. Cuppen, *Presiding*

8:00 PHYS **563.** Organic molecules in protoplanetary disks: Probes of planet formation and chemical evolution. **J. Najita**

8:35 PHYS **564.** Gas phase ion chemistry of complex organic species. **V.M. Bierbaum**, C.A. Cole, Z. Wang, T.P. Snow

9:10 PHYS **565.** Tying interstellar PAH emission spectra and (photo)chemistry to local physical conditions in the emission zones. **C. Boersma**

9:45 Intermission.

10:15 PHYS **566.** Dehydrogenation of PAHs: First steps towards fullerenes in the ISM. **P. Castellanos Nash**, J. Zhen, A. Candian, H. Linnartz, A. Tielens

10:50 PHYS **567.** Photochemical model of the top down formation of fullerenes in the interstellar medium. **O. Berne**, J. Montillaud, C. Joblin

11:25 PHYS **568.** Anharmonic bands in the 3-μm region of acenes: A combined experimental and theoretical study. **A. Petrignani**, E. Maltseva, A. Candian, A. Tielens, J. Oomens, W. Buma

Section C

Colorado Convention Center
Room 503

Computational Chemical Dynamics: Advancing our Understanding of Chemical Processes in Gas-Phase, Biomolecular & Condensed-Phase Systems: A Symposium in Honor of Donald Truhlar

Macromolecular Dynamics

Cosponsored by COMP

J. Gao, B. Mennucci, *Organizers*
B. C. Garrett, *Organizer, Presiding*

8:00 PHYS **569.** Computationally guided design and optimization of inhibitors of macrophage migration inhibitory factor. **W.L. Jorgensen**, D.J. Cole, M.J. Robertson

8:30 PHYS **570.** Multiscale characterization of macromolecular dynamics. **C. Clementi**

9:00 PHYS **571.** Dynamic effects in dihydrofolate reductase catalysis. **R.K. Allemann**, L. Luk, J. Loveridge

9:30 PHYS **572.** Advancing ab initio molecular dynamics via multiple-timestep methods. **R. Steele**

9:50 Intermission.

10:10 PHYS **573.** Toward a molecular theory of early and late events in monomer to amyloid fibril formation. **J.E. Straub**

10:40 PHYS **574.** Large spatiotemporal-scale quantum molecular dynamics simulations: A divide-conquer-recombine approach. **A. Nakano**, R.K. Kalia, K. Nomura, K. Shimamura, F. Shimojo, P. Vashishta

11:10 PHYS **575.** Sorbate dynamics in hierarchical porous materials. **J.I. Siepmann**, P. Bai, E. Haldoupis, M. Tsapatsis

11:30 PHYS **576.** Molecular dynamics simulations of ion transport in carbon nanotubes. **K.L. Shuford**, O. Samoylova, E. Calixte

Section D

Colorado Convention Center
Room 504

Physical Electrochemistry of Electrocatalytic Processes

Electrocatalysis of CO_2

D. A. Scherson, *Organizer*
A. Co, *Organizer, Presiding*
A. R. Asthagiri, *Presiding*

8:30 PHYS **577.** Understanding CO_2 electroreduction on Cu electrodes through first-principles modeling. **A.R. Asthagiri**

9:10 PHYS **578.** Extended π-attraction σ-repulsion model for carbon monoxide adsorbed on platinum-ruthenium-osmium-iridium quaternary alloys. **N. Dimakis**, N.E. Navarro, E.S. Smotkin

9:30 PHYS **579.** Charge-state dependent electrocatalytic activity of discretely charged, atomically-precise $Au_{25}(SR)_{18}^{q}$ nanoclusters (q = -1, 0, +1). **D. Kauffman**, D. Alfonso, C. Matranga, X. Deng, P. Ohodnicki, R. Siva, R. Jin

9:50 PHYS **580.** Investing the electroreduction pathway of carbon dioxide using surface enhanced Raman spectroscopy. J. Billy, E. Coleman, K. Muhlenkamp, **A. Co**

10:10 PHYS **581.** Pyridine-catalyzed CO_2 reduction on p-GaP photoelectrodes: First-principles investigation of possible reaction mechanisms. **M. Lessio**, C. Riplinger, A.B. Muñoz-García, E.A. Carter

Section E

Colorado Convention Center
Room 507

Modeling Complex Biomolecules: From Structure to Dynamics & Function

Dynamics in Function and Inhibitor Design

Cosponsored by COMP

G. Hummer, *Organizer*
A. E. Garcia, *Organizer, Presiding*

8:00 PHYS **582.** Predicting drug-target binding kinetics through enhanced sampling simulations. **F. Gervasio**

‡ *Cooperative Cosponsorship*

8:35 PHYS **583.** Activation and drug design of a muscarinic G-protein coupled receptor. **Y. Miao**, J.A. McCammon

9:10 PHYS **584.** Prediction of mechanically hot spots in protein-protein interactions using perturbation response scanning method. **H. Abdizadeh**, A. Atilgan, C. Atilgan

9:45 PHYS **585.** Nucleotide-dependent interaction of K-Ras4B hypervariable region with Ras active site. T.S. Chavan, H. Jang, L. Khavrutskii, V. Gaponenko, N.I. Tarasova, **R. Nussinov**

10:20 PHYS **586.** Elucidating protein function and dynamics through molecular simulations and Markov state modeling: Allostery through conformational selection. **R.E. Amaro**, R. Malmstrom, S.S. Taylor, A. Kornev

10:55 PHYS **587.** Folding kinetics and local dynamics of the 60 nucleotide rRNA GTPase center RNA. M.J. Rau, **K.B. Hall**

Section F

Colorado Convention Center
Room 505

Modeling Excited States of Complex Systems

Nonadiabatic Effects

B. G. Levine, *Organizer*
S. A. Varganov, *Organizer, Presiding*

8:00 PHYS **588.** Excited state dynamics at complex interfaces: time-domain ab initio studies. **O.V. Prezhdo**

8:40 PHYS **589.** Geometric phase effects in non-adiabatic dynamics near two-state conical intersections. **A.F. Izmaylov**

9:20 PHYS **590.** PYXAID program: a tool for modeling excited state dynamics in complex systems. **A.V. Akimov**, O.V. Prezhdo

9:40 PHYS **591.** Self-trapping of excitons, violation of condon approximation, and efficient fluorescence in conjugated cycloparaphenylenes. **L. Adamska**, J. Liu, S. Fernandez-Alberti, R. Jasti, S.K. Doorn, S. Tretiak

10:00 Intermission.

10:20 PHYS **592.** Current view of surface hopping. **J.E. Subotnik**, B.R. Landry

11:00 PHYS **593.** Multidimensional effects in nonadiabatic statistical theories of spin-forbidden kinetics. **A. Jasper**

11:40 PHYS **594.** Semiclassical Monte-Carlo: A first principles approach to nonadiabatic molecular dynamics. **A. White**, V. Gorshkov, R. Wang, S. Tretiak, D. Mozyrsky

12:00 PHYS **595.** Modeling nonadiabatic photodynamics in aqueous environments with the ab initio multiple spawning and effective fragment potential methods. **K. Keipert**, S.R. Pruitt, M.S. Gordon

Section G

Colorado Convention Center
Room 506

Probing Nano-Plasmonic Phenomena at the Single Molecule, Single Electron, & Single Photon Level

D. J. Masiello, *Organizer*
S. Link, K. A. Willets, *Organizers, Presiding*

8:30 PHYS **596.** Single molecule chemistry probed by SERS and TERS at the nanometer length scale and picosecond time scale. **R.P. Van Duyne**

9:05 PHYS **597.** Optical characterization of pinholes in passivation layers on electrode surfaces. **K. Marchuk**, C. Renault, A.J. Bard, K.A. Willets

9:25 PHYS **598.** Plasmonic application in imaging at the single cancer cell level. **M.A. El-Sayed**

10:00 PHYS **599.** Withdrawn.

10:20 PHYS **600.** Probing magneto-plasmonic phenomena at the single nanostructure level. **K.L. Knappenberger**

10:55 PHYS **601.** Following plasmonically-enhanced chemical reactions with ultrafast Raman spectroscopies. **R.R. Frontiera**

POLY

Division of Polymer Chemistry

M. Jeffries-El, D. Boday and T. White, *Program Chairs*

SOCIAL EVENTS:

POLY Luncheon, 12:30 PM: Sun
POLY Luncheon, 12:30 PM: Mon
POLY Reception, 5:30 PM: Tue
POLY Breakfast, 7:30 AM: Tue
POLY Reception, 5:30 PM: Wed

BUSINESS MEETINGS:

POLY Programming Committee Meeting (Lunch), 12:00 PM: Tue

SUNDAY MORNING

Section A

Sheraton Denver Downtown Hotel
Directors Row E

Next Generation Smart Materials

Bio-inspired and Biomimetic Systems

Cosponsored by PMSE‡

Y. C. Simon, *Organizer*
E. B. Berda, J. Foster, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 POLY **1.** Poly(phthalaldehydes) as stimuli-responsive, depolymerizable materials that are capable of providing amplified responses. **A.M. DiLauro**, S.T. Phillips

9:05 POLY **2.** Making "smarter" heparin-mimicking polymers. **N. Ayres, Y. Huang, Q. Chai**

9:35 POLY **3.** Nucleobase hydrogen bonding in polymers as a source of intelligence. **T.E. Long, K. Zhang**, M. Aiba, S. Cheng, W.D. Chiang

10:05 Intermission.

10:15 POLY **4.** Poly(phosphoester)s: From adhesives to stealth polymers. **F. Wurm**

10:45 POLY **5.** Light-degradable polymers: amplification strategies, response to new wavelengths, and application to a clinical challenge. J. Olejniczak, C. Carling, V. Nguyen Huu, A. Garcia, J. Luo, K. Zhang, **A. Almutairi**

11:15 POLY **6.** Folding single polymer chains. **C. Barner-Kowollik**, J. Willenbacher, O. Altintas

11:45 Concluding Remarks.

Section B

Sheraton Denver Downtown Hotel
Governor's Square 12

Putting Renewable Polymers to Work

D. Boday, E. C. Hagberg, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 POLY **7.** Poly(β-methyl δ-valerolactone) as a scalable and renewable soft segment for aliphatic polyester block polymers. **M.A. Hillmyer**

8:35 POLY **8.** Commercialization of triglyceride-based thermoplastic elastomers for polymer modified asphalt pavements: Where the (bio)rubber meets the road. **E.W. Cochran**, R. Williams, N. Hernandez, M. Yan, A. Hohmann, M.J. Forrester

9:05 POLY **9.** Conversion of agricultural residues into value-added products. **H. Cheng**, A. Biswas

9:35 Intermission.

9:50 POLY **10.** Synthesis and functional properties of renewable polymers. **R.M. Waymouth**, X. Zhang, B. Timothy, A.J. Ingram, K. Chung, W. Ho, J. Hedrick

10:20 POLY **11.** Design and synthesis of eumelanin-inspired polymers derived from vanillin. **T.L. Nelson**, R.P. Hopson, S. Selvaraju, N. Sachinthani

10:40 POLY **12.** Thiol-ene films derived from phenolic acids. G. Yang, H. Tesefay, **M.L. Robertson**

11:10 POLY **13.** Glass transition dynamics of biobased *poly*(ethylene 2,5-furandicarboxylate). **A. Codou**, N. Guigo, M. Moncel, L. Martino, J. Van Berkel, E. De Jong, N. Sbirrazzuoli

Section C

Sheraton Denver Downtown Hotel
Governor's Square 14

Celebrating the Fifth Year Anniversary of Polymer Chemistry (RSC)

Financially supported by Royal Society of Chemistry

D. M. Haddleton, B. S. Sumerlin, W. You, *Organizers, Presiding*

8:30 Introductory Remarks.

8:40 POLY **14.** Nature's functionality on synthetic polymers — zwitterions and inverse zwitteirons. **T. Emrick**

9:10 POLY **15.** Mimicry of photosynthesis: for the synthesis of well-defined polymers. S. Shanmugam, J. Xu, **C. Boyer**

9:40 POLY **16.** New methodology for controlled supramolecular polymerization. **X. Zhang**

10:10 Intermission.

10:30 POLY **17.** Sequential one-pot organocatalytic polymerization of epoxides and cyclic esters/carbonates. **J. Zhao**, D. Pahovnik, Y. Gnanou, N. Hadjichristidis

11:00 POLY **18.** Building smart materials from poly(2-vinyl-4,4-dimethylazlactone) scaffolds. **A.B. Lowe**

11:30 POLY **19.** Self-immolative polymersomes for high-efficiency triggered release and programmed enzymatic reactions. **G. Liu**, X. Wang, S. Liu

Section D

Sheraton Denver Downtown Hotel
Governor's Square 9

General Topics: New Synthesis & Characterization of Polymers

B. Barkakaty, D. Garcia, *Organizers*
A. Carlmark, F. Horkay, *Presiding*

8:00 POLY **20.** Cartilage: architecture and function. **F. Horkay**, P.J. Basser

8:20 POLY **21.** Drug-functionalized cell-penetrating peptides for enhanced delivery and binding in myotonic dystrophy type 1 treatment. **Y. Bai**, L. Nguyen, Z. Song, J. Cheng, S.C. Zimmerman

8:40 POLY **22.** Novel biodegradable, biocompatible and biofunctional block copolymer scaffolds for tissue engineering applications. **P.P. Smith**, A.L. Rightler, B.K. McConnell, F. Zhang, S.O. Streubel, S. Lu, D. Price, S.G. Boyes

9:00 POLY **23.** Protein:polymer conjugates via graft-*from* ring-opening metathesis polymerization. **S.A. Isarov**, J.K. Pokorski

9:20 POLY **24.** Polylactic acid composite with natural fibers in food packaging. **S. Sedaghat**

9:40 POLY **25.** N-heterocyclic carbenes in the organopolymerization of N-substitued N-carboxy-anhydrides to polypeptoid. **I. Falivene**, M. Alghamdi, L. Cavallo

10:00 POLY **26.** Surface-initiated ring opening polymerization of carbonates and siloxanes from cellulose surfaces. S. Pendergraph, G. Klein, M.K. Johansson, **A. Carlmark**

10:20 POLY **27.** Optimizing photo-CuAAC polymerization kinetic for dental restorative materials. **H. Song**, A.D. Baranek, M. McBride, T. Gong, A. Flores, J.W. Stansbury, C.J. Kloxin, C. Bowman

10:40 POLY **28.** Chemical modification reactions of polysaccharides studied in real time by light scattering and viscometry-based methods. V.C. Spier, **A.M. Alb**

11:00 POLY **29.** Radiolabeled polymers to probe the enhanced permeability and retention effect. **M.C. Parrott**

11:20 POLY **30.** Investigating polymerization reactions with thermography: Differentiating between bulk effects, thermal diffusion and oxygen inhibition. **C. Wappl**, R. Geier, H. Freiszmuth, C. Slugovc, G. Gescheidt

11:40 POLY **31.** High performance hydrogels based on melt-assembled networks of sphere-forming block copolymers. **J. Lewis**, T.S. Bailey

12:00 POLY **32.** Smart polymers for on-demand drug delivery. Y. Zhang, K. Cai, **J. Cheng**

Section E

Sheraton Denver Downtown Hotel
Directors Row I

Macromolecular and Nanoparticle Separation Science

Cosponsored by ANYL and PMSE

Financially supported by The Dow Chemical Company, Wyatt Technology, Tosoh BioScience, Waters, NIST

K. Beers, A. K. Brewer, W. Gao, A. M. Striegel, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 POLY **33.** Size exclusion chromatography/gel permeation chromatography – a blessing and curse of science and technology of synthetic polymers. **D. Berek**

9:15 POLY **34.** Industrial polymer analysis using a solvent elimination IR detector. **R. Allen**, S. Moyses, N. Jestel

9:45 POLY **35.** Is SEC-Raman a feasible way of measuring copolymer chemical heterogeneity? **A.M. Striegel**, L. Pitkanen, A.A. Urbas

10:15 Intermission.

10:30 POLY **36.** Probing serum phase oligomer in acrylic emulsion polymerization process by GPC-RI/MS. **T. Zhang**, W. Gao, R. Even, D. Kline

11:00 POLY **37.** Characterization of novel high temperature thermoplastic elastomers polybenzofulvene-block-polyisoprene-block-polybenzofulvene. **J.W. Mays**, W. Wang, T. White, N. Kang, K. Hong, R. Schlegel, M. Beiner, K. Williams, S.P. Gido

11:30 POLY **38.** Ultrahigh performance size exclusion chromatography of synthetic polymers. **M. Janco**, J.N. Alexander, E.S. Bouvier, D. Morrison

12:00 POLY **39.** Advanced polymer chromatography: Method development tools for SEC polymer analysis. **D. Morrison**, M. O'Leary

SUNDAY AFTERNOON

Section A

Sheraton Denver Downtown Hotel
Directors Row E

Next Generation Smart Materials

Bio-inspired and Biomimetic Systems

Cosponsored by PMSE‡

E. B. Berda, Y. C. Simon, *Organizers*
J. Foster, *Organizer, Presiding*
N. Zacharia, *Presiding*

1:30 Introductory Remarks.

1:35 POLY **40.** Progress towards the efficient synthesis of polymers with precisely defined mass, sequence, and stereochemistry. J. Barnes, D. Ehrlich, F. Leibfarth, T.F. Jamison, **J.A. Johnson**

2:05 POLY **41.** Programed block copolymers: At the end it is always good to be smart. **E.B. Coughlin**

2:35 POLY **42.** Tunable solid state fluorescent materials for supramolecular encryption. X. Hou, C. Ke, **J.F. Stoddart**

3:05 Intermission.

3:25 POLY **43.** Dynamic-covalent nanoparticles and self-healing hydrogels. S. Mukherjee, C.C. Deng, W. Brooks, M. Hill, **B.S. Sumerlin**

3:55 POLY **44.** Chirality-selected phase behavior in ionic polypeptide complexes. **M.V. Tirrell**

4:25 POLY **45.** Responsive polypeptide-based star and triblock copolymers: Smart function through morphology transitions. G.A. Strange, A.J. Johnson, I. Smith, J.G. Ray, **D.A. Savin**

4:55 Concluding Remarks.

Section B

Sheraton Denver Downtown Hotel
Governor's Square 12

Putting Renewable Polymers to Work

D. Boday, E. C. Hagberg, *Organizers, Presiding*

1:00 POLY **46.** Diisocyanates and tackifiers from isosorbide. M.D. Zenner, **J.S. Chen**

1:20 POLY **47.** Benzyl chloride functionalized polycarbonates: A versatile platform for the synthesis of functional biodegradable polycarbonates. **R. Ono**, S. Liu, S. Venkataraman, W. Chin, Y. Yang, J. Hedrick

1:50 POLY **48.** Synthesis, characterization, and bimodal blend studies of renewable biobased epoxy resins from vanillyl alcohol. **E.D. Hernandez**, J.M. Sadler, J.J. La Scala, J.F. Stanzione

2:10 POLY **49.** Selective organic catalysis in the synthesis of materials from sustainable resources by ring-opening polymerization. **A.P. Dove**

2:40 Intermission.

2:55 POLY **50.** Renewable polymers in hydraulic fracturing applications. **J.R. Dorgan**

3:25 POLY **51.** Soy-based polymer surfactants for personal care applications. A. Popadyuk, H. Kalita, B.J. Chisholm, **A.S. Voronov**

3:45 POLY **52.** From biorefinery to performance technology: Transforming metathesized renewables oils into high value products. **K.O. Havelka**

4:15 POLY **53.** Renewable feedstocks for the polymer industry. E.C. Hagberg, **P.D. Bloom**

4:45 POLY **54.** Polysaccharide circuit boards for epidermal electronics. **M.A. Daniele**, J.S. Erickson, A.J. Knight, S.A. Roberts, K. Radom, S. Walper, J. Yuen

Section C

Sheraton Denver Downtown Hotel
Governor's Square 14

Celebrating the Fifth Year Anniversary of Polymer Chemistry (RSC)

Financially supported by Royal Society of Chemistry

D. M. Haddleton, B. S. Sumerlin, W. You, *Organizers, Presiding*

1:30 POLY **55.** Hierarchical polymeric nanostructures from precision polymer chemistry. **S. Perrier**

2:00 POLY **56.** Sequence-controlled polymerizations: The Holy Grail is near. **J. Lutz**

2:30 POLY **57.** Protein-polymer conjugates by grafting to and grafting from methods. **H.D. Maynard**, C. Decker, J. Ko, J. Lee, T.H. Nguyen, E. Pelegri-O'Day, N. Matsumoto

3:00 Intermission.

3:20 POLY **58.** Synthesis of protein-polymer conjugates with controllable activity through site-specific conjugation. X. Li, L. Wang, Y. Cai, L. Yuan, H. Wang, G. Chen, **H. Chen**

3:50 POLY **59.** Entropy driven chain effects on ligation. **C. Barner-Kowollik**, A. Lederer, M. Coote, G. Gryn'ova, K. Pahnke, F.G. Schmidt, J. Brandt, N. Guimard

4:20 POLY **60.** Mimicking complex biological membranes and their programmable glycan ligands. **V. Percec**

Section D

Sheraton Denver Downtown Hotel
Governor's Square 9

General Topics: New Synthesis & Characterization of Polymers

B. Barkakaty, D. Garcia, *Organizers*
N. S. Sampson, W. Xi, *Presiding*

1:00 POLY **61.** Solution processable polydiacetylenes (PDAs) through acyclic enediyne metathesis polymerization (AEDMET). **Y. Qin**

1:20 POLY **62.** Very long, linear polymers from tandem isomerization/alternating ring-opening metathesis polymerization (*i*-AROMP). L. Tan, K.A. Parker, **N.S. Sampson**

1:40 POLY **63.** Ring-opening metathesis emulsion polymerization: A comparison of commercial and homemade surfactants and catalysts. S.R. Almahdali, **K. Bukhriakov, V. Rodionov**

2:00 POLY **64.** Withdrawn.

2:20 POLY **65.** Incorporation and use of imidazoles as a dually dopable moiety in conjugated polymers. **J.D. Harris**, K.R. Carter

2:40 POLY **66.** Pushing the limit of the RAFT process: One-pot preparation of multiblock copolymers. **G. Gody**, S. Perrier

3:00 POLY **67.** RAFT polymerization of tertiary amine-based methacrylate pH-responsive monomers for smart MRI contrast agents. **L. Zhu**, S. Powell, S.G. Boyes

3:20 POLY **68.** Stille catalyst-transfer polycondensation using palladium catalysts for the synthesis of well-defined conjugated materials. **Y. Qiu**, T. Kowalewski, K.J. Noonan

3:40 POLY **69.** "Click" by "click" strategy in sequence controlled polymers synthesis. **W. Xi**, S. Pattanayak, C.J. Kloxin, C. Bowman

4:00 POLY **70.** New polymer synthesis strategy based on multicomponent reactions. **R. Kakuchi**, P. Theato

4:20 POLY **71.** Design and synthesis of segmented conjugated polymers via acyclic diene metathesis (ADMET). **G. Singh**, R.M. Peetz

4:40 POLY **72.** Synthesis and polymerization of new 2-substituted vinylimidazolium salts. **D. Smith, T. Muzio**, T.W. Smith

5:00 POLY **73.** Aza-Diels–Alder route to polyquinolines. **D.J. Dibble**, M. Umerani, A. Mazaheripour, Y. Park, A.A. Gorodetsky

Section E

Sheraton Denver Downtown Hotel
Directors Row J

Macromolecular and Nanoparticle Separation Science

Cosponsored by ANYL and PMSE

Financially supported by The Dow Chemical Company, Wyatt Technology, Tosoh BioScience, Waters, NIST

K. Beers, A. K. Brewer, W. Gao, A. M. Striegel, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 POLY **74.** Size and composition-based nanoparticles separations and analyses using field-flow fractionation. **K.R. Williams**

2:15 POLY **75.** Self-organization phenomena in biomacromolecules investigated by field flow fractionation. **A. Lederer**

2:45 POLY **76.** Asymmetrical flow field-flow fractionation for the comprehensive characterization of polymer assemblies. **F.M. Winnik**

3:15 Intermission.

3:30 POLY **77.** Measurement of size and certain structural features of sub-nanokilometer particles in suspension. **P.J. Wyatt**

4:00 POLY **78.** Asymmetric flow field flow fractionation: A versatile tool for nanoparticle separation. **C. Rosu**, R. Cueto, E. Reichmanis, P.S. Russo

4:30 POLY **79.** Semipreparative asymmetric flow field-flow fractionation for nanoparticle characterization. **C. Bria**, A. Ashames, P. Skelly, S.R. Williams

5:00 POLY **80.** Synthesis and characterization of functional polymer nanoparticles via sonogashira coupling. **A. Prasher**, D. Chao, E.B. Berda

Nanotechnology: Delivering on the Promise

Research & Development

Sponsored by PRES, Cosponsored by AGFD, AGRO, ANYL, CARB, CCPA, CCS, CHAS, COLL, COMSCI, CORP, ENFL, HIST, I&EC, IAC, MPPG, PMSE, POLY, SCHB and SOCED

MONDAY MORNING

Section A

Sheraton Denver Downtown Hotel
Directors Row E

Next Generation Smart Materials

Materials with Special Optical, Electronic and Mechanical Behavior

Cosponsored by PMSE‡

E. B. Berda, J. Foster, *Organizers*
Y. C. Simon, *Organizer, Presiding*
C. K. Lyon, *Presiding*

8:30 Introductory Remarks.

8:35 POLY **81.** Mechanochromism of block copolymer photonic gels. **E. Chan**, E.L. Thomas

9:05 POLY **82.** Development of mechanochemical and thermal triggers for release of small organic molecules. **A.J. Boydston**

9:35 POLY **83.** Responsive photonic multilayers from photo-crosslinkable polymers and nanocomposites. **R.C. Hayward**

10:05 POLY **84.** Voxelated liquid crystal elastomers. **T.J. White**, T.H. Ware, J. Wie

10:35 Intermission.

10:45 POLY **85.** Stretchable electronic materials and devices. **Z. Bao**

11:15 POLY **86.** Applying reconfigurable networks of charge-transporting polycyclic aromatic hydrocarbons to problems in energy storage. **B.A. Helms**, P.D. Frischmann, L.C. Gerber, S.E. Doris, C. Li

11:45 POLY **87.** Creating new architectures for π-conjugated semiconducting polymers. **C.K. Luscombe**

12:15 Concluding Remarks.

Section B

Sheraton Denver Downtown Hotel
Governor's Square 12

Putting Renewable Polymers to Work

Cellulosics

D. Boday, E. C. Hagberg, *Organizers, Presiding*

8:00 POLY **88.** High performance cement via cellulose nanocrystal addition. **J.P. Youngblood**, R. Moon, J. Weiss, P. Zavattieri, Y. Cao

8:30 POLY **89.** Effect of the electrical double layer on surface-initiated controlled radical polymerization from cellulose nanocrystals in aqueous media. **J.O. Zoppe**, X. Xu, H.A. Klok

8:50 POLY **90.** Can hemicelluloses be used for durable wood adhesives? **E.E. Malmström**, E. Norström, L. Fogelström, P. Nordqvist, F. Khabbaz

9:10 POLY **91.** Multifunctional fluorescent sensors for imaging the interphase in polymer nanocomposites. **J. Gilman**, D. Fox, J. Woodcock, J. Liddle, S. Stranick, R. Beams, G. Myers, C. Davis, N. Chen, L. Sacui

9:40 Intermission.

9:55 POLY **92.** Structured and functionalized nanocellulose for controlled release and implantation. **J. Foster**

10:25 POLY **93.** Renewable thermoplastic materials from cellulose. **J.H. Wang**, Y. Bai, B. Zhou, Z. Yu, Q. Jia, W. Wang, H. Tan

10:55 POLY **94.** Renewable thermoplastics from lignin. **A.K. Naskar**, C.D. Tran, A.S. Bova

11:15 Concluding Remarks.

Section C

Sheraton Denver Downtown Hotel
Governor's Square 14

Excellence in Graduate Polymer Research

Cosponsored by PRES, PROF, SOCED and YCC
Financially supported by IAB (ACS Polymer Division Industrial Advisory Board)

C. J. Ellison, T. E. Long, *Organizers*
H. N. Cheng, C. J. Landry-Coltrain, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 POLY **95.** Post-electrospinning derivatization of polymer nanofibers with bioactive species using translationally-relevant chemical methods. **J. Zheng**, D.H. Reneker, M. Becker

8:55 POLY **96.** Sequential inverse vulcanization and electropolymerization for conductive plastic sulfur. **P.T. Dirlam**, J. Pyun

9:15 POLY **97.** Manipulating conjugation in electronic polymers: Chemical sensors and precursor routes. **J.G. Weis**, T.M. Swager

9:35 POLY **98.** Poly(Ionic liquid)s and their block copolymers: Synthesis, characterization, self-assembly, and applications. **H. He**, H. Nulwala, K. Matyjaszewski

9:55 Intermission.

10:10 POLY **99.** Facile post-polymerization modification of blocked isocyanate and hydrazide containing polymers. **E.A. Hoff**, B. Abel, C.A. Tretbar, C.L. McCormick, D.L. Patton

10:30 POLY **100.** Sequencing in step-growth polymerization: Influence of segment length on thermomechanical properties of polysulfone-containing segmented polyesters. **J.M. Dennis**, G.B. Fahs, R.B. Moore, S.R. Turner, T.E. Long

10:50 POLY **101.** Olefin cross-metathesis, a mild, modular and efficient approach towards functionalized cellulose esters. **X. Meng**, J.B. Matson, K.J. Edgar

11:10 POLY **102.** Scalable production of mechanically tunable block polymers from sugar. **D.K. Schneiderman**, M. Xiong, F.S. Bates, K. Zhang, M.A. Hillmyer

11:30 Remarks by ACS President, Dr. Diane G. Schmidt, and Photo Session

Section D

Sheraton Denver Downtown Hotel
Governor's Square 15

Electrical, Thermal, & Mass Transport in Polymer Nanocomposites & Alloys

Barrier and Separation Behavior

Cosponsored by PRES

Financially supported by Avery Dennison, 3M, Bayer MaterialScience, Kuraray

J. C. Grunlan, M. Priolo, L. Wagberg, *Organizers*
P. Larsson, D. F. Schmidt, *Presiding*

8:30 Introductory Remarks.

8:35 POLY **103.** Electrospun composite membranes of cellulose acetate (CAc) and poly (vinyl alcohol) (PVA). **L. Baghernejad**, R. Ozer, R. Mohan, O. Shoham, S. Odueyungbo, E.V. Iski

8:55 POLY **104.** Assessing gas permeability in polymer nanolaminates. **E. Dunkerley**, D.F. Schmidt

9:25 POLY **105.** Thermally reduced graphene oxide-PEI multilayer thin films as electrically conductive gas barrier layer. **B. Stevens, J.C. Grunlan**

9:45 POLY **106.** Stretchable gas barrier achieved with partially hydrogen-bonded multilayer nanocoating. **K.M. Holder**, F. Xiang, B.R. Spears, M. Huff, M. Priolo, E. Harth, **J.C. Grunlan**

10:05 Intermission.

10:25 POLY **107.** Multilayered nanocomposites containing high aspect ratio particulates. **S. Nazarenko**

10:55 POLY **108.** Polymer membranes for gas and liquid separations. **B.D. Freeman**

11:25 POLY **109.** Polymer composites for gas separation membranes and sorbents. **W. Koros**

11:55 POLY **110.** Biomaterial-based barrier materials and composites: A review on how to prevent unwanted water interactions and water-induced property deterioration. **P. Larsson, L. Wagberg**

‡ *Cooperative Cosponsorship*

Section E

Sheraton Denver Downtown Hotel
Directors Row I

Macromolecular and Nanoparticle Separation Science

Cosponsored by ANYL and PMSE

Financially supported by The Dow Chemical Company, Wyatt Technology, Tosoh BioScience, Waters, NIST

K. Beers, A. K. Brewer, W. Gao, A. M. Striegel, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 POLY **111.** Polysaccharide characterization using asymmetrical flow field-flow fractionation and multiangle light scattering (AF4-MALS): Successes and challenges. **L. Nilsson**

9:20 POLY **112.** Asymmetrical flow FFF coupled with light scattering for the separation and the structural characterization of glucopolymers with various branching patterns. **A. Rolland-Sabate**, F. Grimaud, R. Iragues, S. Guilois, D. Lourdin, J. Putaux, G. Potocki-Véronèse, A. Buléon

9:55 POLY **113.** Characterization of hyaluronic acid and polymer JR using size exclusion chromatography with advanced detection techniques. **X.M. Liu**, E. Maziarz

10:30 Intermission.

10:45 POLY **114.** Challenges associated with size exclusion chromatography of amphiphilic cellulose ether materials. **D.M. Meunier**, Y. Li, E.M. Partain, M. Brackhagen, P. Oliver

11:20 POLY **115.** New approach to overcome hydrophobic interaction in cellulose ethers for reliable molecular weight characterization. **Y. Li**, D.M. Meunier, D. Redwine, M. Brackhagen, R. Adden

Nanotechnology: Delivering on the Promise

Opportunities and Challenges for Health, Safety and the Environment

Sponsored by PRES, Cosponsored by AGFD, AGRO, ANYL, CARB, CCPA, CCS, CHAS, COLL, COMSCI, CORP, ENFL, HIST, I&EC, IAC, MPPG, PMSE, POLY, SCHB and SOCED

Integrating Chemistry and Polymer Science Research into the Classroom

Sponsored by CHED, Cosponsored by PMSE and POLY

MONDAY AFTERNOON

Section A

Sheraton Denver Downtown Hotel
Directors Row E

Next Generation Smart Materials

Composite Materials and Smart Processes

Cosponsored by PMSE‡

Y. C. Simon, *Organizer*
E. B. Berda, J. Foster, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 POLY **116.** Ionic polymer carbon composites as a new design for electroactive actuators and sensors. **R.B. Moore**

2:05 POLY **117.** Thermal properties of polymer-inorganic composites. **M. White**

2:35 POLY **118.** Covalently linked polymer–clay nanocomposites: Polymer brushes grafted from lamellar organosilicates. **S.L. Burkett**, K.A. Winchell, E.W. Vaimberg

2:55 Intermission.

3:15 POLY **119.** Synthesis and characterization of ionically crosslinked polymer networks. **K.A. Cavicchi**

3:45 POLY **120.** Vinylic vitrimers. **M. Röttger**, R. Nicolay, L. Leibler

4:15 POLY **121.** Combined hydrophobicity and mechanical durability through surface nanoengineering. **P.R. Elliott**, S.P. Stagon, H. Huang

4:45 Concluding Remarks.

Section B

Sheraton Denver Downtown Hotel
Governor's Square 12

Innovations in Macromolecular Network Chemistry

Industrial Innovations in Polymer Chemistry

Cosponsored by BMGT

M. Hunt, C. Lipscomb, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 POLY **122.** Sustainable carbon sources for the chemical industry: CO_2 is becoming a direct and indirect component in polyurethane plastics. **C. Guertler**, K. Malsch, M. Wohak, A. Wolf, A. Bardow, N. von der Assen, W. Leitner, T.E. Mueller

2:05 POLY **123.** Building a portfolio of renewable diols for unsaturated polyester resins. **E.C. Hagberg**, P.D. Bloom

2:35 POLY **124.** From literature research to industrial production and back again: A polymer's tale. **L.M. Stratton**, B. Gordon III, T.W. Smith, K.M. Kayne

3:05 POLY **125.** Living polymerization routes to siloxane macromers. **J.D. Goff**, B. Arkles

3:35 POLY **126.** Enhanced material properties from new isomer configurations of polyetherimides. **P.M. Johnson**

4:05 Intermission.

4:20 POLY **127.** Pushing the boundaries for hydrocarbon extraction in the oil & gas industry through block copolymer technology. **E.B. Murphy**

4:50 POLY **128.** Advances in polyethyelene. **M. Demirors**

5:20 POLY **129.** Abundant, low cost U.S. shale gas supply stimulates polyolefins renaissance. **P. Brant**

Section C

Sheraton Denver Downtown Hotel
Governor's Square 14

Excellence in Graduate Polymer Research

Cosponsored by PRES, PROF, SOCED and YCC
Financially supported by IAB (ACS Polymer Division Industrial Advisory Board)

H. N. Cheng, C. J. Landry-Coltrain, *Organizers*
C. J. Ellison, T. E. Long, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 Recognition of Poster Presenters.

1:45 POLY **130.** Unexpected anomalous diffusion in associating protein hydrogels. **S. Tang**, M. Wang, B.D. Olsen

2:05 POLY **131.** Reducing-environment sensitive synthetic hydrogels for controlled delivery of therapeutics. **P.M. Kharkar**, A.M. Kloxin, K.L. Kiick

2:25 POLY **132.** Photodegradable hydrogels for studying axon guidance and the user-directed formation of neural circuits. **T. Brown**, D. McKinnon, K.S. Anseth

2:45 POLY **133.** Molecular N-dopants and N-dopable conjugated polymers. **B. Naab**, S. Zhang, X. Gu, E. Evans, T. Kurosawa, K. Vandewal, A. Salleo, G.L. Millhauser, S. Barlow, S.R. Marder, Z. Bao

3:05 Intermission.

3:20 POLY **134.** High-throughput screening of electrochromic polymers toward neutral colors. **M.T. Otley**, G.A. Sotzing

3:40 POLY **135.** Chiral transmission to self-assembling nanostructures from circularly polarized light. **J. Yeom**, B. Yeom, H. Chan, K. Smith, S. Dominguez-Medina, J. Bang, G. Zhao, W. Chang, S. Chang, A. Chuvilin, D. Melnikau, A. Rogach, P. Zhang, S. Link, P. Kral, N. Kotov

4:00 POLY **136.** Polymer-particle rheological analysis of adsorbed cement additives for improved processing. **L.R. Murray**, E.G. Soltys, K.A. Erk.

4:20 POLY **137.** Efficient simulation of the molecular scale behavior of polymer melts: Understanding polymer dynamics and rheology. **N.A. Rorrer**, J.R. Dorgan

Section D

Sheraton Denver Downtown Hotel
Governor's Square 15

Electrical, Thermal, & Mass Transport in Polymer Nanocomposites & Alloys

Energy, Electrical & Thermal

Cosponsored by PRES

Financially supported by Avery Dennison, 3M, Bayer MaterialScience, Kuraray

J. C. Grunlan, M. Priolo, L. Wagberg, *Organizers*
S. T. Iacono, J. P. Youngblood, *Presiding*

1:30 Introductory Remarks.

1:35 POLY **138.** Electrical and thermal conductivity of PAN/CNT composite fibers for heating behavior. **A. Chien**, S. Kumar

1:55 POLY **139.** Aqueous MWCNT dispersions and their highly thermally conducting coatings. **J. Texter, X. Ma**, R. Crombez

2:25 POLY **140.** Thermal and other properties in cellulose nanocrystal composite materials. **J.P. Youngblood**, J.A. Diaz, A. Martini, R. Moon

2:55 POLY **141.** Thermal and electrical transport in nanoconfined poly(3-hexylthiophene)-multi-walled carbon nanotube composite fibers. **M.K. Smith**, V. Singh, K. Kalaitzidou, B.A. Cola

3:15 Intermission.

3:25 POLY **142.** Metallized perfluoropolyether nanocomposites: New materials for structural energetics. S.C. Kettwich, J. McCollum, K.S. Kappagantula, N. Clayton, E. Avjian, H.A. Miller, D.W. Ball, M. Pantoya, **S.T. Iacono**

3:55 POLY **143.** Soft, compressible and fully Interdigitated 3D energy storage devices built by layer-by-layer assembly inside aerogels. **M.M. Hamedi, L. Wagberg, G. Nyström, A. Marais, E. Karabulut,** Y. Cui

4:25 POLY **144.** Hybrids of conducting polymers and carbon nanotubes for harvesting electrical energy and thermoelectric cooling. **C. Yu**

Section E

Sheraton Denver Downtown Hotel
Directors Row J

Macromolecular and Nanoparticle Separation Science

Cosponsored by ANYL and PMSE

Financially supported by The Dow Chemical Company, Wyatt Technology, Tosoh BioScience, Waters, NIST

K. Beers, A. K. Brewer, W. Gao, A. M. Striegel, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 POLY **145.** Temperature gradient interaction chromatography: Principle and applications. **T. Chang**

2:15 POLY **146.** Gradient elution at critical point of adsorption: Separation by chemical composition and microstructure. **Y. Brun**, C.J. Rasmussen

2:45 POLY **147.** Use of 2-D chromatographic techniques to elucidate macromolecular structures. **J.A. McConville**, P. Kilz, M. Adler, W. Radke, D. Lohmann

3:15 Intermission.

3:30 POLY **148.** Online 2D *a*TREF-*h*SEC technique for polyolefins characterization. **Y. Yu**, M. Hildebrand, M.A. Stepp, P.J. DesLauriers, C.C. Tso

4:00 POLY **149.** High temperature liquid chromatography of Polyolefin. **R. Cong**, W. deGroot

4:30 POLY **150.** Dual flow refractive index detection for polymer analysis by high temperature gel permeation chromatography. **A.K. Brewer**

5:00 POLY **151.** Exploring a chiral cross-linker by molecular imprinting using chromatographic and batch rebinding techniques. **B. Hebert**, D. Meador, D. Spivak

Nanotechnology: Delivering on the Promise

Bridging the Gap to a Thriving US Marketplace

Sponsored by PRES, Cosponsored by AGFD, AGRO, ANYL, CARB, CCPA, CCS, CHAS, COLL, COMSCI, CORP, ENFL, HIST, I&EC, IAC, MPPG, PMSE, POLY, SCHB and SOCED

Undergraduate Research Posters

Polymer Chemistry

Sponsored by CHED, Cosponsored by PMSE, POLY and SOCED

MONDAY EVENING

Section A

Colorado Convention Center
Halls C/D

Sci-Mix

M. Jeffries-El, D. Boday and T. White, *Organizers*

8:00 - 10:00

POLY **152.** Polyalkylmethacrylate-functionalized inorganic nanoparticles as solid-solid phase change materials: Effect of spacer length, molecular weight and graft density on heat storage capacity. **K.A. Stockmal, S. Granados Focil**

233-234, 243-245, 249-250, 256, 267, 270, 274, 278-279, 282, 284, 286, 288-289, 292-293, 296, 298, 306, 310-313, 315, 319-320, 323, 330, 343, 347, 369-371. See subsequent listings.

STRETCH Your Students' Polymer Knowledge by Putting Some BOUNCE into Your Curriculum

Polymer Science Education and the NGSS

Sponsored by CHED, Cosponsored by PMSE, POLY‡, RUBB and SCC‡

TUESDAY MORNING

Section A

Sheraton Denver Downtown Hotel
Governor's Square 14

Carl S. Marvel Creative Polymer Chemistry Award in Honor of Todd Emrick

M. Jeffries-El, T. P. Russell, *Organizers*
R. C. Hayward, J. Pyun, *Presiding*

8:30 Introductory Remarks.

8:35 POLY **153.** From molecules to functional materials: Controlling structure and properties through synthesis. **R.B. Grubbs**

9:05 POLY **154.** Metal oxide nanoparticle hybrids: New photoresists with extraordinary sensitivity. J. Jiang, B. Zhang, L. Li, E.P. Giannelis, **C.K. Ober**

9:35 POLY **155.** Harnessing biomimetic catch bonds to create mechanically robust nanoparticle networks. B. Iyer, V.V. Yashin, **A.C. Balazs**

10:05 POLY **156.** Exploiting reversible-covalent chemistry to investigate materials and mechanisms. H. Sun, C.P. Kabb, S. Mukherjee, **B.S. Sumerlin**

10:35 POLY **157.** Importance of the intricate linkage of the needs of particular biomedical applications to the design characteristics of functionally-sophisticated nanoscopic macromolecules to achieve efficacy. **K.L. Wooley**

11:05 POLY **158.** Bioconjugate and hybrid systems prepared by atom transfer radical polymerization. **K. Matyjaszewski**

Section B

Sheraton Denver Downtown Hotel
Governor's Square 12

Energy and Materials

Cosponsored by PMSE

S. T. Iacono, *Organizer*
S. Clarson, A. Sellinger, *Organizers, Presiding*

8:30 Introductory Remarks.

8:40 POLY **159.** Stability of substituted benzyltrimethyl ammonium cations in caustic environments. **M.R. Sturgeon**, H. Long, C. Macomber, D.M. Knauss, Y. Yang, B.S. Pivovar

9:10 POLY **160.** Interplay between relaxations and structure in anion-exchange membranes (AEMs). **V. Di Noto**, G. Nawn, K. Vezzù, F. Bertasi, E. Negro, S. Lavina, A. Maes, A.M. Herring, S. Ertem, E. Coughlin

9:30 POLY **161.** Hydroxide conductive benzyltrimethylammonium functionalized polysulfone-polyformal multiblock copolymers for alkaline fuel cells. **D.J. Strasser**, D.M. Knauss

9:50 POLY **162.** Understanding ionomer thin films. **A.Z. Weber**, A. Kusoglu, S. Shi, M. Tesfaye

10:20 Intermission.

10:35 POLY **163.** Diffusion NMR as a tool for understanding ion and solvent transport in anion exchange membranes. **H. Sarode,** Y. Yang, A.M. Herring

10:55 POLY **164.** Hydroxide degradation mechanism for cations in anion exchange membranes: A computational study. **H. Long**, B.S. Pivovar

11:15 POLY **165.** Polymer materials for energy applications: Structure-function studies of porous polymers. **S. Sivaram**

11:35 POLY **166.** Carbon/zirconia/fluoroionomer nanocomposites as polyelectrolyte-membrane fuel cell electrocatalyst support. **S.E. Creager**, J.A. Shetzline

Section C

Sheraton Denver Downtown Hotel

Plaza Court 8

Undergraduate Research in Polymer Science

Financially supported by Sabic Innovative Plastics, IAB (ACS Polymer Division Industrial Advisory Board)

S. E. Morgan, S. I. Nazarenko, *Organizers, Presiding*

8:00 POLY **167.** Hydrolytically stable bio-adaptable thiol-ene network. **D.A. Zamorano**, R. Reit, D. Simon, B.R. Lund, T. Ware, W. Voit

8:15 POLY **168.** Synthesis of p(NIPAM)-p(DMA) copolymers for protein conjugation. **D. Park**, M.N. Zhou, J.W. Lowe, K. Chiu, S.L. Goh

8:30 POLY **169.** Protein adsorption characteristics of amphiphilic starch-containing hybrid polymer films. **A.R. Linehan**, A. Sengupta, P.M. Iovine

8:45 POLY **170.** Expanding the one step acid hydrolysis/Fischer esterification of cellulose nanocrystals. S. Spinella, **V. Hepworth**, A. Maiorana, Q. Qian, R.A. Gross

9:00 POLY **171.** Design and synthesis of pH-responsive polymers to aid in cancerous tumor detection. **K. Farquhar**, L. Zhu, S.G. Boyes

9:15 Intermission.

9:30 POLY **172.** Antioxidant copolymers in biological applications. **D.M. Barber**, T.A. Brenner, L. Qiao, S.L. Goh

9:45 POLY **173.** Fabrication of conducting polymer/silk composite films with topographically nanopatterned surfaces. **N. Ostrovsky-Snider**, S. Severt, J. Larson, A. Murphy

10:00 POLY **174.** Synthesis of hollow polydimethylsiloxane microspheres. **S.J. Fuchs**, J.M. Rankin, K.S. Suslick

10:15 POLY **175.** Synthesis of resorcinarene-core polylactide/polyethylene glycol star block copolymers using click chemistry: Optimizing polymer coupling reactions using No-D NMR spectroscopy. **W.H. Horn**, A.E. Tipton, P.S. Corbin

10:30 POLY **176.** Shrinkage stress in two-stage reactive polymer systems. **B. Earle**, S. Chatani, M. Podgorski, C. Bowman

10:45 POLY **177.** Investigation of trans-1,4-polyisoprene as an organogelator for organic solvents. **P.G. Thomas**, K.A. Cavicchi

Section D

Sheraton Denver Downtown Hotel

Governor's Square 9

General Topics: New Synthesis & Characterization of Polymers

B. Barkakaty, D. Garcia, *Organizers*

K. M. Miller, T. Vokata, *Presiding*

8:00 POLY **178.** Michael addition polyester networks from imidazolium and 1,2,4-triazolium polymerizable ionic liquids. **K.M. Miller**

8:20 POLY **179.** Novel polyurethane/polyhydroxyurethane hybrid polymers and their applications as elastomers and adhesive bonding agents. **E.K. Leitsch**, W.H. Heath, J.M. Torkelson

8:40 POLY **180.** Polyurea glycopolymers from lactose and mannose modified-diamines with different diisocyanate comonomers: Synthesis and anticoagulant properties. **Y. Huang**, M.A. Shaw, E.S. Mullins, N. Ayres

9:00 POLY **181.** Novel poly(borosiloxane)s and their properties. **P. Puneet**, R. Vedarajan, N. Matsumi

9:20 POLY **182.** Reverse anomeric effect (RAE)-mediated syntheses of sugar poly(orthoesters). **L. Li**, K. Knickelbein, J. Wang, M.J. Obrinske, W. Du

9:40 POLY **183.** New monomers and catalysts for nonisocyanate polyurethanes. **R. Lambeth**

10:00 POLY **184.** Synthesis of biodegradable conjugated polymers with controlled backbone flexibility. **T. Vokata**, J. Moon

10:20 POLY **185.** Baylis-Hillman reaction as a versatile platform for the synthesis of densely functionalized polymers. **A. Joy**, C. Peng

10:40 POLY **186.** Redox-switchable copolymerization reactions. **J. Byers**, A.B. Biernesser, K. Delle Chiaie, J. Curley

11:00 POLY **187.** Reverse-selective gas separation membranes based on segmented copolymers of PEO and iptycene-containing polyimides. **R. Guo**, S. Luo, G. Kline

11:20 POLY **188.** Donor-acceptor conjugated polymers with modular electronic properties and very narrow band gaps. **J.D. Azoulay**, B. Zhang

Section E

Sheraton Denver Downtown Hotel

Directors Row I

Macromolecular and Nanoparticle Separation Science

Cosponsored by ANYL and PMSE

Financially supported by The Dow Chemical Company, Wyatt Technology, Tosoh BioScience, Waters, NIST

K. Beers, A. K. Brewer, W. Gao, A. M. Striegel, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 POLY **189.** Polymer separations utilizing 2D liquid chromatography: Inherent limitations and perspectives. **M.R. Schure**

9:15 POLY **190.** Computational/theoretical studies of polymer separations by liquid chromatography at critical condition (LCCC). **Y. Wang**

9:45 POLY **191.** Framework for exploring the effect of physical and chemical heterogeneities on polymer-surface interactions. **C.R. Snyder**, C.M. Guttman, E.A. Di Marzio

10:15 Intermission.

10:30 POLY **192.** Measurement of the surface interaction of solvated chains via model end-tethered polymer layers and self-consistent field theory. **R. Sheridan**, S.V. Orski, R.L. Jones, S. Satija, K. Beers

11:00 POLY **193.** Computations related to nanoparticle characterization and nanocomposite property estimation. **F. Vargas-Lara**, A. Hassan, E.J. Garboczi, J. Douglas

11:30 POLY **194.** Monovalent counter-ion mediated self-assembly of dendrimers. **S. Eghtesadi**

TUESDAY AFTERNOON

Section A

Sheraton Denver Downtown Hotel

Governor's Square 14

Carl S. Marvel Creative Polymer Chemistry Award in Honor of Todd Emrick

M. Jeffries-El, T. P. Russell, *Organizers*

R. C. Hayward, J. Pyun, *Presiding*

1:30 POLY **195.** Surface modification of porous polymer membranes to reduce fouling by oil/water emulsion. **B.D. Freeman**

2:00 POLY **196.** Micelle engineering via crystallization-driven self-assembly. **I. Manners**

2:30 POLY **197.** Tuning dispersion of nanoparticles in polymer matrices. **R.C. Hayward**

3:00 POLY **198.** Getting dopey with polymers and nanoparticles. **J. Pyun**

3:30 POLY **199.** New approaches to designer polymers. **C.J. Hawker**

4:00 POLY **200.** Structuring liquids with nanoparticles. M. Cui, T. Emrick, C. Huang, **T.P. Russell**

5:00 POLY **201.** Tailoring polymer synthesis for materials and devices. **T. Emrick**

5:30 Concluding Remarks.

Section B

Sheraton Denver Downtown Hotel

Governor's Square 12

Energy and Materials

Cosponsored by PMSE

S. T. Iacono, *Organizer*

S. Clarson, A. Sellinger, *Organizers, Presiding*

1:30 POLY **202.** Method of fabricating perfluorosulfonimde (PFSI) electrolyte materials. **J.S. Thrasher**, T.S. Sayler, A.V. Matsnev, R.E. Fernandez

2:00 POLY **203.** Highly conductive alkaline poly(phenylene oxide) poly(vinyl benzyl trimethyl ammonium) diblock membrane for anion exchange membrane fuel cell applications. **T.P. Pandey**, M.W. Liberatore, A.M. Herring

2:20 POLY **204.** Diblock copolymers of poly(2,6-dimethyl-1,4-phenylene oxide)-*b*-poly(vinylbenzyltrimethylammonium) prepared by nitroxide mediated polymerization for anion exchange membranes. **Y. Yang**, D.M. Knauss

2:40 POLY **205.** Transport and morphology of polymerized ionic liquid block copolymer anion exchange membranes with various cations. **K.M. Meek**, F.L. Beyer, Y.A. Elabd

3:10 Intermission.

3:25 POLY **206.** High-modulus, high-conductivity nanostructured polymer electrolyte membranes via polymerization-induced phase separation. **M.W. Schulze**, L.D. McIntosh, M.A. Hillmyer, T.P. Lodge

3:45 POLY **207.** Morphology and transport in a tris(2,4,6-trimethoxyphenyl) phosphonium functionalized PPO for alkaline fuel cells. **Y. Liu**, B. Zhang, Y. Yang, S. Seifert, Y. Yan, M.W. Liberatore, A.M. Herring

4:05 POLY **208.** Withdrawn.

4:25 POLY **209.** Ion transport in polymer electrolyte membranes for state of the art energy conversion technologies. **A.M. Herring**, G.A. Voth, T. Witten, E.B. Coughlin, D.M. Knauss, Y. Yan, M.W. Liberatore

Section C

Sheraton Denver Downtown Hotel

Plaza Court 8

Undergraduate Research in Polymer Science

Financially supported by Sabic Innovative Plastics, IAB (ACS Polymer Division Industrial Advisory Board)

S. E. Morgan, S. I. Nazarenko, *Organizers, Presiding*

1:30 POLY **210.** Rheological and morphological characterization of fractionated rigid-rod sulfone polymers. **J. Tropp**, K.M. Knauer, S.E. Morgan

1:45 POLY **211.** Improving flame resistance and softness of cotton fabric with ultrasonication rinsing of multilayered nanocoating. **M. Krecker**, T. Guin, A. Milhorn, J.C. Grunlan

2:00 POLY **212.** Development of hybrid magnetic cylindrical nanoparticles for pollutant remediation in aqueous environments. **S.M. Ward, A. Pavía-Sanders**, J.A. Flores, J.D. Russell, K.L. Wooley

2:15 Intermission.

2:30 POLY **213.** Dynamic topology of thermally-responsive materials via Diels-Alder chemistry. **M. Markmann,** M.R. Martinez, E.D. Crenshaw, T. Kleine, P.J. Costanzo

2:45 POLY **214.** Withdrawn.

3:00 POLY **215.** Strategies for recovery of Ru catalyst residues in olefin metathesis reactions. **W. Guzman**, J. Suriboot, J. Andrews, D. Bergbreiter

3:15 POLY **216.** Synthesis and characterization of a block copolymer containing and self-immolative block. **A. Engler**, A. Lane, C.G. Willson

3:30 Intermission.

3:45 Panel Discussion.

Section D

Sheraton Denver Downtown Hotel

Directors Row E

Polymer Composites and High Performance Materials

Functional High Performance Polymers

J. W. Gilman, M. Meador, M. Meador, S. E. Morgan, D. Savin, *Organizers*

J. Woodcock, *Presiding*

1:30 POLY **217.** Interactions between structure and properties that control moisture uptake in high-performance polycyanurates. **A.J. Guenthner**, M. Wright, A. Chafin, J.T. Reams, K.R. Lamison, M.D. Ford, S.P. Kirby, J.J. Zavala, V. Vij, J.M. Mabry

2:00 POLY **218.** Tuning the glass transition temperature and energy damping capabilities of thiol-ene thermoset networks. **O. McNair**, A. Janisse, D.A. Savin

2:30 POLY **219.** Alternative high performance polymers for ablative thermal protection systems. **T. Boghozian**

2:50 POLY **220.** Versatile conjugated polymer/di-ureasil hybrid materials: From enhanced emission quantum yields to white light emission. **N. Willis-Fox**, A. Marques, M. Kraft, U. Scherf, H. Burrows, R.C. Evans

3:10 POLY **221.** Intrachain radical chemistry as a facile route to well-defined polymeric nanostructures. **E.B. Berda**, J. Dickinson, J. Cole

3:40 POLY **222.** Oxygen permeation and thermoset degradation with temperature. **M.C. Celina**, N. Giron, A. Quintana

4:10 POLY **223.** Improving mechanical properties of highly branched perfluorinated polymer membranes. **M.J. Quast**, A.D. Argall, C.J. Hager, A. Mueller

4:30 POLY **224.** Development of flexible polyimide-urea aerogels cross-linked with a triisocyanate. **B.N. Nguyen**, M. Meador

Section E

Sheraton Denver Downtown Hotel

Directors Row J

Macromolecular and Nanoparticle Separation Science

Cosponsored by ANYL and PMSE

Financially supported by The Dow Chemical Company, Wyatt Technology, Tosoh BioScience, Waters, NIST

K. Beers, A. K. Brewer, W. Gao, A. M. Striegel, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 POLY **225.** Asymmetric flow field flow fractionation: An effective separation technique for polymers for which SEC/GPC fails. **S. Podzimek**

‡ *Cooperative Cosponsorship*

2:15 POLY **226.** Root causes of molecular weight loss of poly(cyclic butylene terephthalate) in pCBT/clay nanocomposites during processing. **J.W. Lyons**, J.J. Kiefer

2:45 POLY **227.** Leveraging polymer separation science to design new materials. **S. Moyses**, R.W. Allen, N. Jestel

3:15 Intermission.

3:30 POLY **228.** Monitoring kinetics of polymeric processes. M.F. Drenski, C.A. McFaul, A.M. Alb, F. Twigg, C. Jarand, **W.F. Reed**

4:00 POLY **229.** Polymeric antileaching agents that facilitate homogeneous catalysis. **M.L. Harrell**, C. Torres-Lopez, K. Gonzalez, D.E. Bergbreiter

4:30 POLY **230.** Combined hydrophobic/oleophobic membrane separation and extraction for fuel treatment. **A.J. Guenthner**, J.T. Reams, K.T. Greeson, K.R. Lamison, A.S. Vam, S.P. Kirby, A. Kota, G. Kwon, A. Tuteja, J.M. Mabry

5:00 POLY **231.** Surface patterning of ultrafiltration membranes to mitigate particulate and protein fouling. **S. Maruf**, Y. Ding, A.R. Greenberg, J. Pellegrino

TUESDAY EVENING

Section F

Colorado Convention Center
Hall D

Electrical, Thermal, & Mass Transport in Polymer Nanocomposites & Alloys

Cosponsored by PRES

Financially supported by Kuraray, Avery Dennison, Bayer MaterialScience, 3M

J. C. Grunlan, M. Priolo, L. Wagberg, *Organizers*

6:00 - 8:00

POLY **232.** Polyethylene-based composites containing graphene platelets: Enhanced barrier and electrical properties via multilayer coextrusion and interdiffusion. **K.P. Meyers**, J.J. Decker, D.R. Paul, D.A. Schiraldi, S.I. Nazarenko

POLY **233.** Investigating the reactivity of aluminum-based thermites with PFPE additive. **J.M. McCollum**, M. Pantoya, S.T. Iacono

POLY **234.** Effect of reinforcement fabrics on free standing thin film thermite mechanical properties and combustion. **B. Clark**, M. Pantoya, R. Heaps, M. Daniels

POLY **235.** Polyketone nanocomposite with non-covalently functionalized graphene for enhanced moisture barrier property. **I. Jeon**, T. Lee, J. Cho

POLY **236.** Inter- and Intra- molecular interactions in some oligothiophenes and ethylenedioxythiophenes: X-ray single crystal structural analysis. P.T. Pham, **M.M. Bader**

POLY **237.** Molecular modeling of electrical and thermal resistance across carbon nanotube and graphene nanoribbon contacts. **B.L. Farmer, V. Vasrhney**, S. Shenogin, J. Lee, A.A. Voevodin, A.K. Roy

POLY **238.** Withdrawn.

POLY **239.** Improved dielectric breakdown strength of nanocomposites containing surface modified fillers. **M.H. Bell**, M. Mohammadkhani, B.C. Benicewicz, T. Krentz, Y. Huang, L. Schadler, S. Virtanen

POLY **240.** Energy transport in molecules with repeating units occurs ballistically. **N. Rubtsova, C.M. Nyby**, H. Zhang, J. Jayawickramarajah, I.V. Rubtsov

Section F

Colorado Convention Center
Hall D

Energy and Materials

Cosponsored by ENFL and PMSE

S. Clarson, S. T. Iacono, A. Sellinger, *Organizers*

6:00 - 8:00

POLY **241.** Synthesis of dendronized polymers and their self-assembly to nanostructured materials. **P.E. Guzmán**, R.H. Grubbs

POLY **242.** Effects of Confinement on Structure and Proton Conductivity of PFSA. V. Sim, W. Han, **S.A. Ferdousi**, K.L. Yeung

POLY **243.** Design and synthesis of stable angular polycyclic aromatic hydrocarbons. **J.T. Ly, L. Zhang**, A.L. Briseno

POLY **244.** Preparation of polypyridylruthenium light harvesting polymers and application in water oxidation catalyst assembly. **J. Jiang**, G. Leem, Z. Chen, T. Pho, S. Keinan, Z. Fang, E. Puodziukynaite, J.R. Reynolds, K.S. Schanze

POLY **245.** Development and characterization of layer-by-layer assembled ferrocene polymer/enzyme films for usage as biofuel cell anodes. **N.P. Godman**, J. DeLuca, D. Schmidtke, D.T. Glatzhofer

POLY **246.** Synthesis and characterization of semifluorinated polyarylene copolymers. **S.M. Budy**, J. Jin, D.A. Loy, S.T. Iacono

POLY **247.** Bandgap tuning of silicon quantum dots using organic surface ligands. **R. Anderson**, J. Bell, B. Gorman, A. Sellinger, M. Lusk

POLY **248.** Synthesis and characterization of water stable, silicotungstic acid functionalized perfluorocyclobutyl polymer electrolyte. **A. Motz**

POLY **249.** Cyclopentadiene-containing π-conjugated polymers. **L. Chen**, A. Pietrangelo

POLY **250.** Modifying the bandgap of ITO and ZnO by 2eV using novel conjugated aromatic phosphonic and carboxylic acid ligands. **B.W. McNichols**, U. Koldemir, J.L. Braid, A. Morgenstern, M.E. Eberhart, R.T. Collins, D.C. Olson, A. Sellinger

Section F

Colorado Convention Center
Hall D

Excellence in Graduate Polymer Research

Cosponsored by PRES, PROF, SOCED and YCC

Financially supported by IAB (ACS Polymer Division Industrial Advisory Board)

H. N. Cheng, *Organizer*

C. J. Ellison, C. J. Landry-Coltrain, *Organizers*

6:00 - 8:00

POLY **251.** Fluorescence conjugated microporous polymers with amino receptors as metal cation chemosensor. **A. Chen**, J.L. Duffy-Matzner, W.E. Bernier, W.E. Jones

POLY **252.** Roles of quinoidal character, regioregularity, and polydispersity in determining the photovoltaic performance of conjugated copolymers. **T. Zheng**, L. Yu

POLY **253.** Magnetic core-fluorescent conjugated polymer shell nanoparticles prepared by surface-initiated Kumada polymerization. **S. Chatterjee**, C. Rosu, P.S. Russo, E.E. Nesterov

POLY **254.** Fast initiating nickel precatalysts for π-conjugated polymer synthesis. **A.O. Hall**, S. Lee, A.J. McNeil

POLY **255.** Growing green polymers using the sun: Organocatalyzed photoredox mediated polymerization. **J.C. Theriot**, G. Miyake

POLY **256.** Oximes as eversible links in polymer chemistry: Dynamic macromolecular stars. **S. Mukherjee**, A. Bapat, M. Hill, B.S. Sumerlin

POLY **257.** Molecule to morphology chirality-transfer in ABC triblock terpolymers. **A. Sarkar**

POLY **258.** Solid-state self-assembly: For advanced functional materials. **Y. Kim**, N. Kotov

POLY **259.** How processing affects dispersion and thermomechanical properties of waterborne epoxy and cellulose nanocrystal composites. **N. Girouard**, J.C. Meredith, M. Shofner, G. Schueneman

POLY **260.** Functional polymers via post-polymerization modification of poly(methionine). **E.G. Gharakhanian**

POLY **261.** Withdrawn.

Section F

Colorado Convention Center
Hall D

General Topics: New Synthesis & Characterization of Polymers

D. Garcia, T. Saito, *Organizers*

6:00 - 8:00

POLY **262.** One-step synthesis of poly(oxazoline)-based amphiphilic block copolymers using a dual initiator for RAFT polymerization and CROP. **Y. Yu, J. Youk**

POLY **263.** New binuclear α –diimine nickel catalysts for ethylene polymerization. **A.A. Alsaygh**

POLY **264.** Preparation of helical star polymers using tris-nickel Initiators. **D.A. Siriwardane**, J.F. Reuther, B.M. Novak

POLY **265.** Novel styrene sulfonate copolymer and its application. **S. Ozoe**

POLY **266.** Synthesis, morphological behavior, and ODT of poly(cyclohexadiene)-based copolymers. **K. Misichronis**, J. Chen, K.J. Kahk, A. Imel, M.D. Dadmun, J.G. Kennemur, F.S. Bates, J.W. Mays, K. Hong, A.T. Avgeropoulos

POLY **267.** Synthesis and facile end-group quantitation of functionalized PEG azides. **J.E. Semple**, B.T. Sullivan, K.N. Sill

POLY **268.** Effect of ethers on BF_3-initiated cationic ring-opening polymerization of glycidol. **C.M. Staton**, A.A. Chaudhry, E.A. Shcherbina, L.A. Searcy, A.T. Royappa

POLY **269.** Novel functional copolymers of styrene and alkoxy ring-substituted butyl 2-cyano-3-phenyl-2-propenoates. **H. Feng,** G.B. Kharas

POLY **270.** Chain-growth condensation rigid rod polymer brushes: Design and synthesis of a new polymer brush technique. **F.C. Prehn Jr**, S.G. Boyes

POLY **271.** Chemical reactivity of hydroxyl end-groups in bis-MPA based hyperbranched polymers. **M. Syed**, S. Nazarenko

POLY **272.** Comb-type triblock copolymers synthesized by RAFT polymerization and their capability for heavy crude oil emulsification. J. Huang, J. Xu, K. Chen, T. Wang, C. Cui, R. Zhang, L. Li, **X. Guo**

POLY **273.** Polymerization of PEEK AB monomers with oxyalkylene linkages via NAS and Friedel-Crafts reactions. **S. Hennelly**, W.A. Feld

POLY **274.** Synthesis of eumelanin- inspired polyindoles. **K. Sachinthani**, T.L. Nelson

POLY **275.** Synthesis of fluorescently labelled sodium polystyrenesulfonate via atom transfer radical polymerization. **P. Balding**, A.M. Blake, P.S. Russo, W. Huberty, R. Cueto

POLY **276.** Cyclic polymers via a solid-supported ruthenium-based metathesis catalyst system. **J.P. Edwards**, R.H. Grubbs

POLY **277.** Synthesis and characterization of eumelanin-inspired ethynylene-linked polymers. **S. Adhikari**, S. Selvaraju, T.L. Nelson

POLY **278.** Synthesis and characterization of alkoxy-functionalized polyselenophenes. **D. Khambhati**, T.L. Nelson

POLY **279.** Withdrawn.

POLY **280.** Broad spectrum antimicrobial effectiveness for synthetic mimic of antimicrobial peptides. **A.L. Fogel**, S.E. Exley, G. Sahukhal, B. Abel, M.O. Elasri, C.L. McCormick, S.E. Morgan

POLY **281.** PEGylated O_2-riched enzyme conjugatable polymer for long-term high performance electrochemical glucose sensors. **Z. Li**, S. Vaddiraju, F. Papadimitrakopoulos

POLY **282.** Biodegradable, functional polyesters for fused deposition modeling. **K. Dube**, M. Guvendiren, V.B. Damodaran, J.B. Kohn

POLY **283.** Regulation of protein properties via site-specific polymer conjugation. L. Wang, X. Li, H. Wang, L. Yuan, **H. Chen**

POLY **284.** Toward side-selective modification of microdialysis sampling polyethersulfone (PES) membranes. **S. Phillips**, J. Stenken

POLY **285.** Tuning the physical properties of poly(arylene ether)s prepared from 3,5-difluorobenzenesulfonamides. **R. Mitton**, E. Fossum

POLY **286.** Triplet-triplet annihilation upconversion from rationally designed polymeric emitters with tunable interchromophore distances. **X. Yu**, X. Cao, X. Chen, N. Ayres, P. Zhang

POLY **287.** Investigating the effects of a low refractive index counter-diffusive component in two-chemistry holographic photopolymer. **M. Alim**, B. Kowalski, C. Bowman, R. McLeod

POLY **288.** Polycraft: polymer chemistry in the evolving paradigm of education. **S. Parker**, B.R. Lund, W. Voit

POLY **289.** Chemo- and stereoselective polymerization of polar divinyl monomers by metallocenium catalysts. **F. Vidal**, E.Y. Chen

POLY **290.** Starch-containing hybrid polymers: Studying protein adsorption via quartz crystal nicrobalance with dissipation (QCM-D). **A. Sengupta**, A.R. Linehan, P.M. Iovine

POLY **291.** Synthesis and characterization of new low band gap polymers containing ethyl and phenyl ester fuctionalized polythiophene derivatives. **D.M. Shircliff**, B.M. Boardman

POLY **292.** Renewable polymers derived from ferulic acid, biobased diols and fatty acid derivatives via ADMET. I. Barbara, A.L. Flourat, **F. Allais**

POLY **293.** Electrochemical redox-unlocked smart polymeric ring. **A. Feng**, L. Peng, J. Yuan

POLY **294.** Study of polymer dynamics in linear low density polyethylene by solid state NMR. **L. Caire da Silva**, R. Graf, C. Bowers, K.B. Wagener

POLY **295.** Water based PEDOT conducting coating. **X. Liu**, J. Shen, Y. Feng, C. Ma, Z. Xiao, T. Fan, S. Tong, W. Zeng, Y. Liu, Y. Min

POLY **296.** Synthesis of shell- crosslinked nanoparticles from polyhydroxylsaccharides block-polylactides. **J. Wang**, L. Li, M. Obrinske, L. Bitterman, W. Du

POLY **297.** Developement of graphene/polyurea nacomposites based on admiceller polymerization. **T. Karim**

POLY **298.** Flocculation of emulsified oil using a novel amphiphilic and cationic chitosan-based flocculant. **T. Lyu, H. Zhao**

POLY **299.** Effects of Fullerene Chain Ends on Polymer Reptation. A. Zhou, R. Chen, S. Li, X. Sun, Y. Mi, **X. Wang**

POLY **300.** Large molecule incorporation into polyimide aerogel matrix for enhanced aerospace application. **S.L. Vivod**, M.B. Meador, C.R. Pugh

Section F

Colorado Convention Center
Hall D

Innovations in Macromolecular Network Chemistry

Cosponsored by PMSE

B. R. Lund, L. M. Stratton, A. J. Guenthner *Organizers*

6:00 - 8:00

POLY **301.** Novel chlorine-containing hypercross-linked polymers as adsorbent for removing organic pollutants from humid streams. W. Wang, C. Wang, K. Wang, J. Chen, Z. Liu, Z. Hao, **Z. Liu**

POLY **302.** Control of kinetics and stress development in polymer networks with acrylated vs. methacrylated polymer nanoparticles. **P.K. Shah, J.W. Stansbury**

POLY **303.** Light controlled thiol-Michael addition initiated by photocaged superbases. **X. Zhang, W. Xi, S. Chatani, M. Podgorski, C. Bowman**

POLY **304.** Synthesis of a biocompatible hydrogel platform for drug delivery using oxime click chemistry. **K.A. Gilmore**, D.B. Beezer, D.M. Stevens, E.A. Delesky, E.M. Harth

POLY **305.** Thiol-vinyl sulfone and thiol-vinyl sulfone-isocyanate crosslinking reactions to generate glassy and tough network polymers. **M. Podgorski**, D. Nair, E. Becka, C. Bowman

POLY **306.** Thiol-alkyne photopolymerization in miniemulsion: A facile route to functional polymer nanoparticles. **D.N. Amato**, D.A. Amato, M. Brei, R.F. Storey, D.L. Patton

POLY **307.** Visible-light initiator with potential for bottom-up photocuring. **S. Lewis**, M. Barros, K. Sarao, M. Makhija, J.W. Stansbury

POLY **308.** Toward "green" thermosets: Characterization of poly(alkylene mercaptosuccinates). G. Sternhagen, N. Levenhagen, **J.P. Droske**

POLY **309.** Studies on the synthesis and ion conductivities of sp3-hybridized boron-linked macrocycle-based covalent-organic network. **Y. Du**, H. Yang, W. Zhang

Section F

Colorado Convention Center

Hall D

Interacting with the Immune System using Polymeric Systems

B. De Geest, A. P. Esser-Kahn, *Organizers*

6:00 - 8:00

POLY **310.** Light controlled activation of immune cells via photocaged NOD1 agonist. **A.C. Chon**, A. Esser-Kahn

POLY **311.** Effect of spatially predetermined agonist presentation on immune response *via* polymeric systems. **K. Ryu**, K. Slowinska, R. Mancini, A.P. Esser-Kahn

POLY **312.** Synthesis of a photocaged NOD2 agonist for stimulation of innate immune cells. **A.M. Dark**, A. Esser-Kahn

POLY **313.** Enhancing CpG immunotherapy in brain cancer through improved delivery. **E. White**, D. Alizadeh, B. Badie, J.M. Berlin

Section F

Colorado Convention Center

Hall D

Macromolecular and Nanoparticle Separation Science

Joint POLY/PMSE Poster Session

Financially supported by The Dow Chemical Company, Wyatt Technology, Tosoh BioScience, Waters, Green Materials – ICE Science, University of Dallas

K. Beers, A. K. Brewer, W. Gao, A. M. Striegel, *Organizers*

6:00 - 8:00

POLY **314.** Use of high speed/high resolution size based chromatographic separation of polymeric materials with micro viscometric detection. **M.J. O'Leary**

POLY **315.** Online coupling of specialty detectors in GPC for chemical and molar mass detection. J.A. McConville, **D. Lohmann**, T. Hofe, M. Cudaj, G. Guthausen, M. Wilhelm

POLY **316.** Carbohydrate based hyper cross-linked organic polymers with –OH functional group for CO_2 separation. **H. Li**, B. Meng, S.M. Mahurin, S. Chai, D.C. Baker, H. Liu, S. Dai

Section F

Colorado Convention Center

Hall D

Next Generation Smart Materials

Cosponsored by PMSE‡

Y. C. Simon, E. B. Berda, J. Foster, *Organizers*

6:00 - 8:00

POLY **317.** Flexible SiO_2 nanofilms assembled on poly(ethylene terephthalate) substrates through a room temperature fabrication process. **S. Yamamoto, K. Sonobe**, M. Mitsuishi, T. Miyashita

POLY **318.** Degradable nanoparticles for light-assisted cancer invasion inhibition. **H. Chong**, S. Wang

POLY **319.** 3D printing of mechanochromic polycaprolactone on entry-level printers. **G.I. Peterson**, M.B. Larsen, M. Ganter, D. Storti, A.J. Boydston

POLY **320.** Nature-inspired intramolecular cyclization for fast light-triggered nanogel degradation. **C. de Gracia Lux**, J. Lux, G. Collet, S. He, M. Chan, J. Olejniczak, A. Almutairi

POLY **321.** Supramolecular polymers synthesized by thiol-ene click polymerization from supramonomer. **Q. Song**, F. Li, L. Yang, Z. Wang, X. Zhang

POLY **322.** ROS responsive tellurium-containing hyperbranched polymer. **R. Fang**, W. Cao, X. Zhang, H. Xu

POLY **323.** Endothelial cell attachment on shape memory polymer surfaces. **T. Govindarajan**, R. Shandas

POLY **324.** Interfacial fabrication of functional supramolecular polymeric networks for photocatalysis. **B. Yuan**, H. Yang, Z. Wang, X. Zhang

POLY **325.** Cooperative effect of cucurbit[8] uril-based π-π interaction. **Z. Huang**, K. Qin, L. Yang, Z. Wang, X. Zhang

POLY **326.** Withdrawn.

POLY **327.** Application of bioluminescence resonance energy transfer (BRET) in anticancer and antifungal research. **H. Bai**, S. Wang, X. Zhang

POLY **328.** Pursuing ordered microphase separation in mixed polymer brushes. **C.K. Simocko**, A.D. Price, D. Huber, A.L. Frischknecht, S. Hur, G.H. Fredrickson

POLY **329.** Shape memory properties of polymer networks formed using photomediated copper(I)-catalyzed azide alkyne cycloaddition (photo-CuAAC). **M. McBride**, A.D. Baranek, C. Bowman

POLY **330.** Bioderived polymers prepared from *N*-(acryloyl-2-pyrrolidone)s with ether and thio-ether-based residues. **R. Bhat**, A. Pietrangelo

POLY **331.** Fabrication and characterization of a radiopaque embolic hydrogel coil. **T. Lee**, H. Song, I. Jeon, J. Cho

POLY **332.** Novel hydrogelator for the creation of supramolecular structures for biomedical applications. **Y. Gao**, C. Berciu, D. Nicastro, B. Xu, F. Horkay

POLY **333.** Electrochemical redox responsive micelles based on host-guest interactions and star polymers. **L. Peng**, A. Feng, J. Yuan

POLY **334.** Production of polymeric composites with self-healing functionality by multi-axial electrospinning. **J. Seyyed Monfared Zanjani**, B. Saner Okan, M. Yildiz, Y.Z. Menceloglu

POLY **335.** Detecting early metal corrosion via "turn-on" fluorescence in smart epoxy coatings. **D. Ghosh**, W. Ming

POLY **336.** Withdrawn.

POLY **337.** Chemistry of MoS_2 solvent-assisted exfoliation: Correlation between moisture and the In-situ formation of reduction species. **R. Vaia**, D. Nepal, L.F. Drummy, K. Park

POLY **338.** Two-component molecular gels as smart biocompatible soft materials. **J. Miravet**, B. Escuder Gil, C. Berdugo, C. Felip, S. Diaz-Oltra

POLY **339.** Preparation of neutral color polymeric electrochromic devices using an commerical organic dye. **Y. Zhu**, M.T. Otley, X. Zhang, M. Li, G.A. Sotzing

POLY **340.** Rationally engineering phototherapy modules of eosin-conjugated responsive polymeric nanocarriers via intracellular endocytic pH gradients. **G. Liu**, S. Liu

Section F

Colorado Convention Center

Hall D

Polymer Composites and High Performance Materials

J. W. Gilman, M. Meador, M. Meador, D. Savin, *Organizers*

6:00 - 8:00

POLY **341.** Thermal and dynamic mechanical analysis of treated diatomaceous earth and epoxy films. **B.R. Sedai**, F.D. Blum

POLY **342.** Ionic polymer-carbon composites as a new design for electroactive actuators and sensors. **D.G. Mackanic**, R.B. Moore

POLY **343.** New perfluorocyclopentene-derived bisphenol cyanate ester for high performance applications. **C.A. Corley**, D.B. Barbee, S.T. Iacono

POLY **344.** Time delay of open cycle potential (OCP) measurement during the in-situ polymerization of polyaniline with graphene oxide nanosheets. **W. Tang**, C. Yuan, J. Wang, S. Mo, C. Zhao, Y. Liu, Y. Min

POLY **345.** Preparation and characterization of graphene /polyaniline composite with assistance of supercritical carbon dioxide. **W. Tang**, C. Yuan, J. Wang, S. Mo, C. Zhao, Y. Liu, Y. Min

POLY **346.** Graphene-based waterborne coatings and its preparation. **C. Ma**, J. Shen, Y. Feng, X. Liu, Z. Xiao, T. Fan, S. Tong, Y. Liu, Y. Min

POLY **347.** Adsorbed poly(vinyl acetate) on silica: experimental and molecular dynamics simulation studies. **H. Mortazavian, C.J. Fennell, F.D. Blum**

POLY **348.** Raman investigations on polyethylene oxide — TiO_2 nanocomposites. **I. Elamin**, D. Chipara, H. Huang, Y. Zhai, H. Xu, D. Hui, M. Chipara

Section F

Colorado Convention Center

Hall D

Putting Renewable Polymers to Work

D. Boday, E. C. Hagberg, *Organizers*

6:00 - 8:00

POLY **350.** Polymeric materials from biomass. **B.M. Upton**, A.M. Kasko

POLY **351.** Recycle method of waste plastics based on physical degradation theory. **S. Yao**, A. Tominaga, N. Takenaka, N. Oda, H. Sekiguchi, R. Nakano

POLY **352.** Aluminum(III) isopropoxide initiated polymerization of gluconolactone. **D. Saxon**, J. Scanlon

Section F

Colorado Convention Center

Hall D

Undergraduate Research in Polymer Science

S. E. Morgan, S. I. Nazarenko, Organizers

6:00 - 8:00

POLY **353.** Synthesis, characterization, and optical properties of perfluorocyclic arylamine polymers. **D.B. Barbee**, F. Carty, **S.T. Iacono**

POLY **354.** Synthesis, characterization, and utilization of tri(perylene bisimides) as an electron accepting material for polymer solar cells. **M. Roth**, L. Moore, S.E. Morgan

POLY **355.** Incorporation of Diels-Alder chemistry into polymer matrices via an inimer approach. **E.D. Crenshaw, M. Markmann**, T. Kleine, A.E. London, P.J. Costanzo

POLY **356.** Development of fluorocyclic silsesquioxanes as model templates for organically modified silica composites. **C. Thrasher**, A.R. Jennings, S.T. Iacono

POLY **357.** Toward high temperature ellastomers based on poly(arylene ether)s derived from 3,5-difluorobenzene sulfonamides. **J. Schmitz, E. Fossum**

POLY **358.** Tailoring the mechanical properties of conducting polymer films via crosslinking. **B. Farrell**, D. Spence, A. Murphy

POLY **359.** Optimization silk-polypyrrole composite films for use as electromechanical actuators. **J. Larson**, N. Bradshaw, C. Klemke, S. Severt, J. Leger, A. Murphy

POLY **360.** Molecular weight changing polymers via Diels-Alder chemistry. **M.R. Martinez**, M. Markmann, P.J. Costanzo

POLY **361.** Investigation of spin coating a thiol-ene/acrylate shape memory polymer for application in thin film flexible devices. **H. Guduru**

POLY **362.** Investigation of thermally induced microphase separation in dicarboximide functionalized oxanorbornyl diblock copolymers by atomic force microscopy. **T. Kolibaba**, D.A. Waldow

POLY **363.** Biobased replacements of bisphenol A diglycidal ether in epoxy resins. **C. Sago**, A. Maiorana, S. Spinella, R.A. Gross

POLY **364.** Investigation of self-assembled nanomorphologies of functionalized dicarboxide oxanorbornyl diblock copolymers via small angle X-ray scattering and optical birefringence. **J. Rosales**, D.A. Waldow

POLY **365.** Characterization and toxicity of alanine-based polymeric nanoparticles in D. *tigrina* planarian flatworms. **J.P. Wade**, S. Kumar, S. Taylor, E. Economou-Petrovits, R. Lidberg, P. De, L. Ramakrishnan

POLY **366.** Synthesis and characterization of novel ethylene oxide functionalized dicarboxide oxanorbornyl polymers for use as a lithium-ion electrolyte support. **D. Smith**, D.A. Waldow

POLY **367.** Reactivity ratio controlled polycondensation as a route to functional poly(arylene ether ketone)s. **K. Geremia**, E. Fossum

POLY **368.** Energy efficient, closed-loop, water-free protocol for processing of cellulosics with quantitative recovery of an ionic liquid solvent. D. Smith, **R. Carrazzone**, M. Schloder, T.W. Smith

POLY **369.** Multilayered nanocomposites with high aspect ratio graphene platelets: Controlled interdiffusion and improved gas barrier properties. **M. Otto, K. Meyers, S.I. Nazarenko**

POLY **370.** Performance evaluation of variable nitrogen containing five membered ring vinyl monomers and acrylonitrile copolymer. **K.L. Denson**, B. Batchelor, S. Mahmood, D. Yang

POLY **371.** Analysis of thiolene network compatibility with photolithographic solvents. **M. Seymour**, R. Reit, B.R. Lund, W. Voit

POLY **372.** Modeling of block copolymer thin film behavior between neutral and preferential interfaces. **M. Carlson**, W. Durand, G. Blachut, M. Maher, C.J. Ellison, C.G. Willson

POLY **373.** Self-assembly of size tagged triblock copolymer brushes via DNA hybridization. **A.H. Spring**

POLY **374.** Multifunctional polyurethane hydrogels for biomedical applications. **C. Seitz**, M. Nguyen-Kim, J. Borghs, J. Wallenborn

POLY **375.** Synthesis of jeffamine-based organogels and subsequent characterization using cavitation rheology. **S. Walley**, K.C. Bentz, D.A. Savin

POLY **376.** Rheological characterization of cementitious mixtures with excess polyethylene oxide. **E. Soltys**, L. Murray, K.A. Erk

Joint PMSE/POLY Poster Session

Sponsored by PMSE, Cosponsored by POLY‡

WEDNESDAY MORNING

Section A

Sheraton Denver Downtown Hotel

Directors Row J

Next Generation Smart Materials

Smart Nanomaterials, Composites, and Gels

Cosponsored by PMSE‡

E. B. Berda, J. Foster, *Organizers*

Y. C. Simon, *Organizer, Presiding*

D. Balkenende, *Presiding*

8:30 Introductory Remarks.

8:35 POLY **377.** Thermoresponsive supramolecular hydrogels based on diblock methylcellulose derivatives. **H. Kamitakahara**, A. Nakagawa, T. Takano

8:55 POLY **378.** Hollow nanogels and double-shell nanogels with advanced temperature responsiveness. **W. Richtering**, J. Dubbert, M. Karg, J. Pedersen

9:15 POLY **379.** Reversible aggregation of smart PEG-PDMAEMA diblock copolymers in aqueous solution. P. Conor, E. Stubbs, M. Schneider, D. Karis, **E.M. Glogowski**

9:35 POLY **380.** Shape memory polymer foams through emulsion-templating. I. Gurevitch, C. Warwar, **M.S. Silverstein**

9:55 Intermission.

‡ *Cooperative Cosponsorship*

10:15 POLY **381.** Bioderived poly(*N*-acryloyl-2-pyrrolidone)s: Structure/property correlations of a novel class of smart materials. R. Bhat, X. Sun, **A. Pietrangelo**

10:35 POLY **382.** Luminescent organoborane polymers for anion detection. **F. Jaekle**, F. Cheng, F. Guo, P. Chen, F. Pammer

10:55 POLY **383.** Liquid infused surfaces assembled by the layer-by-layer process. **N. Zacharia**, G. Zhu, C. Zhang

11:15 Concluding Remarks.

Section B

Sheraton Denver Downtown Hotel
Governor's Square 12

Energy and Materials

S. Clarson, *Organizer*
S. T. Iacono, A. Sellinger, *Organizers, Presiding*

8:30 POLY **384.** Design, synthesis, and characterization of new sulfonated aromatic polyamides as proton exchange membranes for fuel cells. **F. Liu**, D.M. Knauss

8:50 POLY **385.** Effect of hydration on mechanical properties of anion exchange membranes. M. Vandiver, B. Caire, Y. Li, D.M. Knauss, A.M. Herring, **M.W. Liberatore**

9:10 POLY **386.** Original blend membranes of partially fluorinated copolymers bearing azole functions with sulfonated PEEK for PEMFC operating at low relative humidity. **B.M. Ameduri**

9:40 Intermission.

9:55 POLY **387.** Foldable supercapacitors from triple networks of macroporous cellulose fibers, single-walled carbon nanotubes, and polyaniline nanoribbons. D. Ge, L. Yang, L. Fan, C. Zhang, X. Xiao, Y. Gogotsi, **S. Yang**

10:15 POLY **388.** Polymer materials for energy applications: Structure-function studies of porous polymers. **S. Sivaram**, S. Chatterjee, M. Arukkani

10:35 POLY **389.** Synthesis of perfluoropolyether-based electrolytes for lithium-ion battery applications. **D. Wong, J.M. DeSimone, N.P. Balsara**

10:55 POLY **390.** Design principles for constructing conducting redox polymer based battery materials. C. Karlsson, H. Huang, L. Yang, X. Huang, M. Strømme, R. Emanuelsson, A. Gogoll, **M. Sjödin**

11:15 POLY **391.** Mechanisms of self-discharge in p-doped conducting polymers. H. Olsson, C. Strietzel, Z. Qiu, M. Strømme, **M. Sjödin**

11:35 POLY **392.** Designer nanoporous materials for energy storage and energy conversion applications. **A. van Buuren**, J. Lee, M. Bagge-Hansen, T. Willey, P.G. Allen, B. Wood, J. Biener

Section C

Sheraton Denver Downtown Hotel
Directors Row E

General Topics: New Synthesis & Characterization of Polymers

B. Barkakaty, D. Garcia, *Organizers*
Y. A. Elabd, M. R. Van De Mark, *Presiding*

8:00 POLY **393.** Mechanochemical degradation of three-arm star polymers: Kinetics and modeling. **G.I. Peterson**, D. Church, A.J. Boydston

8:20 POLY **394.** Impact of alkyl chain length on ion conduction and morphology in polymerized ionic liquid diblock copolymers. **J.R. Nykaza**, S. Sharick, E. Davis, Y. Ye, K.A. Page, A. Jackson, F.L. Beyer, K.I. Winey, Y.A. Elabd

8:40 POLY **395.** Investigating the crystallinity of polytetrafluoroethylene (PTFE) by using terahertz time-domain spectroscopy (THz-TDS). **F. Senna Vieira, C. Pasquini**

9:00 POLY **396.** Application of single-chain polymer nanoparticles from consecutive ROMP-RCM process. **Y. Bai**, H. Xing, X. Phang, Y. Lu, S.C. Zimmerman

9:20 POLY **397.** High stiffness in aromatic-aliphatic poly(tyrosol carbonate) by hierarchical control over isomer sequence, phase behavior, and chain orientation. **S.D. Sommerfeld**, S.N. Murthy, Z. Zhang, M. Guvendiren, K. Dube, **J.B. Kohn**

9:40 POLY **398.** Electronic and spintronic properties of poly(3-methylthiophene) polymer brushes. **T.W. LaJoie**, W. You

10:00 POLY **399.** Middle and end labelled PMMA-d3: The effect of chain ends on polymer dynamics. **U.N. Arua**, F.D. Blum

10:20 POLY **400.** Dynamic surface tension comparison of colloidal unimolecular polymers with different hydrophilic groups: Sulfonate, carboxylate, and quaternary amine. **M.R. Van De Mark**

10:40 POLY **401.** Modified ABS for fused filament fabrication 3D printing with improved interlayer adhesion. **K. Yang**, B. Lund, D. Sydney, C. Thompson, R. Smaldone, W. Voit

11:00 POLY **402.** Anomalous thermal characteristics of poly(ionic liquids) derived from 1-butyl-2,3-dimethyl-4-vinylimidazolium salts. **T.W. Smith, M. Zhao**, F. Yang, D. Smith

11:20 POLY **403.** Coordinated experimental and theoretical study of a polydisperse polymer thin film. **B.S. Lokitz**, R. Kumar, M. Kilbey, S.W. Sides, J. Ankner, J.F. Browning, B. Sumpter

11:40 POLY **404.** Probing the interior of dendronized polymers with solvatochromic *p*-nitroanilino groups. **C. Gstrein**, A. Schlüter, B. Zhang

12:00 POLY **405.** Preparation of antibacterial surfaces by liquid-infused nanoporous polymer. **M. Okuom, D. Sabatka, A.E. Holmes**

Section D

Sheraton Denver Downtown Hotel
Directors Row I

Polymer Composites and High Performance Materials

Nanocomposites

J. W. Gilman, M. Meador, S. E. Morgan, D. Savin, *Organizers*
M. Meador, *Organizer, Presiding*

8:30 POLY **349.** Soft, lightweight conductors from nanoscale carbon. **M. Pasquali**

9:00 POLY **406.** Composites of graphene oxide and poly(vinyl acetate) — implications for enhanced mechanical behavior. B.K. Khatiwada, K. Bastola, R. Vaidyanathan, **F.D. Blum**

9:30 POLY **407.** Covalent functionalization of graphene-based platelets for tailored solubility and assembly. B. McGrail, B. Rodier, **E. Pentzer**

10:00 POLY **408.** Polymer grafted nanoparticle hybrids: Applications to gas separations and bimimetic materials. **S. Kumar**, C.J. Durning, B. Benicewicz

10:30 POLY **409.** Assemblies of conjugated polymers on carbon nanotubes. **L. Zhai**

10:50 POLY **410.** Improved carbon nanotube fibers through crosslinking and surface modification. **R. Ripy**, X. Lu, N. Kang, J.W. Mays

11:10 POLY **412.** Facile synthesis of controlled, high molecular weight polyacrylonitrile via low temperature RAFT polymerization. **J.D. Moskowitz**, B. Abel, A.J. Varni, J. Welch, C.L. McCormick, J.S. Wiggins

11:30 POLY **413.** Polymer matrix composites using covalently modified carbon nanotube sheets. **J.S. Baker**, M.A. Meador

Section E

Sheraton Denver Downtown Hotel
Governor's Square 14

Interacting with the Immune System using Polymeric Systems

Molecular Adjuvants

B. De Geest, A. P. Esser-Kahn, *Organizers, Presiding*

8:30 Introductory Remarks.

8:40 POLY **414.** Application of multi-agonist scaffolds to modulate antigen presentation and adaptive immunity. **J. Tom**, A. Esser-Kahn

9:00 POLY **415.** NIAID Adjuvant Program: Lessons and insights from the frontiers of vaccine adjuvant research. **W. Leitner**

9:50 POLY **416.** Syntheses and biological evaluation of toll-like receptor-7 agonistic macromolecules. **N. Shukla**, S.A. David, A. Izzo, C. Hamilton, C. Mutz, D.B. Salunke, P. Gao, R. Balakrishnan, R. Ukani, S. Malladi, T. Day, T. Lewis

10:20 Intermission.

10:50 POLY **417.** Programming immune responses with polymer carriers of Toll-like receptor (TLR) agonists. **G. Lynn**, R. Laga, B. Seder, L. Seymour

11:20 POLY **418.** Controlling the immune system with light: photo-active TLR agonists. **A.P. Esser-Kahn**, R. Mancini, L. Stutts, K. Ryu

WEDNESDAY AFTERNOON

Section A

Sheraton Denver Downtown Hotel
Directors Row J

Next Generation Smart Materials

Smart Nanomaterials, Composites, and Gels

Cosponsored by PMSE‡

E. B. Berda, J. Foster, Y. C. Simon, *Organizers*
M. A. Ayer, N. Zacharia, *Presiding*

1:30 Introductory Remarks.

1:35 POLY **419.** New opportunities in viral nanoparticle protein:polymer conjugates. J.D. Wallat, S. Isarov, J. Zhang, **J.K. Pokorski**

1:55 POLY **420.** Functionalized macro to micro shape memory materials. **V.S. Ashby**, K.R. Houston, S. Turner, S.M. Brosnan

2:15 POLY **421.** Single-chain nanoparticles via reversible acetal crosslinks. **C.K. Lyon**, E.B. Berda

2:35 POLY **422.** Optically responsive supramolecular glasses. **D. Balkenende**, C. Monnier, G. Fiore, C. Weder

2:55 Intermission.

3:15 POLY **423.** Thermally-responsive azo-containing polymeric materials. **M.A. Ayer**, Y.C. Simon, C. Weder

3:35 POLY **424.** Synthesis and phase behavior of alkyne-functionalized di- and triblock copolymers and their cobalt carbonyl adducts. **B. Jiang,** B. Qian, P. Yu, **R.B. Grubbs**

3:55 POLY **425.** Responsive hydrogels for cells in dulture. S. Patil, P. Chaudhury, L. Clarizia, M.J. McDonald, E. Reynaud, P. Gaines, **D.F. Schmidt**

4:15 POLY **426.** Helical polypeptides mediated nonviral gene and siRNA delivery. L. Yin, N. Zheng, H. Lu, N. Gbrielson, K. Kim, X. Deng, R. Zhang, **J. Cheng**

4:35 Concluding Remarks.

Section B

Sheraton Denver Downtown Hotel
Governor's Square 12

Energy and Materials

S. Clarson, *Organizer*
S. T. Iacono, A. Sellinger, *Organizers, Presiding*

1:30 POLY **427.** Organic photovoltaics: Materials microstructure and its effects on device parameters. **A. Salleo**

2:00 POLY **428.** High efficiency BODIPY lamellar organic photovoltaics. **J. Chen**, S.M. Conron, P. Erwin, M. Dimitriou, K. McAlahney, M.E. Thompson

2:20 POLY **429.** Role of linking chemistry on charge separation and photovoltaic performance of all-conjugated block copolymers. J. Mok, Y. Lin, K. Smith, K. Yager, S.B. Darling, D.J. Gosztola, Y. Lee, R. Schaller, E. Gomez, **R. Verduzco**

2:40 POLY **430.** Development of a DBfA Ttpe block copolymer for solar energy harvesting. **M. Hasib**, T.H. Nguyen, S.S. Sun

3:00 Intermission.

3:15 POLY **431.** All-polymer solar cells. **Z. Bao**

3:45 POLY **432.** Supramolecular polymer/fullerene composite nanofibers for organic photovoltaics. **Y. Qin**

4:05 POLY **433.** Toward conjugated polymer photovoltaic cells from low-cost starting materials. **M. Jeffries-El**, M. Ewan, A. Bhuwalka, B.J. Hale, E.W. Muller, B.M. Kobilka

4:35 POLY **434.** Semi-random donor-acceptor copolymers and terpolymers. **W.A. Braunecker**, Z.R. Owczarczyk, S.D. Oosterhout, N. Kopidakis, D.C. Olson

4:55 POLY **435.** Photon upconverting soft materials. **F.N. Castellano**

Section C

Sheraton Denver Downtown Hotel
Directors Row E

Innovations in Macromolecular Network Chemistry

Self-healing or Magnetic

Cosponsored by PMSE

B. R. Lund, *Organizer*
A. J. Guenthner, L. M. Stratton, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 POLY **436.** Oxime-functional hydrogels with tunable gelation and degradation behavior. **S. Mukherjee**, M. Hill, B.S. Sumerlin

2:00 POLY **437.** Reversible dynamic urea bond for the design of functional polymers. H. Ying, Y. Zhang, K. Cai, **J. Cheng**

2:20 POLY **438.** Supramolecular motifs in dynamic covalent PEG-hemiaminal organogel networks. **J.M. Garcia**

2:40 POLY **439.** Malleable and self-healing polymer networks based on dynamic imine bond. **A. Chao, D. Zhang**

3:00 Intermission.

3:20 POLY **440.** Emergent cure chemistry in the development of aerospace materials. **J.M. Mabry**, A.J. Guenthner, J.C. Marcischak, T.S. Haddad, J.T. Reams, M.D. Ford

3:45 POLY **441.** Charged induced formation of crystalline network polymer. **C.T. Yavuz**

4:05 POLY **442.** Magnetically induced free radical polymerization. **M. Soucek**, K. Miller, Z. He

4:30 POLY **443.** New methods for curing thermally stable polycyanurate networks based on magnetic induction heating of coated nanoparticles. **A.J. Guenthner**, C.M. Sahagun, J.M. Mabry

4:50 Concluding Remarks.

Section D

Sheraton Denver Downtown Hotel
Directors Row J

Polymer Composites and High Performance Materials

Biopolymers, Nanocomposites and Bioapplications

J. W. Gilman, M. Meador, M. Meador, S. E. Morgan, *Organizers*
D. Savin, *Organizer, Presiding*

1:30 POLY **444.** Structural nanocellulose composites. **J.P. Youngblood**, S. Chen, J. Liu, R. Moon, G. Schueneman

2:00 POLY **445.** Sustainable, high-performance fiber composites. **C. Kuncho, J. Möller, W. Liu, E. Reynaud,** D.F. Schmidt

2:30 POLY **446.** Processing and properties of polymer nanocomposites with cellulose nanocrystals. **C. Weder**, A. Nicharat, J. Sapkota, J. Foster

3:00 POLY **447.** Hierarchically structured nanocomposites. **J.R. Dorgan**, C. Moran, B. Liu, R. Sosa, L.O. Hollingsworth

3:30 POLY **448.** Stick-slip shear phenomenon of interfaces between cellulose nanocrystals. **S. Keten**, R. Sinko

4:00 POLY **449.** Application of natural fiber welding to the fabrication of biopolymer composite materials. **E. Fox**, E.K. Brown, L. Haverhals, D. Gray, B. Tisserat, T. Price, M. Brusoski, H.C. De Long, P.C. Trulove

4:30 POLY **450.** Ultrastiff nanocomposite hydrogels for biomedical applications. M. Jaiswal, J.R. Xavier, J.K. Carrow, P. Desai, **A.K. Gaharwar**

Section E

Sheraton Denver Downtown Hotel

Governor's Square 14

Interacting with the Immune System using Polymeric Systems

Immunoengineering

B. De Geest, A. P. Esser-Kahn, *Organizers, Presiding*

1:30 POLY **451.** NMR and kinetic studies of nitric oxide loading of poly(acrylonitrile-*co*-1-vinylimidazole) for advanced wound healing. **B. Batchelor**, A. Lowe, S. Mahmood, K.J. Balkus, B.M. Novak

1:50 POLY **452.** Poly(n-acetylgalactosamine)-antigen conjugates induce antigen-specific tolerance. **D.S. Wilson**, M. Damo, S. Kontos, G. Diaceri, J.A. Hubbell

2:15 POLY **453.** Biomaterials for recruitment and differentiation of endogenous regulatory T cells. **S. Little**

2:45 POLY **454.** Polymers for tumor immune therapy: In vitro and in vivo results on multifunctional cylindrical brush polymer conjugates. **M. Schmidt**, S. Gietzen, J. Buehler, C. Hoertz, M. Schinnerer, K. Fischer, A. Birke, M. Barz, C. Kappel, M. Bros, S. Grabbe

3:10 Intermission.

3:40 POLY **455.** Using small molecules to engineer and explore human immunity. **D.A. Spiegel**

4:10 POLY **456.** Modulation of the immune response by lymph node targeting. **H. Liu**

WEDNESDAY EVENING

Section F

Sheraton Denver Downtown Hotel

Plaza Ballroom AB

POLY/PMSE Plenary Lecture and Awards Reception

Cosponsored by PMSE

D. Boday, M. Jeffries-El, T. J. White, *Organizers, Presiding*

5:30 Network.

6:10 Introductory Remarks.

6:15 POLY **457.** Celebration of the award winners. **K.L. Wooley**

7:00 Awards Reception.

THURSDAY MORNING

Section A

Sheraton Denver Downtown Hotel

Directors Row J

Next Generation Smart Materials

Smart Nanomaterials, Composites, and Gels

Cosponsored by PMSE‡

E. B. Berda, J. Foster, Y. C. Simon, *Organizers*

C. K. Lyon, N. Zacharia, *Presiding*

8:30 Introductory Remarks.

8:35 POLY **458.** Size and rigidity dependent pharmacokinetics and biodistribution of cylindrical polymer brushes. **M. Muellner,** S.J. Dodds, T. Nguyen, D. Senyschyn, C. Porter, B. Boyd, F. Caruso

8:55 POLY **459.** Controlling actuation and locomotion: Geometry-composition-humidity gradient correlations for semiautonomic films. **R. Vaia**, D.H. Wang, P. Buskohl, L. Tan

9:15 POLY **460.** Tuning macroscopic properties using stimuli-responsive ionic liquid monomers. **J. Texter**

9:35 POLY **461.** Synthesis and dual-emissive properties of thiophene-substituted difluoroboron β-diketonates in poly(lactic acid). **M. Kolpaczynska**, C.A. DeRosa, W. Morris, C. Fraser

9:55 Intermission.

10:15 POLY **462.** Directed self-assembly of silicon-containing block copolymers for lithography. **M. Maher**, C. Rettner, C. Bates, G. Blachut, M. Carlson, W. Durand, J. Cheng, D.P. Sanders, C.J. Ellison, C.G. Willson

10:35 POLY **463.** Switchable ultrahydrophobic and superhydrophilic polymer surfaces: Synthesis, characterization, and application. **T. Hofe**

10:55 POLY **464.** Reversible single-chain selective point folding via cyclodextrin driven host/guest chemistry in water. **J. Willenbacher**, B. Schmidt, D. Schulze-Sünninghausen, O. Altintas, B. Luy, G. Delaittre, C. Barner-Kowollik

11:15 POLY **465.** Toward self-healing semiconducting polymers. **B.C. Schroeder**, Z. Bao

11:35 Concluding Remarks.

Section B

Sheraton Denver Downtown Hotel

Governor's Square 12

Energy and Materials

S. Clarson, *Organizer*

S. T. Iacono, A. Sellinger, *Organizers, Presiding*

8:30 POLY **466.** Light harvesting using colloidal quantum dots and hybrid organic-inorganic materials. **E. Sargent**

9:00 POLY **467.** Preparation of P3HT/CdS nanocomposites via in-situ nanocrystal growth in P3HT amphiphilic block copolymers. **M. Kern**, C. Tian, S.G. Boyes

9:20 POLY **468.** Rational material, interface, and device engineering for high-performance polymer and perovskite solar cells. **A.K. Jen**

9:50 POLY **469.** Synthesis, characterization, and properties of selectively fluorinated conjugated polymers for organic photovoltaics. **P. Homyak**, E. Coughlin

10:10 POLY **470.** Novel hierarchical composites of inorganic carbon and polysiloxanes for next-generation energy applications. **J.P. Lewicki**, M.A. Worsley, T. Baumann, E.B. Duoss, R.S. Maxwell

10:40 Intermission.

10:55 POLY **471.** Structure measurements for organic photovoltaics manufacturing. **D. DeLongchamp**

11:25 POLY **472.** Photoinduced charge transfer and thermal recombination dynamics of a ternary cascade heterojunction composed of poly(3-hexylthiophene), titanyl phthalocyanine, and Buckminsterfullerene. **J. Park**, O. Reid, G. Rumbles

11:45 POLY **473.** Expanding use of photovoltaics in the developing world: The Nanopower Africa and Power Ethiopia projects. **G. Beaucage**

12:05 POLY **474.** Withdrawn.

Section C

Sheraton Denver Downtown Hotel

Directors Row E

Innovations in Macromolecular Network Chemistry

Medical: Hydrogels and Particles

Cosponsored by PMSE

L. M. Stratton, *Organizer*

A. J. Guenthner, B. R. Lund, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 POLY **475.** Polymeric strategies for the encapsulation of cell lysates in view of anticancer immunotherapy. **L. Lybaert**, B. De Geest

8:55 POLY **476.** Natural p(TA) hydrogel and microgel networks for diverse potential biomedical uses. N. Sahiner, S. Sagbas, M. Sahiner, **N. Aktas**

9:15 POLY **477.** Multiresponsive polymer-protein conjugates as immuno-modulating stategy. **N. Vanparijs, R. De Coen, B. De Geest**

9:35 POLY **478.** Tethered-sphere networks: An ideal platform for property control. **T.S. Bailey**

9:55 Intermission.

10:15 POLY **479.** Printing of polymer hydrogels in micron sizes for the Co- and sequential delivery of drugs. **B.R. Spears**, D. Stevens, E. Harth

10:55 POLY **480.** Cyclic defects in tetrafunctional poly(ethylene glycol) networks and networks with mixed junction functionality. **K. Kawamoto**, M. Zhong, B.D. Olsen, J.A. Johnson

10:35 POLY **481.** Withdrawn.

11:15 POLY **482.** Development of hydrogels and functionalized silica surfaces utilizing novel fluorocyclic precursors. **A.R. Jennings**, C. Thrasher, S.T. Iacono

11:40 Concluding Remarks.

Section D

Sheraton Denver Downtown Hotel

Directors Row I

Polymer Composites and High Performance Materials

Nanoparticles & Nanocomposites

J. W. Gilman, M. Meador, M. Meador, D. Savin, *Organizers*

S. E. Morgan, *Organizer, Presiding*

8:30 POLY **483.** Hyperbranched epoxy with POSS modification for enhanced toughness polymer composites. **S.E. Morgan, Q. Jin, J. Misasi, J.S. Wiggins**

9:00 POLY **484.** Stacking intumescing multilayer thin film onto clay-based nanobrick wall to impart self-extinguishing fire retardant behavior to polyurethane. **K.M. Holder**, M. Huff, M. Cosio, J.C. Grunlan

9:30 POLY **485.** Effect of interfacial modification on the morphology and properties of polybenzimidazole/silica nanocomposite proton exchange membrane for use in fuel cells. **S. Singha**, T. Jana

9:50 POLY **486.** Improvement of mechanical properties of methacrylate based composites by latex particles. **B. Sandmann**, B. Happ, I. Perevyazko, S. Hoeppener, T. Rudolph, F.H. Schacher, M.D. Hager, U. Fischer, P. Burtscher, N. Moszner, U.S. Schubert

10:10 POLY **487.** Properties and synthesis of mixed bimodal nanoparticles via RAFT. **T.L. Neely**, B. Natarajan, L. Schadler, B.C. Benicewicz

10:40 POLY **488.** Development of nanosilica thermoset resins for filament winding and prepreg applications. **J.M. Nelson**

11:10 POLY **489.** Photografting random copolymers to nanoparticles for well-dispersed nanocomposites. **A.W. Hauser**, R.C. Hayward

11:30 POLY **490.** Interface-modified multilayer polymer films for high energy density capacitors. **M.A. Wolak**, M. Mackey, Z. Zhou, J. Carr, L. Zhu, E. Baer

Section E

Sheraton Denver Downtown Hotel

Governor's Square 14

Interacting with the Immune System using Polymeric Systems

Nanoparticulate Vaccination Strategies

B. De Geest, A. P. Esser-Kahn, *Organizers, Presiding*

8:30 POLY **491.** Pollen grains for oral vaccination. **H. Gill**

9:00 POLY **492.** mRNA based startegies for steering and amplifying the adaptive immune response. **B. De Geest**

9:20 POLY **493.** Nanoparticles for brain tumor immunotherapy. **J.M. Berlin**

9:50 Intermission.

10:20 POLY **494.** Modulating adaptive immunity with "carrier-free" polyelectrolyte multilayer films. Y. Chiu, L. Tostanoski, **C. Jewell**

10:50 POLY **495.** Engineering lipid-based vaccine nanoparticles for modulation of immune responses. **J. Moon**

THURSDAY AFTERNOON

Section A

Sheraton Denver Downtown Hotel

Directors Row J

Next Generation Smart Materials

Smart Nanomaterials, Composites, and Gels

Cosponsored by PMSE‡

E. B. Berda, J. Foster, Y. C. Simon, *Organizers*

M. A. Ayer, D. Balkenende, *Presiding*

1:30 Introductory Remarks.

1:35 POLY **496.** Concurrent block copolymer polymersome stabilization and bilayer permeabilization by stimuli-regulated "traceless" crosslinking. **X. Wang**, S. Liu

1:55 POLY **497.** Polymeric nanoparticles from cooperative polymerization and their dynamic behaviors. **L. Li**, C. Yuan, S. Thayumanavan

2:15 POLY **498.** Synthesis and characterization of thermoresponsive, biodegradable polyesters. **J.P. Swanson**, L.R. Monteleone, F. Haso, T. Liu, P.J. Costanzo, A. Joy

2:35 POLY **499.** Depolymerization kinetics and gas capture of polycarbodiimides. **B.L. Batchelor**, J.F. Reuther, B.M. Novak

2:55 Intermission.

3:15 POLY **500.** Stimuli-responsive microporous polymer hydrogels for treatment of severe limb wounds. **B.C. Streifel**, J. Lundin, G. Daniels, J.H. Wynne

3:35 POLY **501.** Enhanced dry adhesion from tapered nanorods and their shape effect. **Y. Cho**, G. Kim, Y. Cho, S. Lee, H. Minsky, K. Turner, D. Gianola, S. Yang

3:55 POLY **502.** To randomize or not to randomize: An investigation into the cell-uptake of polymers. **J. Moraes**, S. Recalcati, G. Gody, R. Peltier, S. Perrier, H.A. Klok

4:15 POLY **503.** Polyelectrolyte exceeding ITO capabilities in flexible electrochromics. **Y. Zhu**, M.T. Otley, X. Zhang, M. Li, G.A. Sotzing

4:35 Concluding Remarks.

Section B

Sheraton Denver Downtown Hotel

Governor's Square 12

Energy and Materials

S. Clarson, *Organizer*

S. T. Iacono, A. Sellinger, *Organizers, Presiding*

1:30 POLY **504.** Conjugated polymers for energy harvesting, storage and modulation. **J.R. Reynolds**

2:00 POLY **505.** Synthesis and characterization of conjugated fulvene chromophores and polymers. **S.M. Budy**, K.J. Knuths, A. Davidson, G.J. Balaich, D.W. Ball, S.T. Iacono

2:20 POLY **506.** Piezoelectric polymer composites: From energy harvesting to artificial muscles. **W. Voit**, C. Baur, G. Ellson

2:40 POLY **507.** Conductance bistability in non-conjugated polymers: Memristors in neuromorphic applications. **S.H. Foulger**

3:10 Intermission.

3:25 POLY **508.** Bioinspired green nanomaterials (GN) design and manufacture for post-combustion carbon capture and sequestration. **S.V. Patwardhan**

3:55 POLY **509.** Microvascular materials for mass and energy transport. **A.P. Esser-Kahn**, D.T. Nguyen

4:15 POLY **510.** Plastron trapping: Fluorinated surface treatment comparison to maintain stable plastrons under flow. **J.R. Alston**, M.A. Khan, R. Campos, A.J. Guenthner, J.M. Mabry

4:35 POLY **511.** Self-repairable polymeric networks that consume carbon dioxide and water. Y. Yang, **M.W. Urban**

4:55 POLY **512.** Safer and more energy efficient antifreeze. **E.V. Clancy**

‡ *Cooperative Cosponsorship*

Section C

Sheraton Denver Downtown Hotel
Directors Row E

Innovations in Macromolecular Network Chemistry

Click Chemistries

Cosponsored by PMSE

A. J. Guenthner, *Organizer*
B. R. Lund, L. M. Stratton, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 POLY **513.** Functional polymer nanoparticles via thiol-ene nanoemulsion photopolymerization. **D.A. Amato**, D.N. Amato, A.S. Flynt, D.L. Patton

1:55 POLY **514.** Raising the glass transition temperature of thiol–ene networks for dental applications. **J. Li**, T.F. Scott

2:15 POLY **515.** Wide bicontinuous compositional windows from co-networks made with telechelic macromonomers. **G.N. Tew**

2:35 POLY **516.** In situ polymerization of thiol-acrylate nanocomposite polymers with encapsulated stem cells. **L.A. Garber**, A. Forghani, J.A. Pojman, D. Hayes, R. Devireddy

2:55 Intermission.

3:15 POLY **517.** Softening polymer substrates for chronically soft neural interface. **W. Voit**

3:35 POLY **518.** Ester-free thiol-X resin: A new material with enhanced mechanical properties. **E. Becka**, M. Podgorski, C. Bowman

3:55 POLY **519.** Photoinitiated Cu(I)-catalyzed azide-alkyne cycloaddition (CuAAC) based networks. **A.D. Baranek**, H. Song, M. McBride, P. Finnegan, T. Gong, C. Bowman

4:15 POLY **520.** High temperature cyanate ester resins from renewable feedstocks: Upgrading through deoxygenation or conversion to hybrid resins. **B.G. Harvey, A.J. Guenthner, W.W. Lai, A. Chafin, M. Garrison, J. Reams, L. Cambrea, H.A. Meylemans, M.C. Davis**

4:35 POLY **521.** Renewable furan-based epoxy-amine thermosets. **G.R. Palmese**

4:55 Concluding Remarks.

Section D

Sheraton Denver Downtown Hotel
Directors Row J

Polymer Composites and High Performance Materials

Computation and Characterization

J. W. Gilman, M. Meador, M. Meador, S. E. Morgan, D. Savin, *Organizers*
A. L. Fogel, *Presiding*

1:30 POLY **522.** Dielectric spectroscopic analysis of cure behavior and relaxation processes in polymer composites. **M.K. Hassan**, C.H. Childers, K.A. Mauritz, J.S. Wiggins

2:00 POLY **523.** Aligned CNT composites: Quantitative analysis by TEM tomography. **J. Liddle**, B. Natarajan, T. Lam, R. Sharma, N. Lachman, D. Jacobs, B. Wardle

2:30 POLY **524.** Mapping the lyotropic phase behavior of diblock copolymer iongels. **T. Bennett**, I. Blakey, K.J. Thurecht, K. Jack

2:50 POLY **525.** Spectroscopic Investigations of polyethylene-carbon nanofibers composites. R. Benitez, **I. Elamin**, B. Jones, L. Jianhua, D. Chipara, K. Lozano, **M. Chipara**

3:10 POLY **526.** Computational design of next generation aerospace material systems. **E. Sapper**, I. Cole, M. Breedon, D. Winkler, F. Chen, C. Chu

3:40 POLY **527.** Connecting molecular to continuum: A multiscale modeling approach using molecular dynamics and finite element analysis to predict composite failure. **S.J. Tucker**, S. Christensen

4:10 POLY **411.** Lignin expanded acrylonitrile-butadiene-styrene (ABS) thermoplastic for composite applications. **A.K. Naskar**, S.K. Akato, D.L. Erdman

Section E

Sheraton Denver Downtown Hotel
Governor's Square 14

Interacting with the Immune System using Polymeric Systems

Macromolecular Engineering of the Immune Response

B. De Geest, A. P. Esser-Kahn, *Organizers, Presiding*

1:30 POLY **528.** Supramolecular peptide immunomodulators. C. Mora Solano, R.R. Pompano, T. Sun, J. Chen, A.S. Chong, **J.H. Collier**

2:10 POLY **529.** Engineering amphiphiles that target lymphoid tissues and optimally engage immune cells for more effective vaccines. **D.J. Irvine**

2:50 Intermission.

3:20 POLY **530.** Designing novel protein mimics from simple synthetic polymers. **G.N. Tew**

3:50 POLY **531.** Effect of 3D presentation of glycomimetic polymers on lectin interaction. **A.M. Kasko**, W. Liau, K. Lin

PMSE

Division of Polymeric Materials Science and Engineering

A. H. Tsou, Q. Lin, C. M. Stafford and M. Becker, *Program Chairs*

OTHER SYMPOSIA OF INTEREST:

Smart and Responsive Composites from Renewable Building Blocks *(see CELL, Tue, Wed)*

Integrating Chemistry and Polymer Science Research into the Classroom *(see CHED, Mon)*

Energy and Materials *(see POLY, Tue, Wed, Thu)*

POLY/PMSE Plenary Lecture and Awards Reception *(see POLY, Wed)*

Nanotechnology: Delivering on the Promise *(see PRES, Sun, Mon)*

WCC Rising Stars Awards Symposium *(see WCC, Mon)*

SOCIAL EVENTS:

Social Hour: Tue
Reception: Wed

BUSINESS MEETINGS:

Business Meeting: Sun, Mon

SUNDAY MORNING

Section A

Sheraton Denver Downtown Hotel
Directors Row J

Advances in X-ray and Neutron Scattering Techniques for Elucidating Polymer Morphology

Tutorial: Learnings & Developments

Y. Men, *Organizer*
R. Jones, A. I. Norman, *Organizers, Presiding*

9:15 Introductory Remarks.

9:30 PMSE **1.** Synchrotron facility for characterization of hierarchical structures — from microns to Angstroms in less than 3 minutes. **J. Ilavsky**

10:00 PMSE **2.** Travels in reciprocal space: A tutorial on images, microstructures, scattering, and Fourier transforms. A. Bons, **J. Butler**

10:30 Intermission.

10:45 PMSE **3.** Newest developments and adaptive strategies in laboratory SAXS (and WAXS) for polymer research. **S.W. Barton**, K. Joensen, S. Skou

11:15 PMSE **4.** Size, shapes, and crystalline structure of polymeric materials with a SAXS/WAXS instrument. **S. Rodrigues**, S. Desvergne-Bleneau, P. Panine, M. Fernandez-Martinez, F. Bossan

Section B

Sheraton Denver Downtown Hotel
Governor's Square 16

ACS Award in Applied Polymer Science: Symposium in Honor of Geoffrey W. Coates

W. Dichtel, *Organizer, Presiding*

8:25 Introductory Remarks.

8:30 PMSE **5.** Polymer brushes: Versatile 2D materials for interface engineering. D. Calabrese, M. Welch, **C.K. Ober**

9:00 PMSE **6.** Fun with block copolymers: New materials and processes using directed self assembly for nanoscale patterning. **P.D. Hustad**

9:30 PMSE **7.** Dynamic complex emulsion droplets. **T.M. Swager**, L. Zarzar

10:00 Intermission.

10:15 PMSE **8.** New strategies for living radical polymerization. **C.J. Hawker**

10:45 PMSE **9.** Pushing the limits of α-diimine-based catalysts for olefin polymerization. **B.K. Long**, J. Rhinehart, N. Mitchell, L. Brown

11:15 PMSE **10.** Controlling sequence, stereochemistry, and functionality in linear polymers prepared by ring-opening metathesis polymerization. **M.A. Hillmyer**

Section C

Sheraton Denver Downtown Hotel
Governor's Square 11

Design Principles of Functional Macromolecular Materials

Financially supported by IBM; Solvay; Aldrich; RSC: Journal of Materials Chemistry A, B & C, Soft Mater and Chemical Science

A. J. Boydston, L. M. Campos, K. L. Wooley, *Organizers*
E. Pentzer, *Organizer, Presiding*

8:00 PMSE **11.** Challenges facing directed assembly of block copolymers: Nanopatterning at the sub-10 nm scale. **J.M. Buriak**

8:30 PMSE **12.** Efficient intramolecular singlet fission in organic molecules. **M. Sfeir**, E. Busby, J. Xia, Q. Wu, J. Low, R. Song, J.R. Miller, X. Zhu, L.M. Campos

9:00 PMSE **13.** Putting side chains to work in conjugated materials. **S.W. Thomas**

9:20 Intermission.

9:35 PMSE **14.** Functional electronic polymer design. **Z. Bao**

10:05 PMSE **15.** Precursor conversion, nucleation, and growth of colloidal metal phosphide quantum dots. **B.M. Cossairt**, D. Gary, B. Glassy

10:35 PMSE **16.** Efficient syntheses of π-conjugated semiconducting polymers. **C.K. Luscombe**

11:05 PMSE **17.** Chemical transformations in bimetallic nanoparticle alloys. **J. Millstone**, L. Marbella, C.M. Andolina

Section D

Sheraton Denver Downtown Hotel
Directors Row H

Nanostructured Porous Polymers: Synthesis, Properties Applications

Nanostructured Porous Polymers for Membrane Application

B. D. Freeman, *Organizer*
D. L. Gin, H. Lin, *Organizers, Presiding*

8:30 PMSE **18.** Ion sorption and transport in ion-exchange membranes. **B.D. Freeman**

9:00 PMSE **19.** Controlled assemblies of cyclic peptide-polymer conjugates toward sub-nanometer porous membrane. **T. Xu**

9:30 PMSE **20.** Influence of nanoimprint lithography on the structure and permselectivity of ultrafiltration membranes. **S. Maruf**, M. Farr, E. Kujundzic, J. Yoshimura, Z. Ott, A.R. Greenberg, Y. Ding

10:00 Intermission.

10:30 PMSE **21.** CO_2-philic graphene oxide thin film composite membranes. **H. Park**, H. Kim, H. Yoon, B. Yoo, Y. Cho

11:00 PMSE **22.** Iptycene-containing polymeric membranes for efficient gas separation. **R. Guo**, J. Wiegand, S. Luo

11:30 PMSE **23.** Advanced materials and membranes for gas separations. **C. Liu**

Section E

Sheraton Denver Downtown Hotel
Governor's Square 17

Stimulus-Responsive Assemblies and Materials

Chemical Control of Materials Properties

J. Cha, A. P. Goodwin, *Organizers*
C. Bowman, *Organizer, Presiding*

8:30 PMSE **24.** Supramolecular concepts for patterning hydrogels. **A. Nelson**

9:00 PMSE **25.** Dynamic hydrazone-crosslinked hydrogels provide an adaptable matrix for 3D cell culture. **D. Domaille**, D. McKinnon, K.S. Anseth, J. Cha

9:30 PMSE **26.** Synthesis and evaluation of thermally-responsive coatings based upon Diels-Alder chemistry and renewable materials. D.N. Amato, G.A. Strange, J.P. Swanson, K.L. Varney, D.V. Amato, **P.J. Costanzo**

9:50 PMSE **27.** "Scaffolded" thermally remendable polymers with improved self-healing capabilities. **G. Berg**, A.D. Baranek, C. Bowman

10:10 PMSE **28.** Incorporation of dithiomaleimide mechanophores into polymeric materials. M. Karman, **Y.C. Simon**

10:30 Intermission.

10:45 PMSE **29.** Optically programmed buckling of polymer nanocomposite gels. **R.C. Hayward**

11:15 PMSE **30.** Damage precursor detection in polymer matrix composites. **E.M. Nofen**, J. Wickham, J. Zou, A. Chattopadhyay, L. Dai

11:35 PMSE **31.** Photolabile layer-by-layer films. **S.W. Thomas**

Section F

Sheraton Denver Downtown Hotel
Governor's Square 15

Graphene and Carbon Nanotubes: Synthesis, Devices and Applications

Energy Harvesting and Storage

A. D. Taylor, *Organizer*
G. S. Tulevski, *Organizer, Presiding*

8:30 PMSE **32.** Harvesting energy with semiconducting single-walled carbon nanotubes: From photovoltaics to thermoelectrics. **J. Blackburn**, A. Ferguson, A. Avery, A. Dowgiallo, R. Ihly, K. Mistry, J.C. Johnson

9:00 PMSE **33.** Few-walled carbon nanotubes for energy storage. **J. Liu**

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9:30 PMSE **34.** Ultrafast spectroscopic signature of charge transfer between single-walled carbon nanotubes and C_{60}. **A. Dowgiallo**, K. Mistry, J.C. Johnson, J. Blackburn

9:50 Intermission.

10:10 PMSE **35.** Influence of nanotube polydispersity on SWCNT-Si solar cells. **E. Hobbie**

10:40 PMSE **36.** Porous graphene from polymer templates and their use in energy storage applications. K. Liu, Y. Chen, **Y. Zhu**

11:10 PMSE **37.** Time resolved microwave conductivity on single-walled carbon nanotube fullerene heterojunctions. **R. Ihly**, K. Mistry, T. Clikeman, B. Larson, O.V. Boltalina, S.H. Strauss, G. Rumbles, J. Blackburn

Next Generation Smart Materials

Bio-inspired and Biomimetic Systems

Sponsored by POLY, Cosponsored by PMSE

Macromolecular and Nanoparticle Separation Science

Sponsored by POLY, Cosponsored by ANYL and PMSE

SUNDAY AFTERNOON

Section A

Sheraton Denver Downtown Hotel

Directors Row J

Advances in X-ray and Neutron Scattering Techniques for Elucidating Polymer Morphology

Tutorial: Learnings & Developments

A. I. Norman, *Organizer*

R. Jones, Y. Men, *Organizers, Presiding*

1:15 Introductory Remarks.

1:30 PMSE **38.** Basics of small-angle neutron scattering. **B. Hammouda**

2:00 PMSE **39.** Small angle X-ray scattering for morphological analysis of semicrystalline polymers: Modeling of the interface distribution function. **T. Thurn-Albrecht**, A. Seidlitz

2:30 Intermission.

2:45 PMSE **40.** New methods for measuring nanostructures: Grazing-transmission and variance scattering. **K. Yager**

3:15 PMSE **41.** Recent developments in high intensity high resolution in-house SAXS. **L. Jianhua**, A. Takase

Section B

Sheraton Denver Downtown Hotel

Governor's Square 16

ACS Award in Applied Polymer Science: Symposium in Honor of Geoffrey W. Coates

W. Dichtel, *Organizer, Presiding*

1:30 PMSE **42.** Targeted applications as inspirations to develop strategies toward polymer materials and nanoscopic devices derived from natural products. **K.L. Wooley**

2:00 PMSE **43.** Stille catalyst-transfer polycondensation of thiophene. **K.J. Noonan**

2:30 PMSE **44.** Development of epoxide/CO_2 copolymerization technology. **S. Allen**

3:00 Intermission.

3:15 PMSE **45.** Polymerization in 2- and 3D. **W. Dichtel**, B.J. Smith, G. Hwang, R.P. Bisbey, A.D. Chavez

3:45 PMSE **46.** Synthesis of functional materials using ROMP initiators. **R.H. Grubbs**

4:15 PMSE **47.** Catalysis for polymer synthesis. **R.M. Waymouth**

4:45 PMSE **48. Award Address** (ACS Award in Applied Polymer Science sponsored by Eastman Chemical). Advances in polymer chemistry enabled through catalyst design and discovery. **G.W. Coates**

Section C

Sheraton Denver Downtown Hotel

Governor's Square 11

Design Principles of Functional Macromolecular Materials

Financially supported by IBM; Solvay; Aldrich; RSC: Journal of Materials Chemistry A, B & C, Soft Mater and Chemical Science

A. J. Boydston, L. M. Campos, E. Pentzer, K. L. Wooley, *Organizers*

P. McGrier, *Presiding*

1:00 PMSE **49.** Mega-supramolecules for energy conservation and fire safety using long end-associative telechelics in fuel. **J.A. Kornfield**

1:30 PMSE **50.** Block copolymer templates for functional nanostructured materials. **H. Tran**, L.M. Campos

1:55 PMSE **51.** Dual stimuli responsive hydrogels. **A. Nelson**

2:25 PMSE **52.** Manipulating morphological characters with architecturally diverse block polymers for lithographic applications. **H. Minehara, L.M. Pitet, S. Kim, E.W. Meijer, C.J. Hawker**

2:45 Intermission.

3:00 PMSE **53.** Controlling molecular conformations of functional macromolecular materials. **L. Fang**

3:25 PMSE **54.** Cyano substituted benzothiadiazoles: Novel acceptor units allowing systematic lowering of conjugated polymer LUMO levels. **A. Casey**, Y. Han, Z. Fei, A.J. White, T.D. Anthopoulos, M.J. Heeney

3:45 PMSE **55.** Overcoming chirality-selected phase behavior in polypeptide complexes. **D. Priftis**, L. Leon, Z. Song, S. Perry, K.O. Margossian, A. Tropnikova, J. Cheng, M.V. Tirrell

4:05 PMSE **56.** Triggered delivery of therapeutic hydrogen sulfide from macromolecular and supramolecular carriers. **J.B. Matson**, J. Foster

Section D

Sheraton Denver Downtown Hotel

Directors Row H

Nanostructured Porous Polymers: Synthesis, Properties Applications

Nanostructured Porous Polymers for Membrane Application

D. L. Gin, H. Lin, *Organizers*

B. D. Freeman, *Organizer, Presiding*

R. Guo, *Presiding*

1:30 PMSE **57.** Nanoporous block copolymer membranes for ultrafiltration: A simple approach to size tunability. H. Ahn, **T.P. Russell**

2:00 PMSE **58.** Pore-size tuning in self-assembled block copolymer membrane. **K. Peinemann**, X. Qiu, H. Yu, S. Nunes

2:30 PMSE **59.** Membranes with artificial free-volume enabled by block copolymer self-assmebly. **N. Petzetakis**

3:00 Intermission.

3:30 PMSE **60.** Recent advances in the design of nanoporous polymers based on lyotropic liquid crystals for membrane applications. **D.L. Gin**, B.M. Carter, S.M. Dischinger, L.A. Robertson, M.G. Cowan, X. Feng, M.E. Tousley, S. Nejati, Y. Choo, R.D. Noble, M. Elimelech, C.O. Osuji

4:00 PMSE **61.** Nanoparticle-embedded water filtration membranes. H.A. Weinstein, N.S. Rentz, **L.F. Greenlee**

4:30 PMSE **62.** Synthesis of passive polymeric membranes for CO_2 separation. **S. Chatterjee**, T. Hong, S.M. Mahurin, J.W. Mays, A.P. Sokolov, T. Saito

Section E

Sheraton Denver Downtown Hotel

Governor's Square 17

Stimulus-Responsive Assemblies and Materials

Functional Materials and Surfaces

C. Bowman, J. Cha, *Organizers*

A. P. Goodwin, *Organizer, Presiding*

1:30 PMSE **63.** Remotely controlled stimuli-responsive materials. **S. Minko**

2:00 PMSE **64.** Self-healing electronic materials. **Z. Bao**

2:30 PMSE **65.** Composite organic conducting polymers with multiple (thermally accessible) conducting phases. **J. Galan-Mascaros**, Y. Koo, P. Maldonado-Illescas

2:50 PMSE **66.** Remarkable pressure responses of metal–organic frameworks: Proton transfer, linker coiling, order-to-disorder transition. A. Ortiz, A. Boutin, K.J. Gagnon, A. Clearfield, **F. Coudert**

3:10 PMSE **67.** UV-responsive organic thin-film transistors with a benzothiophene semiconductor dispersed in a polymer matrix. C. Smithson, D. Ljubic, **Y. Wu**, S. Zhu

3:30 Intermission.

3:45 PMSE **68.** Origami and kirigami nanocomposites. **N. Kotov**, T. Shyu, P. Damasceno, S.C. Glotzer

4:15 PMSE **69.** Color control in stimuli-responsive cholesteric liquid crystal composites. **T.J. White**, K. Lee, V. Tondiglia

4:45 PMSE **70.** Liquid crystal elastomers with a reversible and multistimulus response. H. Kim, T. Adetiba, **A. Agrawal**, B. Zhu, H. Chen, J. Jacot, **R. Verduzco**

5:05 PMSE **71.** Responsive liquid crystal/polymer aperiodic and periodic composites. **T.J. Bunning**, S. Serak, L. De Sio, E. Ouskova, R. Vergara, C. Umeton, N. Tabirian, T.J. White

Section F

Sheraton Denver Downtown Hotel

Governor's Square 15

Graphene and Carbon Nanotubes: Synthesis, Devices and Applications

Chemistry and Materials Science of 2-D Materials

A. D. Taylor, *Organizer*

G. S. Tulevski, *Organizer, Presiding*

1:00 PMSE **72.** Carbon nanomaterial heterostructure devices. **M. Hersam**

1:30 PMSE **73.** Flexible and conductive MXene-based nanocomposites with high volumetric capacitance. **Y. Gogotsi**, M. Zhao, Z. Ling, C.E. Ren, M.R. Lukatskaya, M.W. Barsoum

2:00 PMSE **74.** Synthesis of novel aromatic architectures through the benzannulation of aryl acetylenes. **W. Dichtel**, S. Hein, H. Arslan

2:30 PMSE **75.** Self-folding polymer-graphene bilayer sensors. T. Deng, C. Yoon, **Q. Jin**, M. Li, Z. Liu, D.H. Gracias

2:50 Intermission.

3:10 PMSE **76.** Hydrogenated graphene: Formation, stability, and applications. **P.E. Sheehan, K.E. Whitener**, W.K. Lee, J. Felts, J. Robinson, P. Campbell

3:40 PMSE **77.** Synthesis of polybenzoquinolines as graphene nanoribbon precursors. **Y. Park**, D.J. Dibble, M. Umerani, A. Mazaheripour, A.A. Gorodetsky

4:00 PMSE **78.** Nematic order drives macroscopic patterns of graphene oxide in drop drying. **S. Zhang**

4:20 PMSE **79.** Protein adsorbed graphene oxide nanosheets for intracllular protein and vaccine delivery. **H. Li**, B. De Geest

Section G

Sheraton Denver Downtown Hotel

Governor's Square 10

General Papers/New Concepts in Polymeric Materials

Polymer Nanotechnology

Q. Lin, *Organizer*

D. Zhang, S. Zhou, *Presiding*

1:30 PMSE **80.** Formation of sub-10 nm features with modified PS-PMMA. **S. Zhou**, D. Janes, C.G. Willson, C.J. Ellison

1:50 PMSE **81.** Photolithographic control of nanostructures in cross-linkable block copolymers. **G. Chado**, C. He, M.P. Stoykovich

2:10 PMSE **82.** Interfacial interactions between conjugated polymers and carbon nanotubes. **S. Zhang**

2:30 PMSE **83.** Graphene fiber induced polymer transcrystallization. **J. Abdou**, S. Zhang

2:50 PMSE **84.** ROMP-derived stimuli-responsive organoboron nanostructures. **G. Pawar**, J.B. Sheridan, F. Jaekle

3:10 Intermission.

3:30 PMSE **85.** Designing the porosity of bacterial cellulose nanopapers. **A. Mautner**, K. Lee, K. Li, A. Bismarck

3:50 PMSE **86.** Alternating donor-acceptor conjugated polymers entailing amide/imide-based accepting moieties toward semiconducting materials. **D. Zhang**

4:10 PMSE **87.** Nanothermometer: Measuring temperature change in nanometer scale on photothermal Au nanoparticles. **H. Sakalak**, H. Cavusoglu, B. Buyukbekar, G. Demirel, M. Citir, M. Yavuz

4:30 PMSE **88.** Microfabrication of microfluidic devices via reaction-diffusion. **M. Kleiman**, K. Brubaker, D.T. Nguyen, A. Esser-Kahn

Next Generation Smart Materials

Bio-inspired and Biomimetic Systems

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Macromolecular and Nanoparticle Separation Science

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MONDAY MORNING

Section A

Sheraton Denver Downtown Hotel

Directors Row J

Advances in X-ray and Neutron Scattering Techniques for Elucidating Polymer Morphology

Thin Films, Membranes & Fibrous Polymers

R. Jones, *Organizer*

Y. Men, A. I. Norman, *Organizers, Presiding*

8:30 PMSE **89.** Functional Group Depth Profiling with Resonant Soft X-ray Reflectivity. **D. Sunday**, E. Chan, C.M. Stafford

8:50 PMSE **90.** Simultaneous SAXS/WAXS investigation of out-of-equilibrium polymer films. **P. Panine**, S. Desvergne, M. Fernandez-Martinez, S. Rodrigues, F. Bossan

9:20 PMSE **91.** Resonant soft X-ray scattering for soft materials. **C. Wang**, A. Young, A. Hexemer, H. Padmore

9:50 PMSE **92.** Structure and morphology of P3HT and P3HT-containing donor-acceptor block copolymers as elucidated by x-ray scattering methods. **T. Thurn-Albrecht**

10:20 Intermission.

10:35 PMSE **93.** Structure studies of natural cellulose microfibrils by synchrotron small-angle X-ray scattering. **B.S. Hsiao**, B.T. Chu, Y. Su

11:05 PMSE **94.** Structure evolution of polymer grafted nanoparticle assemblies by selective solvent annealing of the canopy. **J. Che**, C.A. Grabowski, H. Koerner, R.A. Vaia

11:25 PMSE **95.** Small-angle X-ray studies of the morphological change of anion exchange membranes under uniaxial extensional strain. **B.R. Caire**, M. Vandiver, S. Seifert, M.W. Liberatore

‡ *Cooperative Cosponsorship*

11:45 PMSE **96.** Infrared and neutron reflectometry of sulfonated poly(ether ether ketone) interfaces with Pt and SiO_2. **J.H. Doan**, J.A. Dura, E.S. Smotkin

Section B

Sheraton Denver Downtown Hotel

Governor's Square 16

Cooperative Research Award: Symposium in Honor of Andy Tsou and Benjamin Hsiao

Financially supported by ExxonMobil

B. T. Chu, D. Schulz, *Organizers, Presiding*

8:30 Introductory Remarks.

8:30 PMSE **97.** Crystallization of polyolefins under flow and deformation. **B.S. Hsiao**, A.H. Tsou

9:00 PMSE **98.** Miscibility and crystallization in hydrocarbon block and block-random copolymers. **R.A. Register,** B.S. Beckingham, A.B. Burns

9:30 PMSE **99.** Supramolecular assembly: Giant polyhedrons and giant surfactants based on "nanoatoms". **S.Z. Cheng**

10:00 PMSE **100.** Fluorinated block copolymers: New materials as environmentally benign anti-fouling coatings. B. Wenning, D. Calabrese, **C.K. Ober**

10:30 PMSE **101.** Electrospun fibrous membrane for reducing postoperative peritoneal adhesion and for targeted drug delivery. **C.C. Han**

11:00 PMSE **102.** Cellulose nanofibers as a key component in separation membranes. **B.T. Chu, B. Hsiao**

Section C

Sheraton Denver Downtown Hotel

Governor's Square 11

Design Principles of Functional Macromolecular Materials

Financially supported by IBM; Solvay; Aldrich; RSC: Journal of Materials Chemistry A, B & C, Soft Mater and Chemical Science

A. J. Boydston, L. M. Campos, E. Pentzer, K. L. Wooley, *Organizers*

J. B. Matson, *Presiding*

8:30 PMSE **103.** Understanding mechanochemistry from first principles. **T. Martínez**

9:00 PMSE **104.** Linking molecular design of the polymer functionalization to tune grafted particle assembly or dispersion within domains and interfaces of polymer matrices. **A. Jayaraman**

9:25 PMSE **105.** Isophthalic acid - pyridine H-bonding: A simple yet versatile supramolecular synthon for the design of functional polymers. **L. Montero de Espinosa**, S. Balog, C. Weder

9:45 PMSE **106.** Synthesis and spontaneous segregation of functional bottlebrush polymer additives. **S.L. Pesek**, X. Li, I. Mitra, G. Stein, R. Verduzco

10:05 Intermission.

10:20 PMSE **107.** Design principles for charge storage within redox-active covalent organic frameworks. C.R. DeBlase, H.D. Abruna, **W. Dichtel**

10:50 PMSE **108.** Ring-opening metathesis oolymerization (ROMP) via electroorganic synthesis. **K. Ogawa**, A. Goetz, A.J. Boydston

11:15 PMSE **109.** Polymer mechanochemistry at surfaces. **H. Klok**

11:35 PMSE **110.** Flow IEG: A scalable route to sequence and architecturally defined unimolecular macromolecules. **F.A. Leibfarth**, J.A. Johnson, T.F. Jamison

Section D

Sheraton Denver Downtown Hotel

Directors Row H

Nanostructured Porous Polymers: Synthesis, Properties Applications

Nanostructured Porous Polymers for Sorbents

H. Lin, *Organizer*

B. D. Freeman, D. L. Gin, *Organizers, Presiding*

8:30 PMSE **111.** Porous organic polymers: synthesis and absorption/transport properties. **S.T. Nguyen**

9:00 PMSE **112.** Directing structural features and gas sorption properties of nanoporous polymers. O. Buyukcakir, **A. Coskun**

9:30 PMSE **113.** Nanoporous selective absorbents based on semicrystalline syndiotactic polystyrene. **S. Nazarenko**

10:00 Intermission.

10:30 PMSE **114.** Porous organic polymers for electrocatalysis and photoresponsive gas adsorption. **W. Zhang, Y. Zhu, G. Lu, H. Yang, Y. Jin**

11:00 PMSE **115.** Rational design of porous organic polymers for decontamination. **G. Barin, J.R. Long**

11:30 PMSE **116.** Effect of cross-link density on carbon dioxide separation in PDMS norbornene membranes. **T. Hong**, Z. Niu, S.M. Mahurin, D. Jiang, B.K. Long, J.W. Mays, A.P. Sokolov, T. Saito

Section E

Sheraton Denver Downtown Hotel

Governor's Square 17

Stimulus-Responsive Assemblies and Materials

Tunable Particles and Surfaces

C. Bowman, A. P. Goodwin, *Organizers*

J. Cha, *Organizer, Presiding*

8:30 PMSE **117.** One-step preparation of thermo/photosensitive nanogels and their use as stabilizers of Pickering high internal phase emulsions. **F.M. Winnik**, X. Zhang

9:00 PMSE **118.** Building responsive materials from compartmentalized microparticles. **J. Lahann**

9:30 PMSE **119.** Polymer directed self assembly of pH-responsive antioxidant nanoparticles. **R.K. Prudhomme**

9:50 PMSE **120.** Responsive porous polymers through emulsion-templating. M. Ovadia, I. Gurevitch, **M.S. Silverstein**

10:10 PMSE **121.** Nanogel-based stimulus-responsive capsules with tunable wall permeability. **A. Pich**

10:30 Intermission.

10:45 PMSE **122.** Responsive nanomaterials: Combining nanostructures, cells, and ultrathin polymer films. **V.V. Tsukruk**

11:15 PMSE **123.** Reversible tuning of pore size and CO_2 adsorption in a series of azobenzene functionalized porous organic polymers (POPs). **Y. Zhu**, W. Zhang

11:35 PMSE **124.** Star polyelectrolytes based microcapsules with multiresponsiveness to ionic strength, pH, and temperature. **W. Xu**, P.A. Ledin, F. Plamper, C. Synatschke, A. Mueller, V.V. Tsukruk

Section F

Sheraton Denver Downtown Hotel

Governor's Square 9

Graphene and Carbon Nanotubes: Synthesis, Devices and Applications

Low-D Carbon Devices and Materials

G. S. Tulevski, *Organizer*

A. D. Taylor, *Organizer, Presiding*

8:30 PMSE **125.** How will carbon nanotubes impact the next generation of electronics? **A. Franklin**

9:00 PMSE **126.** Materials science and applications of exceptionally electronic-type sorted semiconducting carbon nanotubes in field effect transistors and photovoltaics. **M. Arnold**

9:30 PMSE **127.** Synthesis and photophysical investigation of a series of porphyrin-containing polymers that helically wrap single-walled carbon nanotubes. **M.G. Glesner**, H. Yoo, J. Olivier, P. Deria, M.J. Therien

9:50 Intermission.

10:10 PMSE **128.** Semiconducting SWCNT enrichment via conjugated polymer extraction. **P.R. Malenfant**, J. Ding, Z. Li, J. Lefebvre, F. Cheng, C. Homenick, J. Dunford, N. Du, G.P. Lopinski, R. James, C. Kingston, B. Simard, J. Humes, J. Kroeger

10:40 PMSE **129.** Graphene photonics and plasmonics. **F. Xia**

11:10 PMSE **130.** Dose-controlled, floating evaporative self-assembly and alignment of semiconducting carbon nanotubes (SWCNTs) from organic solvents. **Y. Joo**, G.J. Brady, M. Arnold, P. Gopalan

11:30 PMSE **131.** Novel route to fabericate graphene oxide quantum dots (GOQDs) and graphene quantum dots (GQDs). T. Fan, C. Yuan, W. Tang, S. Tong, S. Mo, C. Zhao, Y. Liu, **Y. Min**

Section G

Sheraton Denver Downtown Hotel

Governor's Square 10

General Papers/New Concepts in Polymeric Materials

Polymeric Biomaterials and Applications

Q. Lin, *Organizer*

A. K. Gaharwar, P. B. Smith, *Presiding*

8:50 PMSE **132.** Elastomeric and mechanically stiff nanocomposite for bone tissue engineering. P. Kerativitayanan, **A.K. Gaharwar**

9:10 PMSE **133.** Biobased composites for tissue engineering from tung oil and collagen. **R.L. Quirino**, D.B. Page, A. Stewart, A. Scholz

9:30 PMSE **134.** Enhanced bone cell functions on poly(⊠-caprolactone) networks grafted with polyhedral oligomeric silsesquioxane nanocages. L. Cai, C.H. Sprague, C. Foster, **S. Wang**

9:50 PMSE **135.** Poly(ε-caprolactone) networks tethered with dangling poly(L-lysine) chains for promoting smooth muscle cell functions. X. Liu, **S. Wang**

10:10 Intermission.

10:30 PMSE **136.** Derivatives of chitin and chitosan for biomedical applications bearing nitric oxide-releasing *S*-nitrosothiol substituents. **A. Lutzke,** A. Pegalajar-Jurado, B.H. Neufeld, M.M. Reynolds

10:50 PMSE **137.** Producing lignin-based polyols through microwave-assisted liquefaction for rigid polyurethane foam production. **B. Xue**, R. Sun

11:10 PMSE **138.** Glycerol based hyperbranched poly(ester)s for the controlled release of the plant growth regulator naphthylacetic acid. **T. Zhang**, B.A. Howell, P.B. Smith

11:30 PMSE **139.** Design of biobased hyperbranched polyesters: Structure and molecular weight. **P.B. Smith**, T. Zhang, B.A. Howell, S.J. Martin

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MONDAY AFTERNOON

Section A

Sheraton Denver Downtown Hotel

Directors Row J

Advances in X-ray and Neutron Scattering Techniques for Elucidating Polymer Morphology

Block Copolymers & Polymer Blends

A. I. Norman, *Organizer*

R. Jones, Y. Men, *Organizers, Presiding*

1:30 PMSE **140.** Thermodynamic interactions and shear-aligned structures in triblock copolymers derived from vegetable oils. S. Wang, S. Vajjala Kesava, E. Gomez, **M.L. Robertson**

2:00 PMSE **141.** Characterizing the distribution and thermodynamics of selectively associating additives in polymer blends. **D. Sunday,** Y. Tein, R. Kline

2:30 PMSE **142.** Structure transitions in symmetric crystalline-crystalline diblock copolymers with synchrotron simultaneous SAXS/WAXS investigations. F. Xue, **S. Jiang**

3:00 Intermission.

3:15 PMSE **143.** Co-solvency and co-non-solvency of polymers in mixed solvents. **B. Hammouda**

3:45 PMSE **144.** Microstructural origins of yield, strain hardening and hysteresis in thermoplastic elastomers under uniaxial deformation: an in situ tensile-SANS study. **C. Lopez-Barron**, A. Eberle

4:15 PMSE **145.** SANS study on the phase behaviors of responsive star polyelectrolytes. **W. Xu**, I. Choi, F. Plamper, C. Synatschke, A. Mueller, Y. Melnichenko, V.V. Tsukruk

Section B

Sheraton Denver Downtown Hotel

Governor's Square 16

Polymeric Biomaterials

Novel Polymeric Biomaterials: Synthesis, Modification and Fabrication

Cosponsored by CELL

Financially supported by Genzyme; RSC 'Journal of Materials Chemistry B' and 'Biomaterials Science'; Genzyme; TA Instruments; Malvern Instruments; University of Delaware Materials Science & Engineering

M. Grunlan, X. Jia, *Organizers, Presiding*

1:20 PMSE **146.** Responsive materials for the directing and delivering stem cells and therapeutics. M.S. Rehmann, P.M. Kharkar, **A.M. Kloxin**

1:50 PMSE **147.** Withdrawn.

2:10 PMSE **148.** Efficient syntheses of polysaccharides and their biomedical applications. **W. Du, L. Li, J. Wang**, M. Obrinske

2:30 PMSE **149.** Tailoring the activity of lysozyme by combining grafting-from and grafting-To RAFT polymerization. **R. Falatach, C. McGlone, S. Averick, R.C. Page, D. Konkolewicz, J. Berberich**

2:50 Intermission.

3:10 PMSE **150.** Silk proteins for stabilization and drug delivery systems. **D.L. Kaplan**

3:40 PMSE **151.** Conjugated polymer nanoparticles for intracellular organelle specific drug delivery. M. Kumar, T. Vokata, E. Mendez, **J. Moon**

4:00 PMSE **152.** Improving network crosslinking of peptide-immobilized hydrogels formed by visible light-initiated thiol-acrylate photopolymerization. **C. Lin, J. Bragg**

4:20 PMSE **153.** Multifunctional polyesters and polyurethanes with peptide-like pendant functional groups. **A. Joy, Y. Xu, J.P. Swanson**

TECHNICAL PROGRAM

Section C

Sheraton Denver Downtown Hotel

Governor's Square 11

Design Principles of Functional Macromolecular Materials

Financially supported by IBM; Solvay; Aldrich; RSC: Journal of Materials Chemistry A, B & C, Soft Mater and Chemical Science

A. J. Boydston, L. M. Campos, E. Pentzer, K. L. Wooley, *Organizers*

Y. Xia, *Presiding*

1:00 PMSE **154.** Structural evolution of polyelectrolyte-complex-core micelles and ordered-phase bulk materials. **M.V. Tirrell**

1:30 PMSE **155.** Design of functional materials to tailor glycan interactions at the cell-matrix interface. **K. Godula**

1:55 PMSE **156.** Designing dynamic rearrangement of polymeric structures using the principles found in lungs. **A.P. Esser-Kahn, M. Kleiman, D.T. Nguyen, K. Brubaker**

2:20 PMSE **157.** Kinetic control of modulus properties in peptide functionalized hydrogels. **M. Becker,** B.D. Vogt, G. Hua, Z.K. Zander, C. Wiener

2:45 Intermission.

3:00 PMSE **158.** Sustainable and degradable thermosets and polyesters from sugar-derived dilactones. J. Gallagher, M.A. Hillmyer, **T.M. Reineke**

3:30 PMSE **159.** Design of hydrogels as synthetic extracellular matrix mimics using modular building blocks and facile techniques. **A.M. Kloxin**

4:00 PMSE **160.** Poly(oligonucleotide): Development and biomedical utility of nucleic acid-programmed polymers and nanoparticles. **N.C. Gianneschi**

Section D

Sheraton Denver Downtown Hotel

Directors Row H

Nanostructured Porous Polymers: Synthesis, Properties Applications

New Approaches and Applications of Nanostructured Porous Polymeric Materials

D. L. Gin, *Organizer*

B. D. Freeman, H. Lin, *Organizers, Presiding*

1:30 PMSE **161.** Hierarchically porous conductive hydrogels as a novel material platform for energy storage and biosensor technologies. **G. Yu**

2:00 PMSE **162.** Surface modification of metal-organic framework nanoparticles using random polymer. **T. Li**, S. Darnall, I. Lee, T. Xu

2:20 PMSE **163.** Photocrosslinked honeycomb-patterned films with submicron pores fabricated using monodisperse silica nanoparticles as templates for regulating MC3T3-E1 cell functions. X. Wu, **S. Wang**

2:40 PMSE **164.** Grafting of poly(oligoethylene glycol) (meth)acrylate brushes on the surface of cylindrical mesopores of ordered silica via activator regenerated by electron transfer ATRP. **A.S. Manchanda**, M. Kruk

3:00 PMSE **165.** Block copolymer packing limits and interfacial reconfigurability in the assembly of periodic mesoporous organosilicas. **B.A. Helms**, A.W. Wills, P. Ercius, E.R. Rosenberg, R. Runser

3:20 Intermission.

3:40 PMSE **166.** High surface area methylsilsesquioxane polymer gels made by fluoride catalyzed rearrangement. J. Furgal, H. Yamane, Y. Chujo, **R.M. Laine**

4:00 PMSE **167.** Nanoporous materials from crosslinked gemini surfactant lyotropic liquid crystal network phases. **J. Jennings, M. Mahanthappa**

4:20 PMSE **168.** Microporous inorganic/organic hybrids via oxysilylation of a cubic symmetry nanobuilding block $[(HMe_2SiOSiO_{1.5})_8]$ with $R_xSi(OEt)_{4-x}$ in Hydrophobic media. **D. Pan**, E. Yi, J. Furgal, M. Schwartz, P. Doan, R.M. Laine

4:40 PMSE **169.** Biomimetic amphiphobic surfaces on paper. **S. Oyola-Reynoso**, I. Tevis, Z. Li, J. Halbertsma-Black, M. Thuo

5:00 PMSE **170.** Hierarchical porosity in emulsion-templated polymers. S. Israel, **M.S. Silverstein**

Section E

Sheraton Denver Downtown Hotel

Governor's Square 17

Stimulus-Responsive Assemblies and Materials

Inspiration from Biology

C. Bowman, A. P. Goodwin, *Organizers*

J. Cha, *Organizer, Presiding*

1:30 PMSE **171.** Peptide supramolecular polymerizations. **S.I. Stupp**

2:00 PMSE **172.** Phase behavior and self-assembly of stimulus response peptide polymers. **A. Chilkoti**

2:30 PMSE **173.** Molecular description of LCST behavior of elastin-like peptides poly(VPGVG) and poly(VGPVG). **N.K. Li**, Y.G. Yingling

2:50 PMSE **174.** Temperature-triggered self-assembly of nanovesicles from collagen-like peptide-containing diblock bioconjugates. **T. Luo**, L. He, P. Theato, K.L. Kiick

3:10 PMSE **175.** Regulating supramolecular polymerization of polypeptide-grafted macromolecules. **H. Xia**, Y. Zhang, H. Fu, Y. Ren, J. Cheng, Y. Lin

3:30 Intermission.

3:45 PMSE **176.** Responsive, switchable, and self-assembled properties of zwitterionic biomaterials. **S. Jiang**

4:15 PMSE **177.** Stimulus-responsive polymer-lipid assemblies as biomolecule-activated imaging contrast agents. **A.P. Goodwin**

4:45 PMSE **178.** Infrared invisibility stickers inspired by cephalopods. **L. Phan,** D. Ordinario, **E. Karshalev**, M. Shenk, **A.A. Gorodetsky**

5:05 PMSE **179.** Photoresponsible mussel-derived surgical tissue glue. **E. Jeon**, B. Hwang, Y. Yang, H.J. Cha

Section F

Sheraton Denver Downtown Hotel

Governor's Square 9

Graphene and Carbon Nanotubes: Synthesis, Devices and Applications

Composite Materials

G. S. Tulevski, *Organizer*

A. D. Taylor, *Organizer, Presiding*

1:30 PMSE **180.** Graphene/polymer derived ceramics with anisotropic properties. **L. Zhai**

1:50 PMSE **181.** Efficient, low-cost, simple method to enhance the thermal efficiency of ceramic by spray deposition of silane-modified graphene. S. Tong, J. Wang, S. Mo, C. Yuan, **Y. Liu**, Y. Min

2:10 PMSE **182.** Conductive nanocomposites of polyethylene/oxidized polyethylene (PE/OPE) blends with thermally reduced graphene and carbon black. **M.Z. Iqbal**, A.A. Abdala, M.W. Liberatore

2:30 PMSE **183.** 3D graphene/58 S bioactive glass scaffolds as a biocompatible scaffold for retinal ganglion cells. **Q. Yao**, S. Yu, Y. Liu

2:50 PMSE **184.** Antibacterial surface acting via photothermal effects. **H. Liwei**, Y. Lihua

Section G

Sheraton Denver Downtown Hotel

Governor's Square 10

General Papers/New Concepts in Polymeric Materials

Polymer Synthesis

Q. Lin, *Organizer*

X. Guo, S. Zavada, *Presiding*

1:30 PMSE **185.** Polymerization of N-NCAs in ionic liquids: Heterophase synthesis of polypeptoids. **S.M. Brosnan**, C. Secker, H. Schlaad, K. Tauer, M. Antonietti

1:50 PMSE **186.** Design and synthesis of a degradable triblock copolymer, poly(ethylene glycol)-*block*-polyphosphoester-*block*-poly(L-lactide) for biomedical applications. **R. Li, F. Zhang, S. Zhang**, H. Wang, K.L. Wooley

2:10 PMSE **187.** Synthesis of silver oxide nanoparticles in spherical polyelectrolyte brushes. A. Ahmad, X. Liu, Y. Xu, **X. Guo**

2:30 PMSE **188.** Proton-transfer polymerization (HTP): Converting methacrylates into polyesters by an N-heterocyclic carbene. **M. Hong**, E.Y. Chen

2:50 PMSE **189.** Synthesis and polymerization of substituted oxazine ring of polybenzoxazine. **F.P. Cassidy**, K. Chiou, H. Ishida

3:10 Intermission.

3:30 PMSE **190.** Rapid, puncture-initiated, autonomous healing *via* oxygen-mediated polymerization. **S.R. Zavada**, K.L. Gordon, N.R. McHardy, T.F. Scott

3:50 PMSE **191.** Biodegradable comb-dendritic tri-block copolymers consisting of poly(ethylene glycol) and poly(L-lactide) or poly(⊠-caprolactone) and pre-osteoblastic cellular response to the spherulitic surfaces. X. Wu, J. Dou, S. **Wang**

4:10 PMSE **192.** Self-assembly of giant polymer capsules with purely hydrophilic polymers: The hydrophilic effect. **S.M. Brosnan**, H. Schlaad, M. Antonietti

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Undergraduate Research Posters

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Macromolecular and Nanoparticle Separation Science

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MONDAY EVENING

Section A

Colorado Convention Center

Halls C/D

Sci-Mix

M. Becker, Q. Lin, C. M. Stafford, A. H. Tsou, *Organizers*

8:00 - 10:00

128. See previous listings.

297, 299-300, 304-305, 307-308, 314-319, 322-324, 328-332, 336, 339-344, 351-352, 355, 357, 359-365, 371-375, 377-385, 388-390, 392-394, 397-398, 401-402, 404-406, 408, 411-412. See subsequent listings.

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TUESDAY MORNING

Section A

Sheraton Denver Downtown Hotel

Directors Row J

Advances in X-ray and Neutron Scattering Techniques for Elucidating Polymer Morphology

High Strength Polymers and Composites

Y. Men, *Organizer*

R. Jones, A. I. Norman, *Organizers, Presiding*

8:30 PMSE **193.** Elucidating the relationships between polyethylene architecture and mechanical properties. A. Kannan, **D. Bucknall**, A. Eberle, T. Shaffer, A.I. Norman, S. Weigand

9:00 PMSE **194.** Molecular weight dependency of crystallization, recrystallinzation and melting lines in isotactic polypropylene and polybutene-1. Y. Lu, Y. Wang, **Y. Men**

9:30 PMSE **195.** Investigating the crystallization kinetics and structure development of hybrid polymer-nanocomposite materials using SAXS/WAXS and thermal techniques. **E.L. Heeley**, P.G. Taylor, Y. El Aziz, A. Basindale, D. Hughes

10:00 Intermission.

10:15 PMSE **196.** Topology of soft materials using neutron and X-ray scattering. **G. Beaucage**

10:45 PMSE **197.** Morphological origin of the embrittlement of polymers upon crystallization: The case of PET. **L. Balzano**

11:15 PMSE **198.** Phase behavior of polymer-grafted nanoparticles in a polymer matrix. **K. Mongcopa**, R. Ashkar, P. Butler, R. Krishnamoorti

Section B

Sheraton Denver Downtown Hotel

Governor's Square 16

Polymeric Biomaterials

Novel Polymeric Biomaterials: Synthesis, Modification and Fabrication

Cosponsored by CELL

Financially supported by Genzyme; RSC 'Journal of Materials Chemistry B' and 'Biomaterials Science'; Genzyme; TA Instruments; Malvern Instruments; University of Delaware Materials Science & Engineering

M. Grunlan, X. Jia, *Organizers, Presiding*

8:25 PMSE **199.** Degradable porous polymer biomaterials through emulsion-templating. T. Bialystocki, D. David, L. Perry, D. Rosenfeld, S. Levenberg, **M.S. Silverstein**

8:55 PMSE **200.** Cell encapsulating tough hydrogel materials. **A.P. Dove**

9:25 PMSE **201.** Development of flexible and elastic, biodegradable and bioactive polycarbonates. **Z. Zhang**, S.D. Sommerfeld, J. Bushman, M. Guvendiren, D. Zunger, P. Mishra, H. Kaplan, J.B. Kohn

9:45 PMSE **202.** Advanced biocompatible and high strength underwater tissue bioadhesive. **H. Kim**, S. Lim, B. Hwang, H.J. Cha

10:35 Intermission.

10:05 PMSE **203.** Molecular understanding, design, and development of zwitterionic biomaterials. **S. Jiang**

10:55 PMSE **204.** Antimicrobial coatings for biomedical applications: Challenges and opportunities offered by natural polymers. **K. Neoh**, M. Li, R. Wang, E. Kang, E. Chiong

11:15 PMSE **205.** Low-temperature plasma surface modification of porous polymeric materials for environmental and medical applications. **M.N. Mann**, A. Pegalajar-Jurado, E.R. Fisher

11:35 PMSE **206.** Highly selective antibacterial activity through control of polymer amphiphilicity based on the exploration of non-ionic hydrophilic counits. **A. Punia**, N. Yang

Technical program information known at press time. The official technical program for the 249th ACS National Meeting is available at: www.acs.org/denver2015

‡ *Cooperative Cosponsorship*

Section C

Sheraton Denver Downtown Hotel
Governor's Square 11

Design Principles of Functional Macromolecular Materials

Financially supported by IBM; Solvay; Aldrich; RSC: Journal of Materials Chemistry A, B & C, Soft Mater and Chemical Science

A. J. Boydston, L. M. Campos, E. Pentzer, K. L. Wooley, *Organizers*
B. M. Cossairt, *Presiding*

8:30 PMSE **207.** Modeling block copolymer thin film orientation in the presence of neutral and preferential interfaces. **W. Durand**, M. Carlson, G. Blachut, M. Maher, C.J. Ellison, C.G. Willson

8:55 PMSE **208.** Design rules for membranes in artificial solar fuels generators. **N.A. Lynd**

9:15 PMSE **209.** Functional degradable poly(carbonate)s: Design, synthesis, and self-assembly. **R.J. Williams**, R.K. O'Reilly, A.P. Dove

9:35 PMSE **210.** Efficient synthesis of rigid ladder polymers via palladium catalyzed annulation. **Y. Xia**

10:00 PMSE **211.** Photolithographic olefin metathesis polymerization. **R. Weitekamp**, H. Atwater, R.H. Grubbs

10:20 Intermission.

10:35 PMSE **212.** Synthetic polymer anion exchange membranes. **W. Zhang**, Y. Liu, M.W. Liberatore, A.M. Herring, E. Coughlin

10:55 PMSE **213.** Synthesis and design of functional porous organic polymers. **P. McGrier**

11:20 PMSE **214.** Designing a hydrophobic monomer library with LogP values. **R.T. Mathers**

11:40 PMSE **215.** Structural design principles for high performance polysaccharide binders in silicon anodes. T. Kwon, Y.K. Jeong, J. Choi, **A. Coskun**

Section D

Sheraton Denver Downtown Hotel
Directors Row H

Nanoscale Spectroscopic and Microscopic Characterization

Hybrid SPM/AFM

Financially supported by ExxonMobil Chemicals; Bruker; Nanosurf

A. H. Tsou, D. Yablon, *Organizers*
J. Hobbs, *Presiding*

8:30 PMSE **216.** AFMIR : A powerful tool for Infrared Nanoscopy. **A. Dazzi**, A. Deniset-Besseau, C.A. Marcott, K. Kjoller

9:00 PMSE **217.** Investigation of microscopic properties of polymer surface in contact with liquids: A combined SFM-Raman study. **S. Hild**

9:30 PMSE **218.** Infrared nanoimaging and nano-FTIR spectroscopy. **R. Hillenbrand**

10:00 Intermission.

10:15 PMSE **219.** Multimodal and multispectral nano-imaging: Accessing the structure underlying the function in molecular and soft-matter. **M.B. Raschke**

10:45 PMSE **220.** Nanoscale chemical, mechanical and thermal analysis of polymers using AFM-IR. **K. Kjoller**, M. Lo, Q. Hu, C. Prater

11:05 PMSE **221.** Bimodal AFM for elucidation of polyolefin morphology. **A.H. Tsou**, D. Yablon, H. Bradshaw, E.J. Blok, R.N. Dharmarajan

Section E

Sheraton Denver Downtown Hotel
Governor's Square 17

Stimulus-Responsive Assemblies and Materials

Biomedical Applications of Stimulus-Responsive Assemblies

C. Bowman, J. Cha, A. P. Goodwin, *Organizers*
D. Domaille, *Presiding*

8:30 PMSE **222.** Facile synthesis of clickable, pH responsive functional polyphosphoramidates. **H. Wang**, F. Zhang, R. Li, S. Zhang, K.L. Wooley

8:50 PMSE **223.** Dual-triggered polymeric nanoparticles as activatable fluorescent probes for the detection of inflammation and tumors. **J. Lux**, M.L. Viger, V.A. Nguyen Huu, G. Collet, M. Guma, A. Foucault-Collet, B. Bartok, G.S. Firestein, A. Almutairi

9:10 PMSE **224.** Carrier-free, light-activated nanoparticle system for the simultaneous delivery of nucleic acids and cancer drug. **K. Zhang**, B. Li, J.J. Zhao, X. Tan

9:30 PMSE **225.** Enzyme-responsive nanoparticles for tissue targeting. **N.C. Gianneschi**

10:00 PMSE **226.** Stimuli-responsive anisotropic colloidal nanoparticles. **C. Lu, M.W. Urban**

10:20 Intermission.

10:35 PMSE **227.** Light/magnetic responsive polymer/inorganic hybrid assemblies for cancer theranostics. **Z. Nie**, Y. Liu, J. Lin, X. Chen

11:05 PMSE **228.** Magnetic field triggered drug release from polymersomes for cancer therapeutics. H. Oliveira, J. Thévenot, O. Sandre, **S. Lecommandoux**

11:25 PMSE **229.** Versatile platform to temperature-responsive PEG-based materials: Facile post-polymerization functionalization of PEO-*co*-PAGE with n-alkane thiols. **T. Kawamori**, D. Klinger, J. Gopez, T. Murakami, C.J. Hawker

Section F

Sheraton Denver Downtown Hotel
Governor's Square 15

ACS Award in Polymer Chemistry: Symposium in Honor of Nikos Hadjichristidis

Well-Defined Polymers: From Design to Applications

Financially supported by ExxonMobil

Y. Gnanou, *Organizer*
J. Frechet, *Organizer, Presiding*

8:30 PMSE **230.** Branched polymers: Stars, grafts, and gels by ATRP. **K. Matyjaszewski**

9:00 PMSE **231.** Advance of sequential controlled polymerizations for the design of molecular brush block copolymers: Sophisticated functional single molecule materials and hierarchically-assembled cluster properties. **K.L. Wooley**

9:30 PMSE **232.** Model thermoplastic polyurethanes with sequence controlled monodisperse hard segments. L. Ren, P. Shah, N. Kang, **R. Faust**

10:00 Intermission.

10:30 PMSE **233.** Tailored block copolymers and their processing for self-assembled thin films applications. D. Calabrese, B. Wenning, M. Chavis, **C.K. Ober**

11:00 PMSE **234.** Synthesis of star and star-block copolymers by living radical polymerisation. **D.M. Haddleton**

11:30 PMSE **235.** Photoinduced ATRP and CuAAC click reactions and their combinations for macromolecular syntheses. S. Doran, E. Murtezi, S. Dadashi-Silab, M. Ciftci, G. Yilmaz, M. Tasdelen, **Y. Yagci**

Section G

Sheraton Denver Downtown Hotel
Governor's Square 10

Polymer Modeling: Structure, Dynamics and Function

Solutions, Melts and Surfaces

Financially supported by ExxonMobil; Dow Chemical

R. Locker, G. C. Rutledge, *Organizers*
M. A. Pasquinelli, *Presiding*

8:30 PMSE **236.** Equilibration of high molecular-weight polymer melts: A hierarchical universal strategy. G. Zhang, L. Moreira, T. Stuehn, **K.C. Daoulas**, K. Kremer

9:00 PMSE **237.** Molecular simulation of polymer adsorption on rough surfaces. A. Venkatakrishnan, A. Frost, J. Lewnard, A. Shim, K. Anderson, **V.K. Kuppa**

9:20 PMSE **238.** Effects of ionic liquid structure on the thermodynamics of cellulose dissolution. **B. Rabideau**, A.E. Ismail

9:40 PMSE **239.** Threading of ring poly(ethylene oxide) molecules by linear chains or other rings in the melt: molecular dynamics simulations followed by a geometric analysis. **D.G. Tsalikis**, V.G. Mavrantzas

10:00 PMSE **240.** Tubes, topology, and entangled rings. **S. Milner**

10:30 PMSE **241.** Molecular dynamics study on the influence of copolyeseter composition on adhesion with soda-lime glass. **B. Hanson**, J.G. Ray, M.A. Pasquinelli

10:50 PMSE **242.** Deformation of poly(amido amine) dendrimers at surfaces. **K.A. Maerzke**, N. Henson, P. Welch, C.F. Welch

11:10 PMSE **243.** Hydrogen bond organization and related structural order in bis-MPA based dendrimers versus hyperbranched polymers. **M. Syed**, B. Olson, S.I. Nazarenko

Energy and Materials

Sponsored by POLY, Cosponsored by PMSE

Smart and Responsive Composites from Renewable Building Blocks

Cues from Nature: Environmentally-Triggered Functionality in Biopolymers

Sponsored by CELL, Cosponsored by PMSE

Macromolecular and Nanoparticle Separation Science

Sponsored by POLY, Cosponsored by ANYL and PMSE

TUESDAY AFTERNOON

Section A

Sheraton Denver Downtown Hotel
Directors Row J

Advances in X-ray and Neutron Scattering Techniques for Elucidating Polymer Morphology

High Strength Polymers and Composites

R. Jones, *Organizer*
Y. Men, A. I. Norman, *Organizers, Presiding*

1:30 PMSE **244.** Studying the nonequilibrium nature of extension-Induced nucleation in polymer melts with ultrafast X-ray scattering. **L. Li**

2:00 PMSE **245.** Characterization of crystallinity in polyolefins by wide angle X-ray diffraction. **R. Ortega**, J. Butler, D. Winter

2:30 PMSE **246.** Switching Chirality of hybrid left-right crystalline helicoids built of achiral polymer chains: When right-to-left becomes left-to-right. M. Rosenthal, M. Burghammer, A.P. Melnikov, D.V. Anokhin, G. Bar, E.T. Samulsky, **D. Ivanov**

3:00 Intermission.

3:15 PMSE **247.** Depth-sectioning method for X-ray diffraction: isolating the real-time structure development in pressure driven flows. **L. Fernandez-Ballester**

3:45 PMSE **248.** Neutron scattering characterization of amino-polymer/silica composite CO_2 adsorbents: Morphology, mobility, and consequences for performance. **A. Holewinski**, M. Sakwa-Novak, C.W. Jones

4:15 Concluding Remarks.

Section B

Sheraton Denver Downtown Hotel
Governor's Square 16

Polymeric Biomaterials

Drug Delivery and Controlled Release

Cosponsored by CELL

Financially supported by Genzyme; RSC 'Journal of Materials Chemistry B' and 'Biomaterials Science'; Genzyme; TA Instruments; Malvern Instruments; University of Delaware Materials Science & Engineering

M. Grunlan, X. Jia, *Organizers, Presiding*

1:25 PMSE **249.** Lanthanide-containing polycations for imaging and monitoring polyplex dynamics. L. Xue, S. Kelkar, **T.M. Reineke**

1:55 PMSE **250.** Synthesis and evaluation of peptide-based polymers for biomedical applications. L. Chan, C. Ngambenjawong, D. Chu, M. Cieslewicz, X. Wang, H. Wei, Y. Cheng, N. White, P. Horner, **S. Pun**

2:25 PMSE **251.** Gene-delivering non-viral systems from PEI-g-PEG and PEI-functionalized telechelic PEG: Effect of polymer architecture on gene transfection efficiency and cyto-toxicity. L. Cedrone, M. George, V. Mityushin, W. Holmes, R. Bellin, **S. Granados Focil**

2:45 PMSE **252.** Self-assembly of PEGylated poly(amino acid)s and their use in DNA complexation. **C. Scholz**, D. Ulkoski, A. Meister, J. Kressler

3:05 Intermission.

3:20 PMSE **253.** Designer antimicrobial materials. **A. Shukla**

3:50 PMSE **254.** Phenylboronic acid-installed polycarbonates: synthesis and use as drug carriers. Y. Aguirre-Chagala, J.L. Santos, **M. Herrera-Alonso**

4:20 PMSE **255.** Temporal control over multiple biological signals using photochemical reactions. **M.A. Azagarsamy, K.S. Anseth**

4:40 PMSE **256.** Comb polymers for non-viral gene delivery. **R. Letteri, S. Parelkar, R. Elder, A. Jayaraman, T. Emrick**

Section C

Sheraton Denver Downtown Hotel
Governor's Square 11

Drug Delivery and Drug Device Combination Products

Nanotechnology for Oncology

A. S. Kulshrestha, P. Timmins, *Organizers*
S. Sridharan, *Organizer, Presiding*
S. R. Raghavan, *Presiding*

1:30 PMSE **257.** Polyacrylamide nanogels for potential cancer therapy. **K. Neoh**, S. Lu, E. Kang, R. Mahendran, E. Chiong

1:55 PMSE **258.** Development and evaluation of CD44-targeted lipid-based nanoparticles in an orthotopic non-small cell lung cancer xenograft mouse model. **S.R. Benhabbour**, J.M. DeSimone, R. Mumper, A. Webster, C. Luft

2:20 PMSE **259.** Bio-inspired cocoon-like DNA-nanoclew for anticancer drug delivery. **W. Sun**, R. Mo, Y. Lu, Z. Gu

2:45 PMSE **260.** Invertible micellar polymer assemblies for targeted delivery of curcumin to osteosarcoma cells. O. Kudina, K.L. Shogren, C.T. Gustafson, M.J. Yaszemski, A. Maran, **A.S. Voronov**

3:10 PMSE **261.** Modulation of immune response along with bax and bcl-2 mediated enhanced apoptosis in breast cancer cells via paclitaxel loaded vitamin E nanoemulsion. **V.K. Pawar**, M.K. Chourasia

3:35 PMSE **262.** Nanogels from metal-chelating crosslinkers applied to copper-64 PET imaging of tumors and metastases. **J. Lux**, A.G. White, M. Chan, C.J. Anderson, A. Almutairi

Section D

Sheraton Denver Downtown Hotel

Directors Row H

Nanoscale Spectroscopic and Microscopic Characterization

Nanomechanical Characterization

Financially supported by ExxonMobil Chemicals; Bruker; Nanosurf

A. H. Tsou, D. Yablon, *Organizers*

M. B. Raschke, *Presiding*

1:30 PMSE **263.** Nanomechanical characterization of polymers by atomic force microscopy: dynamic and quasi static approaches. C. Dietz, A. Voss, M. Schulze, **R. Stark**

2:00 PMSE **264.** AFM-based viscoelasticity measurement for polymeric materials. **K. Nakajima**

2:30 PMSE **265.** Molecular scale imaging of semicrystalline polymers. **J.K. Hobbs**, N. Mullin, R. Savage

3:00 PMSE **266.** Deformation rate dependence of nanomechanical properties as measured by atomic force microscopy. **B. Pittenger**, T. Mueller

3:20 Intermission.

3:30 PMSE **267.** Viscoelastic AFM nanomechanics in non-ambient environments. **J. Killgore**

4:00 PMSE **268.** Advances in nanomechanical characterization of polymer materials with scanning probe microscopy. **D. Yablon**

4:20 PMSE **269.** Studies of stimuli responsive polymer composites grafts by colloidal probe microscopy. S.L. Skiles, J. Spear, D. Bergbreiter, **J.D. Batteas**

4:40 PMSE **270.** Photothermally excited contact resonance imaging in air and water. **M. Kocun**, A. Labuda, A. Gannepalli, R. Proksch

Section E

Sheraton Denver Downtown Hotel

Governor's Square 17

Stimulus-Responsive Assemblies and Materials

Biomedical Applications of Stimulus-Responsive Assemblies

C. Bowman, J. Cha, *Organizers*

A. P. Goodwin, *Organizer, Presiding*

1:30 PMSE **271.** Maltodextrins image bacterial infections and drug resistance by positron emission tomography. **N. Murthy**

2:00 PMSE **272.** Tailored supramolecular structures for the controlled release of therapeutics and for polymeric antimicrobials. **J.L. Hedrick**

2:30 PMSE **273.** Photocleavable linkers for cell and protein micropatterning. **S.V. Wegner,** O. Senturk, J.P. Spatz

2:50 PMSE **274.** Stimuli-responsive self-folding soft-grippers for drug delivery. **H. Kwag**, K. Malachowski, J. Breger, M.O. Wang, J. Fisher, F.M. Selaru, D.H. Gracias

3:10 PMSE **275.** Light-responsive strategy for reversible control of elastic modulus in PEG-based hydrogels. **A. Rosales**, K. Mabry, E. Nehls, K.S. Anseth

3:30 Intermission.

3:45 PMSE **276.** Squeezable tubules from self-assembly of amphiphilic macrocycles. **M. Lee**

4:15 PMSE **277.** Triggering the de novo synthesis of phospholipid membranes. **N.K. Devaraj**

4:45 PMSE **278.** Stimuli-responsive uptake and release of polyelectrolytes by amphoteric microgels. **W. Richtering, A. Gelissen**, F. Plamper, A. Schmid, D. Pergushov, I. Potemkin, A. Pich

5:05 PMSE **279.** Molecular-level interactions in the design of reversible and recyclable flocculants. **K.L. Morrissey**, R.Z. Chapman, L. Zolnierowski, M. Keirn, G. Henry, M.P. Stoykovich

Section F

Sheraton Denver Downtown Hotel

Governor's Square 15

ACS Award in Polymer Chemistry: Symposium in Honor of Nikos Hadjichristidis

Well-Defined Polymers: From Design to Applications

Financially supported by ExxonMobil

J. Frechet, Y. Gnanou, *Organizers*

M. Moller, *Presiding*

1:00 PMSE **280.** Hypersonic phononic particle brush materials. **G. Fytas**

1:30 PMSE **281.** Regular highly branched polymers: From polymeric to colloidal properties. **D. Vlassopoulos**

2:00 PMSE **282.** Dynamic covalent polymers as viscosity modifiers. T. Nguyen, R. Nicolay, **L. Leibler**

2:30 Intermission.

3:00 PMSE **283.** Ring opening metathesis polymerization for the synthesis of complex macromolecular architectures. **M. Pitsikalis**

3:30 PMSE **284.** Smart hybrid nanocarriers to treat pancreatic cancer. **H. Iatrou**

4:00 PMSE **285.** Synthesis, structure-property studies in lactic acid derived polymers: Multiarm branched polymers and copolymers of by "core-first" and "arm-first" approach. **S. Sivaram**

4:30 PMSE **286.** Polymeric surfaces exhibiting photocatalytic activity and controlled wettability with anisotropic features. **S.H. Anastasiadis**, M.A. Frysali, L. Papoutsakis, G. Kenanakis, E. Stratakis, M. Vamvakaki, S. Pispas

5:00 PMSE **287.** Directed self-assembly of block copolymers. **A. Avgeropoulos**

Section G

Sheraton Denver Downtown Hotel

Governor's Square 10

Polymer Modeling: Structure, Dynamics and Function

Self-Assembly and Structure Development

Financially supported by ExxonMobil; Dow Chemical

R. Locker, G. C. Rutledge, *Organizers*

V. K. Kuppa, *Presiding*

1:00 PMSE **288.** Ultracoarse-grained simulation of biopolymers. **G.A. Voth**

1:30 PMSE **289.** Multiresolution modeling of polymers: Wavelet-based reconstruction. C.S. Adorf, A. Agarwal, **B. Rabideau**, C.R. Iacovella, A.E. Ismail

1:50 PMSE **290.** Computational analysis of solvent effects on electron transfer in organic radical battery cathode materials. **R.E. Larsen,** T.W. Kemper, W. Braunecker, B.K. Hughes, D. Bobela, A. Ferguson, T. Gennett

2:10 PMSE **291.** Effect of short chain branching on the properties of semi-crystalline polyethylene. V. Kumar, R. Locker, **G.C. Rutledge**

2:30 PMSE **292.** Usage of Poly(NIPAm) in the biofuel production. **J.V. Ribeiro**, R.C. Bernardi, K. Schulten

3:00 PMSE **293.** Coarse-grained simulations of solvent-assisted self-assembly of block copolymer thin films. **S. Hur**, M. Mueller, P.F. Nealey, J.J. De Pablo

3:20 PMSE **294.** Folding behavior of polypeptide-grafted comb-like macromolecules. **Y. Ren**, Y. Zhang, H. Xia, J. Cheng, Y. Lin

3:40 PMSE **295.** Molecular dynamics simulations of structure and effective interactions of diblock copolymer grafted nanoparticles in a homopolymer blend matrix. **C. Estridge**, A. Jayaraman

Energy and Materials

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Macromolecular and Nanoparticle Separation Science

Sponsored by POLY, Cosponsored by ANYL and PMSE

TUESDAY EVENING

Section A

Colorado Convention Center

Hall D

Joint PMSE/POLY Poster Session

Cosponsored by POLY‡

Q. Lin, *Organizer*

6:00 - 8:00

Graphene and Carbon Nanotubes: Synthesis, Devices and Applications.

PMSE **296.** Synthesis, characterization of graphene incorporated polyamide resin. **A. Musa**, A. AlSheikh, T.A. Saleh

PMSE **297.** Graphene filler and graphenated nanogels. **I. Yaghoubi Rad, J.W. Stansbury**

Nanoscale Spectroscopic and Microscopic Chraracterization of Polymers.

PMSE **298.** Quantitative modulus mapping of polymer thin films using tapping mode. **M. Kocun**, A. Labuda, R. Proksch

Polymeric Biomaterials.

PMSE **299.** Structure and properties of bisoxalamide-based segmented block-copolymers with controlled crystal thickness. **D. Anokhin**, M. Rosenthal, Y. Odarchenko, N. Sijbrandi, P. Dijkstra, J. Feijen, D. Ivanov

PMSE **300.** Synthesis and characterization of anorganic bone/polyglycolide composites. **L. Gauza**, K. Papke, K. Thorpe, J. Redepenning

PMSE **301.** Influence of nanocarbons on collagen molecular ordering and fibril alignment. **E.C. Green**, M.L. Minus, D. Aishanjiang

PMSE **302.** Folding graft copolymer with pendant drug segments for co-delivery of anticancer drugs. W. Tai, Y. Lu, R. Mo, **Z. Gu**

PMSE **303.** Plasma modification of 3D, bioresorbable, polymeric scaffolds: Customizing surface chemistry to fabricate bioreactive and bionon reactive materials. **M.J. Hawker**, A. Pegalajar-Jurado, E.R. Fisher

PMSE **304.** Solute stabilization via amphiphilic polymers possessing different architectures. **H. Luo**, J.L. Santos, M. Herrera-Alonso, B.A. Aguilar-Castillo

PMSE **305.** 4D printing for spatially and temporally dynamic bioscaffolds. **J.M. McCracken**, R.G. Nuzzo

PMSE **306.** Positive effect of biaxial stretching on the mechanical behavior of PLA-Talc nanocomposites. **S. Ouchiar**, G. Stoclet, C. Cabaret, J. Gloaguen, V. Gloaguen, J. Lefebvre

PMSE **307.** Development of a hyperbranched polymer theranostic for prostate cancer. **A. Pearce**, B.E. Rolfe, A.V. Fuchs, P.J. Russell, A.K. Whittaker, K.J. Thurecht

PMSE **308.** Synthesis, characterization, and antibacterial activity evaluation of a water-soluble chitosan derivative and its application on paper. **G. Rodríguez Galindo**, R. Manriquez Gonzalez, J. Andrade Ortega, J. Casas Solís, E. Delgado

PMSE **309.** Impact of cross-linking on rate of release of pyridoxine from Zein fibers and films. **G.W. Selling**, E. Lafond, K.D. Utt

PMSE **310.** Targeted CT imaging of human hepatocellular carcinoma using low-generation dendrimer-entrapped gold nanoparticles modified with lactobionic acid. Y. Cao, Y. He, H. Liu, Y. Luo, M. Shen, J. Xia, **X. Shi**

PMSE **311.** Withdrawn.

PMSE **312.** Thermomechanical properties of poly(L-lactide)/poly(D-lactide) blends. **G. Stoclet**

Stimulus-Responsive Assemblies and Materials.

PMSE **313.** In situ functionalization of azlactone-based polymer brushes. **B.M. Aden**, B.S. Lokitz, M. Kilbey

PMSE **314.** Single-molecule resolution of polymer diffusion on a thermo-responsive polymer brush. **H. Chin**, D.K. Schwartz

PMSE **315.** CO_2 adjustable and magnetic recyclable catalyst-supports based on "smart" hybrid nanoparticles. **A. Feng**, J. Yuan

PMSE **316.** Thermally-responsive phosphorus-filled nanobrick wall multilayer thin film eliminates polyurethane melt dripping and reduces heat release associated with fire. A. Cain, Y. Li, R.D. Davis, C. Nolen, **M. Huff**, J.C. Grunlan

PMSE **317.** Surface charge generation in nanogels for activated cellular uptake at tumor-relevant pH. **L. Li**, K. Raghupathi, C. Yuan, S. Thayumanavan

PMSE **318.** Ketal-containing poyacrylates and polyacrylamides as building blocks for multi-responsive nanomedicines. **B. Louage**, B. De Geest

PMSE **319.** Biocompatible mesoporous carbon nanocapsule as a nanoreactor: In situ synthesis of imaging nanoparticles and surface modifications for stimuli responsive theranostic applications. **G. Mishra**, A. Rammohan, A. Mukhopadhyay, S. Sivakumar, A. Sharma

PMSE **320.** Diffusion of photoabsorbing degradation byproducts in photodegradable polymer networks. **S. Norris**, A.M. Kasko, T. Chou

PMSE **321.** Light-triggered chemical amplification to accelerate degradation and release from polymeric particles. **J. Olejniczak**, V. Nguyen Huu, J. Lux, M.R. Grossman, A. Almutairi

PMSE **322.** Swellable polysiloxane elastomers as substrates for passive radio frequency identification (RFID) gas sensors. **C. Rumens**, M. Ziai, K. Belsey, J. Batchelor, S.J. Holder

PMSE **323.** Strong attraction among the carboxylic acid-functionalized hydrophilic fullerene giant anions and the spontaneous, reversible self-assembly in dilute solution. **P. Yin, T. Liu**

Well-Defined Polymers: From Design to Applications — ACS Award in Polymer Chemistry Symposium in Honor of Nikos Hadjichristidis.

PMSE **324.** Phosphazene-catalyzed ring-opening polymerization of ε-caprolactone and epoxide. **H. Alamri**

PMSE **325.** Synthesis and characterization of poly(vinyl ether)-based graft polymers by combination of living polymerization techniques. **R. Alghamdi**, H. Bouchecif, N. Hadjichristidis

PMSE **326.** Triblock and pentablock terpolymers of functionalized vinyl ethers by base-assisted living cationic polymerization. **A. Al-sulami**, H. Bouchecif, N. Hadjichristidis

PMSE **327.** Withdrawn.

PMSE **328.** Ruthenium N-heterocyclic carbene star polymer. **K. Bukhriakov**, C. Mugemana, V. Rodionov

PMSE **329.** Anion-conducting block copolymer membranes for artificial photosynthesis. **P. Cotanda**, N.P. Balsara

PMSE **330.** Methyl methacrylate polymerization by Frustrated Lewis Pairs (FLPs): Polymerization and termination mechanism. **L. Falivene**, L. Caporaso, L. Cavallo

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‡ *Cooperative Cosponsorship*

PMSE **331.** Organopolymerization of acrylic monomers by N heterocyclic carbenes. **I. Falivene**, L. Caporaso, L. Cavallo

PMSE **332.** Mechanistic insight into the etylene reactivity promoted by phosphine–sulfonamide palladium(II) complexes. **I. Falivene**, L. Caporaso, L. Cavallo

PMSE **333.** Carbon dioxide based building blocks for polycarbonate synthesis by polycondensation and ring opening polymerization. **D. Pati**, X. Feng, N. Hadjichristidis, Y. Gnanou

PMSE **334.** Development of nanoporous membranes by block copolymer self-assembly for biofuel production. **N. Petzetakis**

PMSE **335.** Enzyme-inspired soft materials for catalysis by design. **V.O. Rodionov**

PMSE **336.** Synthesis of macromolecular architectures with a high hydrophobic/hydrophilic contrast by ring-opening metathesis polymerization. **V.O. Rodionov,** C. Jehanno, K. Bukhriakov

PMSE **337.** Facile metal-free "grafting-from" route from acrylamide-based substrate toward complex macromolecular combs. **J. Zhao**, H. Alamri, N. Hadjichristidis

General Papers/New Concepts in Polymeric Materials.

PMSE **338.** Nitric oxide releasing polymeric systems for wound healing applications. **K.A. Arabea**, A. Pegalajar-Jurado, K.A. Wold, M.M. Reynolds

PMSE **339.** Design, surface modification, and evaluation of cell-growth directive properties of 3D hydrogel scaffolds. **A. Badea**, J.M. McCracken, R.G. Nuzzo

PMSE **340.** Study of antibacterial properties of silver chloride/ poly (3-hydroxylbutyrate-co-3-hydroxylvalerate) (AgCl/PHBV) composite: A potential scaffold for bone tissue regeneration. **R.A. Bakare**

PMSE **341.** Crystallinity determination of poly(3-hexyl thiophene) thin films by means of fast scanning calorimetry. **J. Balko**, A. Rinscheid, A. Wurm, C. Schick, R. Lohwasser, M. Thelakkat, T. Thurn-Albrecht

PMSE **342.** Role of PEO-segment lengths in surface properties of antigouling PEG-silane amphiphile. **M. Barry**, M.A. Rufin, P.A. Adair, M. Grunlan

PMSE **343.** Synthesis of highly swellable functional poly(dimethylsiloxane) composites for use as selective gas and solvent sensors. **K. Belsey**, C. Rumens, S.J. Holder

PMSE **344.** Determining temperature change on photothermal Au nanorod and Au nanocage using smart polymers. **B. Buyukbekar**, H. Cavusoglu, H. Sakalak, M. Citir, G. Demirel, M. Yavuz

PMSE **345.** MALDI MS results for organotin polyamines from reaction of 3-amino-1,2,4-triazole and organotin dihalides. **C.E. Carraher**, Jr., V. Suresh, R. Crichton, M.R. Roner

PMSE **346.** Synthesis of organotin polyamines from reaction of 3-amino-1,2,4-triazole and organotine dihalides. **C.E. Carraher**, Jr., R. Crichton, M.R. Roner

PMSE **347.** Inhibition of cancer cell lines by organotin polyesters synthesized from reaction of the salt of D-camphoric acid and organotin dihalides. M.R. Roner, **C.E. Carraher,** Jr., A. Moric-Johnson, L. Miller, A. Campbell

PMSE **348.** Initial study of the ability of organotin polyethers derived from the anticoagulant dicumarol to inhibit cancer cell lines. M.R. Roner, **C.E. Carraher**, Jr., A. Moric-Johnson, L. Miller, N. Sookedo

PMSE **349.** Inhibition of cancer cell lines by the organotin polyether esters synthesized from reaction of the salt of alpha-cyano-4-hydroxycinnamic acid and organotin dihalides. **C.E. Carraher**, Jr., M.R. Roner, A. Moric-Johnson, L. Miller, V. Suresh

PMSE **350.** Use of the dioctyltin polyether ester synthesized from reaction of alpha-cyano-4-hydroxycinnamic acid and dioctytin dichloride itself acting as the MALDI MS matrix. **C.E. Carraher**, Jr., V. Suresh, M.R. Roner

PMSE **351.** Interfacial profile control in cross-linkable block copolymers for improved pattern transfer. **G. Chado**, C. He, M.P. Stoykovich

PMSE **352.** Behavior of compatibilizers with different chemical structure in polyethylene-MMT nanocomposites. **C. Chapple**, N. Shabestary

PMSE **353.** Carbon nanotube polymer nanocomposites for potential solder application. **C. Chen**, S. Ganguli, A.K. Roy

PMSE **354.** Tuning of the glass transition temperature of epoxy polymer. **C. Chen**, S. Ganguli, A.K. Roy

PMSE **355.** Cyclopentadiene-Based π-Conjugated Polymers. **L. Chen**

PMSE **356.** Fully physical double network hydrogels with high strength and fatigue resistance. **Q. Chen**, L. Zhu, H. Chen, J. Zheng

PMSE **357.** Redox active polymers for size-exclusion transport in nonaqueous redox flow batteries. N. Gavvalapalli, J. Hui, **K.J. Cheng**, T. Lichtenstein, M. Shen, J.S. Moore, J. Rodriguez-Lopez

PMSE **358.** Step-growth dental composites with improved mechanical performance from photopolymerized thiol-vinyl sulfone resins. **M.J. Claudino**, P.K. Shah, M. Podgorski, E. Becka, J.W. Stansbury, C. Bowman

PMSE **359.** Nonviral gene therapy applications of multifunctional fluorescent quantum dots. **J.M. Davis, M. Ellis, N. Mundt, K. Fichter**

PMSE **360.** Controlling transport through a cubic-phase lyotropic liquid-crystalline polymer nanofiltration membrane via anion exchange. **S. Dischinger**, B.M. Carter, D. Gin, R.D. Noble

PMSE **361.** Shape memory polyurethane aerogels. **S. Donthula**, F. Zheng, C. Sotiriou-Leventis, N. Leventis

PMSE **362.** Synthesis of Gd-doped quantum dots for theranostic applications with multiple imaging modalities. **M.A. Ellis**, N. Mundt, K. Fichter

PMSE **363.** Chemically modified dendritic starch: A novel nanomaterial for siRNA delivery. **S.A. Engelberth**, N. Hempel, M. Bergkvist

PMSE **364.** Mechanical properties and electromagnetic interference shielding effect of epoxy composite reinforced with Ni-plated basalt chopped fiber. **W. Eom**, H. Kim

PMSE **365.** Synthesis of highly gas-selective triptycene-based polymers of intrinsic microporosity (TPIMs). **B.S. Ghanem**, R. Swaidan, E. Litwiller, I. Pinnau

PMSE **366.** Synthesis of poly(2-methacryloxy ethyltrimethyl ammonium chloride) brushes by ATRP on magnetic nanoparticles. L. Qin, H. Han, Y. Xu, L. Li, X. **Guo**

PMSE **367.** In situ preparation of Ag/Au nanoparticle bilayer via layer-by-layer assembly in spherical polyelectrolyte brushes. F. Zhao, J. Wang, Y. Tian, L. Li, **X. Guo**

PMSE **368.** Phase behavior of spherical polyelectrolyte brushes solution in supercritical carbon dioxide. L. Liu, Y. Wen, Y. Cang, J. Zhang, Z. Yu, X. Hou, R. Zhang, **X. Guo**

PMSE **369.** Influence of compressed gas on the solubility of inorganic salt in reverse micelle. J. Zhang, Y. Cang, Y. Wen, L. Liu, X. Hou, Z. Yu, R. Zhang, **X. Guo**

PMSE **370.** Assessment of subcutaneous injection pads as acceptable skin mimics. **R. Gupta**, D. Karvani, C. Clawson, S. Pansare, S. Patel, S. Dutta Ray

PMSE **371.** Characterization of the distribution of deuterium as a function of molecular weight in D-labeled commercial polyolefins. **B.M. Habersberger**

PMSE **372.** Functional β-sheet stabilized polypeptide microspheres by NCA-ROP and noncovalent entrapment. **S. Harris Wibowo**, G. Qiao

PMSE **373.** Pyrene-modified polyelectrolytes/MWNT LbL assemblies extinguish flames on polyurethane foam. A. Cain, M. Plummer, B. Stevens, T. Smith, P. Odenborg, **K.M. Holder, J.C. Grunlan**

PMSE **374.** Intumescent nanocoating extinguishes flame on fabric using aqueous polyelectrolyte complex deposited in single step. A. Cain, S. Murray, K.M. Holder, C. Nolen, **M. Huff**, J.C. Grunlan

PMSE **375.** Extending soft lithography methods to generate patterned hydrogels. **H.G. Jayasinghe**, Y. Vasquez

PMSE **376.** Investigation of effect of bulky and hydroxyl groups in the polyimide membrane for gas separation. S. Nam, **D.J. Kim,** H. Koh, S. Ha

PMSE **377.** Reversible transformation of planar sheets into nanocapsules by host-guest trigger. **Y. Kim**, M. Lee

PMSE **378.** Elastomeric microfluidic reactors for use with 2D and 3D surfaces. **A. Konda**, M.A. Stoller, S.A. Morin

PMSE **379.** Withdrawn.

PMSE **380.** Can we tune the color of organic charge transfer systems by varying their donor-acceptor interaction geometry? **P. Li,** J. Hwang, J.M. Maier, M.D. Smith, K.D. Shimizu

PMSE **381.** Design, synthesis, and gas transport properties of spirobifluorene-based intrinsically microporous polyimides (SPIM-PI). **X. Ma**, B. Ghanem, R. Swaidan, E. Litwiller, I. Pinnau

PMSE **382.** Assessment of freeze drying as a technique to obtain silver nanopowders and easing its incorporation in silver/chitosan composites for its potential use as an antibacterial film in medical devices. **G. Madrigal**, P. Zuniga, A. Dickerman, C. Chaves-Villarreal

PMSE **383.** Synthesis and characterization of robust terephthalaldehyde-phloroglucinol (TPOL) aerogels as precursors for nanoporous carbons. **H. Majedifar**, M.A. Saeed, S. Donthula, N. Leventis, C. Sotiriou-Leventis

PMSE **384.** Donor-acceptor core-shell nanoparticles for organic photovoltaics. **K. McKenna**, J. Ferguson, H.P. Rathnayake

PMSE **385.** Highly specific quantum dot bioconjugates for single molecule imaging. **N. Mundt**, M. Butts, K. Fichter

PMSE **386.** Comparison of ion transport property of the ion exchange membrane by molecular dynamic simulation. **S. Nam**, C. Park, D.J. Kim

PMSE **387.** Alginate microspheres with encapsulated *lactibacillus* for potential bladder cancer therapy. **K. Neoh**, L. Shi, E. Kang, R. Mahendran, E. Chiong

PMSE **388.** Plasma surface modifications of nitric oxide releasing polymer films for increased hydrophilicity. **B.H. Neufeld**, A. Pegalajar-Jurado, M. Hawker

PMSE **389.** Crystallization kinetics and interfacial behavior of multiwalled carbon nanotubes based polypropylene composites. **S. Parija**, A.R. Bhattacharyya

PMSE **390.** Glass transitions of individual microdomains in phase-mixed poly(urethane urea) elastomers investigated by solid-state NMR. **N.V. Patil**, W. Hu, A. Hsieh

PMSE **391.** Thiol-ene/anhydride networks for tunably degradable neural substrates. **R. Reit**, V. Agrawal, B.R. Lund, W. Voit

PMSE **392.** Ferrocene-based polyamide aerogels: Graphitization, transmetalation, and use in heterogeneous catalysis. **M.A. Saeed**, C.A. Wisner, S. Donthula, A. Mumtaz, C. Sotiriou-Leventis, N. Leventis

PMSE **393.** Self-healing potential of triazole-pyridine based metallopolymers. **B. Sandmann, B. Happ, S. Kupfer, S. Gräfe, F.H. Schacher, M.D. Hager, U.S. Schubert**

PMSE **394.** Metal-free cycloaddition of internal alkynes and multifunctional azides under solvent-free conditions. **B. Sandmann**, B. Happ, M.D. Hager, J. Vitz, R. Paulus, P. Burtscher, N. Moszner, U.S. Schubert

PMSE **395.** In vivo evaluation of mithramycin analog nanoformulations. **D. Scott, P. Cao, J. Rohr, Y. Bae**

PMSE **396.** Effect of different fillers on the durability and mechanical properties of LDPE and PVC composites. **M.N. Siddiqui**, H.H. Redhwi, M. Younas, S. Hussain

PMSE **397.** Synthesis of donor-acceptor conjugated copolymers via acyclic diene metathesis (ADMET) and Suzuki polycondensation (SPC). **G. Singh**, H. Ardolic, M. Montano, R.M. Peetz

PMSE **398.** Synthesis and characterization of PTT using novel catalyst. **G. Song**, M. Huang, X. Li, W. Zhou, W. Yang

PMSE **399.** Applications of addition fragmentation chain transfer. **N. Sowan**, L. Cox, Y. Ding, C. Bowman

PMSE **400.** Computational design of polyethylene glycol (PEG) brushes for display of biofunctional molecules for delivery applications. **F. Stanzione**, A. Jayaraman

PMSE **401.** Increasing hydrophobic interactions in a polyelectrolyte for improved oxygen barrier in multilayer nanocomposite thin films. **B. Stevens, J.C. Grunlan**

PMSE **402.** Programmed shape change of 2D thermoplastic structures into 3D components. **M. Vannoy**, A. Konda, S.A. Morin

PMSE **403.** Synthesis and structure-property relationship of novel azobenzene-containing diamines and polyimides. **D.H. Wang, M.L. Baczkowski, J. Wie**, T.J. White, **L. Tan**

PMSE **404.** Controlled formation and dissolution of polymer suspension with visible light. **Z. Wang**, Y. Liao

PMSE **405.** Microfluidic encapsulation and photopolymerization of single cell-laden microgel. **B. Xia**, J. Oakey, K. Krutkramelis

PMSE **406.** pH-responsive polymeric microspheres for micronutrients fortification of salt. **X. Xu**, Y. Zeng, E. Rosenberg, R. Langer, A. Jaklenec

PMSE **407.** Withdrawn.

PMSE **408.** Biodegradable nitric oxide-releasing *S*-nitrosated derivatives of citrate elastomer for biomedical applications. **P. Yapor**

PMSE **409.** Shape memorizing micro and nano polymer particles. **L. Cox**, Y. Ding, J. Xiao, M.P. Stoykovich, Z. Zhang, Z. Li, J. Killgore

PMSE **410.** Arylene–ethylene polymer with high ethylene/ethane adsorption selectivity. **C. Yu**, M.G. Cowan, R.D. Noble, W. Zhang

PMSE **411.** Effects of substrate on the gradient structure and surface properties of fluorinated polyacrylates latex blends film. **H. Yuanyuan**, Z. Chaocan, C. Yanjun

PMSE **412.** Capillary instability of polymer lithographic structures: Influence of viscosity, substrate confinement and local curvature. **Z. Zhang**, G. Hilton, Y. Ding

Energy and Materials

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Innovations in Macromolecular Network Chemistry

Sponsored by POLY, Cosponsored by PMSE

Next Generation Smart Materials

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WEDNESDAY MORNING

Section B

Sheraton Denver Downtown Hotel
Governor's Square 16

Polymeric Biomaterials

Sensors and Medical Devices

Cosponsored by CELL

Financially supported by Genzyme; RSC 'Journal of Materials Chemistry B' and 'Biomaterials Science'; Genzyme; TA Instruments; Malvern Instruments; University of Delaware Materials Science & Engineering

M. Grunlan, X. Jia, *Organizers, Presiding*

8:25 PMSE **413.** Synthesis and characterization of poly(N-acryloylamino-Ethoxyethanol)-based antifouling materials. **H. Chen**, M. Zhang, R. Hu, C. Zhao, J. Zheng

8:45 PMSE **414.** PEO-silane amphiphiles to prevent protein adsorption on silicone: Dependence on concentration versus PEO-segment length. **M.A. Rufin**, M.E. Barry, P.A. Adair, M.L. Hawkins, J.E. Raymond, M.A. Grunlan

9:05 PMSE **415.** Reducing protein adsorption with polymer-grafted hyaluronic acid coatings: Optimization of material properties and a study on coating mechanism. **O. Karacsony**, G. Dunér, N. Washburn, R.D. Tilton

9:25 PMSE **416.** Self-cleaning membranes for implanted glucose biosensors. **M.A. Grunlan**, R. Fei, A.K. Means, A.A. Abraham, G.L. Coté

9:45 Intermission.

10:00 PMSE **417.** Noncovalent strengthening mechanisms in mussel adhesion and mussel mimetic polymers. D.G. Barrett, D.E. Fullenkamp, S. Manohar, **P.B. Messersmith**

10:30 PMSE **418.** Surface porous PEEK with high strength for load-bearing orthopaedic implants. N.T. Evans, F.B. Torstrick, C.S. Lee, K.M. Dupont, D.L. Safranski, W.A. Chang, A.E. Macedo, A. Lin, J.M. Boothby, D.C. Whittingslow, R.A. Carson, R.E. Guldberg, **K. Gall**

11:00 PMSE **419.** Direct deposition of body temperature responsive polymeric medical sealants. **A.M. Behrens**, B.J. Casey, M.J. Sikorski, A.D. Sandler, P. Kofinas

11:20 PMSE **420.** Mixed-charge copolymers for complete and fast wound healing. J. Jhong, **A. Venault**, Y. Chang

Section C

Sheraton Denver Downtown Hotel

Governor's Square 11

Drug Delivery and Drug Device Combination Products

Drug Device Combination

A. S. Kulshrestha, *Organizer*

S. Sridharan, *Organizer, Presiding*

J. Lange, *Presiding*

9:00 PMSE **421.** Hemofoam: A biopolymer-based foam for treating noncompressible hemorrhage. **S.R. Raghavan**, M. Dowling, J. White

9:25 PMSE **422.** Withdrawn.

9:50 PMSE **423.** Design control process for drug delivery injection device - Symlin™ pen for parenteral diabetes treatment. **L. Tsou**, M. Barnett, L. Sheridan

10:15 PMSE **424.** Development of devices for self-injection: Using tribological analysis to optimize injection force. S. Burren, L. Urbanek, **J. Lange**

10:40 PMSE **425.** Usability of devices for self-injection: A novel approach for device platforms. **J. Lange**, P. Richard, N. Bradley

11:05 PMSE **426.** Drug delivery injection systems for biopharmaceutical products. **J. Gonzalez**, J. Haynes

Section D

Sheraton Denver Downtown Hotel

Directors Row H

Nanoscale Spectroscopic and Microscopic Characterization

X-ray and Electron Microscopy

Financially supported by ExxonMobil Chemicals; Bruker; Nanosurf

D. Yablon, *Organizer*

A. H. Tsou, *Organizer, Presiding*

8:30 PMSE **427.** Molecular orientation, packing, and domain purity: Impact on organic photovoltaic devicees. **H.W. Ade**

9:00 PMSE **428.** X-ray spectroscopic characterization of organic semiconductor nanowires. **A. Mazaheripour**, N. Hüsken, J. Jocson, G. Kladnik, A. Cossaro, L. Floreano, A. Verdini, A.M. Burke, K. Miller, A. Masurkar, J. Kymissis, D. Cvetko, A. Morgante, A.A. Gorodetsky

9:20 PMSE **429.** Nanoscale characterization of polymers by soft X-ray spectromicroscopy. **A.P. Hitchcock**

9:50 Intermission.

10:05 PMSE **430.** Energy filtered TEM for element specific imaging of new poly(isoprene-b-benzofulvene) block copolymers. **S.P. Gido**

10:35 PMSE **431.** Spectroscopic characterization of (hydrated) polymers and polymer interfaces in the *(cryo)*-STEM. **M. Libera**

11:05 PMSE **432.** TEM vs. SAXS observations of microstructure in stretched polyethylene blown films. **J. Butler**, A. Bons, S. Wapp, A. Kanaan, J. Morris, D. Bucknall, D. Fiscus, A. Eberle

11:35 PMSE **433.** Increased polymer order at silica interfaces using single silanol functional groups. **H. Varol**, A. Sanchez, J. Baio, C. Malm, T. Weidner, M. Mermet-Guyennet, N. Martzel, D. Bonn, M. Bonn, E. Backus, S. Parekh

Section E

Sheraton Denver Downtown Hotel

Governor's Square 17

General Papers/New Concepts in Polymeric Materials

Novel Polymeric Materials

Q. Lin, *Organizer*

C. O. Hayes, S. Tallury, *Presiding*

8:30 PMSE **434.** Directly patternable polyhedral silsesqioxane and benzocyclobutene dielectric materials for microelectronics packaging. **C.O. Hayes**, P. Liu, B. Mueller, P. Chen, P. Thedford, W. Bell, P.A. Kohl, G. Dong, C.G. Willson

8:50 PMSE **435.** Withdrawn.

9:10 PMSE **436.** Star-shaped molecules with POSS core and azobenzene dye arms. **P.A. Ledin**, I.M. Tkachenko, W. Xu, I. Choi, V.V. Shevchenko, V.V. Tsukruk

9:30 PMSE **437.** Silicone microspheres through ultrasonic spray pyrolysis. **J.M. Rankin**, N.K. Neelakantan, K.S. Suslick

9:50 PMSE **438.** Designing block copolymer architectures toward sub-10 nm features in robust thin films. **J.H. Hayat**, A. Nese, C.G. Hardy, C. Tang

10:10 Intermission.

10:30 PMSE **439.** Thiol-maleimides for high glass transition thiol-click networks. **S. Parker**, R. Reit, B.R. Lund, W. Voit

10:50 PMSE **440.** Structure property relationships of *ortho*-functional benzoxazine monomers toward high performance thermosets. K. Zhang, S. Ohashi, **H. Ishida**

11:10 PMSE **441.** Synthesis and liquid crystalline behavior of the novel discotic benzenetrisamide-based benzoxazine. **S. Ohashi**, K. Zhang, H. Ishida

11:30 PMSE **442.** Engineering superior toughness in commercially viable block copolymer modified epoxy resin. **T. Li**, L.F. Francis, F.S. Bates

Section F

Sheraton Denver Downtown Hotel

Governor's Square 15

ACS Award in Polymer Chemistry: Symposium in Honor of Nikos Hadjichristidis

Well-Defined Polymers: From Design to Applications

Financially supported by ExxonMobil

J. Frechet, Y. Gnanou, *Organizers*

M. A. Hillmyer, *Presiding*

8:00 PMSE **443.** Supramolecular helical polymerization of homochiral, heterochiral, racemic, and achiral building blocks. **V. Percec**

8:30 PMSE **444.** Micro- and macromolecular design of aliphatic polyesters. **A. Albertsson**

9:00 PMSE **445.** Functional and light-actuated microgels — from responsive hydrogels toward microscopic locomotor systems. **M. Moeller**, M. Ahmed, H. Zhang

9:30 PMSE **446.** Critical role of well-defined polymers in rational product development. **D.J. Lohse**

10:00 Intermission.

10:30 PMSE **447.** Single site catalysts for olefin oligomerisation, polymerisation, polyolefins depolymerisation, and related reactions. **J.M. Basset**

11:00 PMSE **448.** Preparation of polycarbonates and Its block copolymers through copolymerization of carbon dioxide and epoxides. **X. Feng**, N. Hadjichristidis, Y. Gnanou

11:30 PMSE **449.** Molecular engineering of substituted polyacetylenes by living anionic polymerization. **J. He**, Y. Zhang, J. Li, Y. Yu

Section G

Sheraton Denver Downtown Hotel

Governor's Square 10

Polymer Modeling: Structure, Dynamics and Function

Structure-Function Relationships

Financially supported by ExxonMobil; Dow Chemical

R. Locker, G. C. Rutledge, *Organizers*

A. Jayaraman, *Presiding*

8:30 PMSE **450.** Using molecular simulations for rational design of polymeric materials for drug and DNA delivery. **A. Jayaraman**, R. Elder, A. Ghobadi

9:00 PMSE **451.** Morphological and rheological properties of aqueous micellar network of polyelectrolyte block copolymers. **N.K. Li**, W.H. Fuss, Y.G. Yingling

9:20 PMSE **452.** Understanding the effects of physical and chemical features of solvent additives on the bulk heterojunction morphology of blends of conjugated polymers and fullerene derivatives using molecular simulations. **H. Marsh**, A. Jayaraman

9:40 PMSE **453.** Supramolecular interaction between surface crystal and side chain crystal and its application. **S. Yao**, T. Okuma, **A. Maeda**, K. Hirakawa, **Y. Hasebe**, F. Yamasaki, R. Nakano, H. Sekiguchi

10:00 PMSE **454.** Molecular aspects of yielding of glassy polymers. **M. Hütter**, N. Lempesis, G.G. Vogiatzis, G.C. Boulougouris, L. van Breemen, M.E. Delhorme, L.E. Govaert, H.E. Meijer, D.N. Theodorou

10:30 PMSE **455.** Molecular scale modeling of polymer rheology: Investigations into slip and migration. **N.A. Rorrer**, J.R. Dorgan

10:50 PMSE **456.** Molecular basis of deformation behavior of chemically crosslinked epoxy thermosets. **S. Chattaraj**, P. Pant, D. Pawaskar, H. Nanavati

11:10 PMSE **457.** Molecular modelling of alkane nucleation under shear and extensional flow. **D. Nicholson**, G.C. Rutledge

Next Generation Smart Materials

Smart Nanomaterials, Composites, and Gels

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Smart and Responsive Composites from Renewable Building Blocks

Innovative Film & Ordered Assemblies/ Advanced Nanoreactor Systems

Sponsored by CELL, Cosponsored by PMSE

WEDNESDAY AFTERNOON

Section B

Sheraton Denver Downtown Hotel

Governor's Square 16

Polymeric Biomaterials

Instructive Tissue Engineering Matrices

Cosponsored by CELL

Financially supported by Genzyme; RSC 'Journal of Materials Chemistry B' and 'Biomaterials Science'; Genzyme; TA Instruments; Malvern Instruments; University of Delaware Materials Science & Engineering

M. Grunlan, X. Jia, *Organizers, Presiding*

1:25 PMSE **458.** Materials for angiocrine factor delivery and harnessing of pro-regenerative inflammation. **E. Botchwey**

1:55 PMSE **459.** Inherent mechanical gradients influence cell behavior in electrospun Fiber mats. M.C. Calhoun, T.M. Nelson, J.J. Lannutti, **J.O. Winter**, R. Dupaix

2:15 PMSE **460.** Engineering cell-instructive environments for the assembly of functional tissues. X. Xu, H. Zhang, K.T. Dicker, S. Liu, J.M. Fox, **X. Jia**

2:35 PMSE **461.** Guidance of smooth muscle cell migration on photocrosslinked polymer substrates with stiffness gradient. X. Liu, **S. Wang**

2:55 Intermission.

3:15 PMSE **462.** Addressing infection while engineering biomimetic tissues. **E. Loboa**

3:45 PMSE **463.** Surface gradients in biopolymeric films containing biochemical and physical cues for investigating cell-material interactions. **J.L. Almodovar**, C. Picart

4:05 PMSE **464.** Recombinant resilin-based biomaterials for tissue engineering applications. **L. Li**, Z. Tong, E. Levendoski, X. Jia, S. Thibeault, K.L. Kiick

4:25 PMSE **465.** Self-folding photopatterned hydrogel scaffolds for 3D cell culture. **H. Kwag**, J. Serbo, L. Romer, D.H. Gracias

Section C

Sheraton Denver Downtown Hotel

Governor's Square 11

Drug Delivery and Drug Device Combination Products

Controlled Release

S. Sridharan, *Organizer*

A. S. Kulshrestha, *Organizer, Presiding*

L. Tsou, *Presiding*

1:30 PMSE **466.** Controlled localized drug release from an injectable-solid peptide hydrogel. **D.J. Pochan**

1:55 PMSE **467.** Controlled release of salicylic acid from a glycerol/adipic acid hyperbranched poly(ester). **B.A. Howell**, T. Zhang, P.B. Smith

2:20 PMSE **468.** Bio-inspired synthetic vesicles for glucose-responsive insulin delivery. W. Tai, J. Di, **Z. Gu**

2:45 PMSE **469.** Noncovalent interaction-stabilized polymeric micelles for targeted delivery of anticancer drug. **J.P. Tan**, A. Attia, C. Yang, S. Gao, J.L. Hedrick, A. Nelson, Y. Yang

3:10 PMSE **470.** Smart hydrogels based on poly(L-histidine) for drug delivery to treat pancreatic cancer. **H. Iatrou**, P. Bilalis, A. Karatzas, K. Dimas, D. Vlassopoulos, C. Tsimblouli, Y. Marakis, E. Sereti

3:35 PMSE **471.** Stabilization and delivery of human growth hormone from polymer nanofibers. Y. Gao, J. Harris, **M. Becker**

Section D

Sheraton Denver Downtown Hotel

Directors Row H

Nanoscale Spectroscopic and Microscopic Characterization

Spectroscopic Characterization

Financially supported by ExxonMobil Chemicals; Bruker; Nanosurf

A. H. Tsou, D. Yablon, *Organizers*

H. W. Ade, *Presiding*

1:30 PMSE **472.** Probing molecular mechanisms underlying failure in semicrystalline polymers. **C.R. Snyder**

2:00 PMSE **473.** Theoretical and experimental vibrational spectroscopy of ionomers. **E.S. Smotkin, J. Doan**, E. Kingston, K. Anderson, A. Vong

2:20 PMSE **474.** Chemical, morphological, and mechanical characterization of the interphase of polymer matrix composites. **D. Nepal**, A. Ecker, J. Moller, S. Barr, R.J. Berry, T. Breitzman

2:40 Intermission.

3:00 PMSE **475.** Characterization of polymer chain macrostructures: Complete chain architectures. **A.E. Tonelli**

3:30 PMSE **476.** IR spectroscopy of Cd^{2+} exchanged Nafion and sulfonated poly(ether ether ketone), vs. state-of-hydration, for quantum dot preparation. **K. Anderson**, E. Kingston, E.S. Smotkin

‡ *Cooperative Cosponsorship*

3:50 PMSE **477.** Dynamic mechanical relaxations in ultrahigh molecular weight polyethylene fibers probed by solid-state NMR. N.V. Patil, **W. Hu**

Section E

Sheraton Denver Downtown Hotel
Governor's Square 9

General Papers/New Concepts in Polymeric Materials

Novel Polymeric Materials

Q. Lin, *Organizer*
M. Galizia, N. Guigo, *Presiding*

1:30 PMSE **478.** Learning from peptides and realizing by polymers: Translating bioinspired sequences toward synthetic polymers to explore sequence specific interactions. **H. Boerner**

1:50 PMSE **479.** Photodegradable and biodegradable biomaterials based on alkoxyphenacyl and coumarin chromophores. **A. Joy, S. Sun**, E. Chamsaz

2:10 PMSE **480.** Formation of ⊠-sheet hollow microspheres by NCA-ROP and surface-anchored peptide assembly. **S. Harris Wibowo**, G. Qiao

2:30 PMSE **481.** Cellular toxicity and uptake behavior of triphenyl phosphonium-containing conjugated polymer nanoparticles. **E. Mendez, R. Manian, J. Moon**

2:50 PMSE **482.** Phototriggered crosslinking of multifunctional nanoparticles by Michael-type addition. **Y. Liang**, K.L. Kiick

3:10 Intermission.

3:30 PMSE **483.** Predictive calculation of hydrogen and helium solubility in glassy and rubbery polymers. **M. Galizia, Z.P. Smith, G.C. Sarti, B.D. Freeman, D.R. Paul**

3:50 PMSE **484.**
Heterogeneous thiol-Michael addition polymerization for the design of functional microparticles. **C. Wang, M. Podgórski**, C. Bowman

4:10 PMSE **485.** Constructing bicontinuous polymeric nanospheres from amphiphilic block copolymers: Control of pore size and thermal phase transitions. **S.J. Holder**, B. McKenzie, M.J. Wirix, J.F. de Visser, O. Monaghan, P.H. Bomans, F. Nudelman, N.A. Sommerdijk

4:30 PMSE **486.** PEGMEMA-Titania hybrid particles from commercial dual functional organophosphonic acid linkers: a powerful approach to coating applications. **E. Cao**, E. Prouzet, V. Héroguez

Section F

Sheraton Denver Downtown Hotel
Governor's Square 15

ACS Award in Polymer Chemistry: Symposium in Honor of Nikos Hadjichristidis

Well-Defined Polymers: From Design to Applications

Financially supported by ExxonMobil

J. Frechet, Y. Gnanou, *Organizers*
J. W. Mays, *Presiding*

1:00 PMSE **487.** Complex periodic polymer microphases. **E.L. Thomas**

1:30 PMSE **488.** Nanostructured block copolymers for lithium batteries. **N.P. Balsara**

2:00 PMSE **489.** Tailoring molecular packing for uncommon polymeric self-assemblies. J. Haataja, N. Houbenov, R. Milani, P. Metrangolo, H. Iatrou, N. Hadjichristidis, **O.T. Ikkala**

2:30 Intermission.

3:00 PMSE **490.** Molecular scale dynamics of ring polymers: a neutron spin echo study. **D. Richter**

3:30 PMSE **491.** New high temperature thermoplastic elastomers based on polybenzofulvene. **J.W. Mays**, W. Wang, T. White, N. Kang, K. Hong

4:00 PMSE **492.** Order and disorder in short block polymers. **F.S. Bates**, T. Gillard, C. Leighton, S. Lee

4:30 PMSE **493.** Nanostructured membranes by in situ block polymer synthesis. **M.A. Hillmyer**

5:00 PMSE **494. Award Address** (ACS Award in Polymer Chemistry sponsored by ExxonMobil Chemical). Well-defined polymers: From design to applications. **N. Hadjichristidis**

Section G

Sheraton Denver Downtown Hotel
Governor's Square 10

Polymer Modeling: Structure, Dynamics and Function

Polymer Modeling in Industry

Financially supported by ExxonMobil; Dow Chemical

R. Locker, G. C. Rutledge, *Organizers*
S. Tallury, *Presiding*

1:00 PMSE **495.** Advances in atomistic polymer modeling: Thermosets and interfaces. **P. Saxe**, C. Freeman, D. Rigby

1:30 PMSE **496.** Driving innovation for advanced materials and systems formulation modeling. **P. Veld**

2:00 PMSE **497.** Molecular-level deformation in stacked lamellar polyethylene. **R. Locker**, J. Kim, A.H. Tsou, G.C. Rutledge

2:30 PMSE **498.** Modeling applications for improved understanding of block copolymer morphology. **J. Weinhold**, V.V. Ginzburg, P.D. Hustad

3:00 Concluding Remarks.

Next Generation Smart Materials

Smart Nanomaterials, Composites, and Gels

Sponsored by POLY, Cosponsored by PMSE

Innovations in Macromolecular Network Chemistry

Self-healing or Magnetic

Sponsored by POLY, Cosponsored by PMSE

Smart and Responsive Composites from Renewable Building Blocks

Advanced Nanoreactor Systems/New Paradigms to Smart Material Chemistry & Engineering

Sponsored by CELL, Cosponsored by PMSE

THURSDAY MORNING

Section A

Sheraton Denver Downtown Hotel
Governor's Square 10

General Papers/New Concepts in Polymeric Materials

Polymer Processing and Properties

Q. Lin, *Organizer*
M. W. Frey, M. Krecker, S. Tallury, *Presiding*

8:30 PMSE **499.** Thick growing multilayer thin film with high gas barrier and fire resistance. **M. Krecker**, T. Guin, D. Hagen, J.C. Grunlan

8:50 PMSE **500.** Processing polyamides in superheated water. **G.C. Evans**, A.J. Lesser

9:10 PMSE **501.** Rheological characterization of filled polyamide 11 and polyamide 12 solutions in polyols. **K.A. Patankar**, V.V. Ginzburg, G.F. Billovits

9:30 PMSE **502.** Wheat gluten modified by rubbery cross-linker for improved mechanical properties and reduced water absorption. **C. Diao**, H. Xia, R. Parnas

9:50 PMSE **503.** Halogen-bonded mesogens direct polymer self-assemblies over millimeter length scale. N. Houbenov, R. Milani, M. Poutanen, J. Haataja, V. Dichiarante, J. Sainio, J. Ruokolainen, G.P. Resnati, P. Metrangolo, **O.T. Ikkala**

10:10 Intermission.

10:30 PMSE **504.** Effects of solvents on the morphology and conductivity of poly(3,4ethylenedioxythiophene):poly(-styrenesulfonate) nanofibers. **M.W. Frey**, M. Pehlivaner Kara

10:50 PMSE **505.** Nonisothermal crystallization of biobased poly(ethylene 2,5-furandicarboxylate). **N. Sbirrazzuoli**, A. Codou, N. Guigo, J. van Berkel, E. Dejong

11:10 PMSE **506.** Dynamic strain hole burning of elastomers filled with nanoparticles. **S. Li**, G. Zhan, Y. Mi, **X. Wang**

11:30 PMSE **507.** Heat- or water-driven malleability in covalent network polyimines. **P.J. Taynton**, W. Zhang

Section B

Sheraton Denver Downtown Hotel
Governor's Square 16

Polymeric Biomaterials

Instructive Tissue Engineering Matrices

Cosponsored by CELL

Financially supported by Genzyme; RSC 'Journal of Materials Chemistry B' and 'Biomaterials Science'; Genzyme; TA Instruments; Malvern Instruments; University of Delaware Materials Science & Engineering

M. Grunlan, X. Jia, *Organizers, Presiding*

8:25 PMSE **508.** Chondroinductive biomaterials for cartilage regeneration. **M.S. Detamore**

8:55 PMSE **509.** OGP functionalized phenylalanine-based poly(ester urea) for enhancing osteoinductive potential of human mesenchymal stem cells. G.M. Policastro, F. Lin, K. Stakleff, M. Graham, R. Katsarava, **M. Becker**

9:25 PMSE **510.** Dynamic polymer substrates with Increasing stiffness for regulation of smooth muscle cells. X. Liu, L. Cai, **S. Wang**

9:45 Intermission.

10:05 PMSE **511.** Antioxidant biomaterials for regenerative engineering applications. **G. Ameer**

10:35 PMSE **512.** Nanoengineered polymeric biomaterials for musculoskeletal tissue engineering: A growth-factor-free approach. J.R. Xavier, J.K. Carrow, T. Thakur, P. Desai, L. Cross, M. Jaiswal, **A.K. Gaharwar**

11:05 PMSE **513.** Novel mechanochemical reaction cascade for sensing bond breakage in hydrogels. **K.R. Fitch, A.P. Goodwin**

Section C

Sheraton Denver Downtown Hotel
Governor's Square 11

Drug Delivery and Drug Device Combination Products

Non-fouling Antimicrobial and Transdermal Therapies

A. S. Kulshrestha, S. Sridharan, *Organizers, Presiding*

9:00 PMSE **514.** Modulating *Vibrio cholerae* quorum-sensing-controlled communication using autoinducer-loaded nanoparticles. **R.K. Prudhomme**

9:25 PMSE **515.** Facile synthesis of antifouling dendrimer for drug and bioprobe delivery. **Y. Han**, M. Ye, Y. Qian, H. Hu, J. Tang, M. Sui, X. Liu, Y. Shen

9:50 PMSE **516.** In vivo visible light-triggered drug release from an implanted depot. **C. Carling**, M. Viger, V.A. Nguyen Huu, A. Garcia, A. Almutairi

10:15 PMSE **517.** Pentobra: A novel multifunctional antibiotic to fight bacterial resistance. **S. Deshayes**, N. Schmidt, G. Wong, A.M. Kasko

Section D

Sheraton Denver Downtown Hotel
Directors Row H

General Papers/New Concepts in Polymeric Materials

Design of Functional Polymeric Materials

Q. Lin, *Organizer*
W. Braunecker, H. Gao, *Presiding*

8:30 PMSE **518.** Developing one-pot polymerization methods to access uniform hyperbranched ppolymers. **H. Gao**

8:50 PMSE **519.** Design, synthesis, and structure-function studies of novel triblock copolymers. **J.E. Semple**, B.T. Sullivan, B.K. Burke, T. Vojkovsky, K.N. Sill

9:10 PMSE **520.** Rational design of a crown-ether-bearing copolymer by overcoming the compositional drift in *N*-(2-hydroxypropyl) methacrylamide copolymerization. **J. Moraes**, I. Simionca, H. Ketari, H.A. Klok

9:30 PMSE **521.** Preparation and evaluation of hybrid adsorbent for the removal of trace organic contaminants from water and wastewater. **B. Bhattarai**, M. Manickavachagam, R.P. Suri

9:50 PMSE **522.** Claisen rearrangement catalyzed by mechanical force. **K. Kumar**, K. Fitch, P.K. Shah, J.W. Stansbury, A. Weidner, A.P. Goodwin

10:10 Intermission.

10:30 PMSE **523.** Organic radical polymer brushes for mechanistic charge transfer studies. **W.A. Braunecker**, B.K. Hughes, A. Ferguson, J.C. Johnson, P. Ndione, S. Nanayakkara, T. Gennett

10:50 PMSE **524.** Control of spacer arm strategy to synthesize amphiphilic polymers with highly selective bactericidal activity. **A. Puni**a, N. Yang

11:10 PMSE **525.** Design of multifunctional quantum dot conjugates for biomedical applications. J.M. Davis, B. Agana, N. Mundt, M. Ellis, D. Klaus, **K. Fichter**

11:30 PMSE **526.** Autonomous movement of nanomotors fueled by biological substrates using compartmentalization and substrate recycling strategies. **M. Nijemeisland**, L. Abdelmohsen, J. van Hest, D.A. Wilson

Section E

Sheraton Denver Downtown Hotel
Governor's Square 9

General Papers/New Concepts in Polymeric Materials

Stimulus-Responsive Materials

Q. Lin, *Organizer*
L. Peng, S. Tallury, *Presiding*

8:30 PMSE **527.** Withdrawn.

8:50 PMSE **528.** Interfacial behavior and assembly of multiresponsive star graft copolymers. **W. Xu**, Z. Iatridi, C. Tsitsilianis, V.V. Tsukruk

9:10 PMSE **529.** Electrochemical redox responsive supramolecular hydrogels based on host-guest interaction between β-cyclodextrin and ferrocene. **L. Peng**, A. Feng, J. Yuan

9:30 PMSE **530.** Encapsulation of charge-transfer complexes for mechanochromic sensors applications. **A. Lavrenova, J. Farkas, C. Weder, Y.C. Simon**

9:50 PMSE **531.** Use of peripherally alkylated dithieno[3,2-*b*:2,3-*d*]pyrrole units in conjugated polymers and small molecules for sensing applications. **J. Green**, Y. Han, M.J. Heeney

10:10 Intermission.

10:30 PMSE **532.** Controlling the self-assembly of semicrystalline block copolymers toward manipulating the phase transition of bicontinuous nanospheres. **O. Monaghan**, B. McKenzie, N.A. Sommerdijk, S.J. Holder

10:50 PMSE **533.** Synthesis and characterization of photomechanically responsive bis(azobenzene)-functionalized aromatic polyamides and poly(amide-imides). **D.H. Wang**, J. Wie, J. Che, R. Vaia, T.J. White, L. Tan

11:10 PMSE **534.** Electrically tunable plasmonic behavior of nanocube-polymer nanomaterials induced by a redox active electrochromic polymer. T.A. König, **P.A. Ledin**, J.A. Kerszulis, M.A. Mahmoud, M.A. El-Sayed, J.R. Reynolds, V.V. Tsukruk

11:30 PMSE **535.** Reversible temperature-responsive vesicles formed by polyoxometalate-polymer hybrids in aqueous solution. **J. Zhou**, T. Liu

Section F

Sheraton Denver Downtown Hotel

Plaza Court 8

General Papers/New Concepts in Polymeric Materials

New Concepts in Polymeric Materials

Q. Lin, *Organizer*

H. Dong, A. Shirke, *Presiding*

8:30 PMSE **536.** Efficient Cu(I) acetate-catalyzed cycloaddition of multifunctional alkynes and azides under solvent-free conditions. **B. Sandmann**, B. Happ, M.D. Hager, J. Vitz, R. Paulus, E. Rettler, P. Burtscher, N. Moszner, U.S. Schubert

8:50 PMSE **537.** Withdrawn.

9:10 PMSE **538.** Toughening a glassy polymer with naturally derived cellulose nanofibrils. **H. Dong**, J. Steele, J.F. Snyder, J.A. Orlicki, G. Napadensky, R.S. Reiner, A.W. Rudie

9:30 PMSE **539.** Surfactant-direct assembly of water soluble conjugated polyelectrolytes. **G. Braggin**, S. Zhang

9:50 PMSE **540.** Sustainable large-scale solvent driven actuation by self-healable polyelectrolyte multilayers. **Y. Gu**, X. Huang, N. Zacharia

10:10 Intermission.

10:30 PMSE **541.** Preparation of poly(methyl methacrylate/butyl acrylate) nanoparticles by miniemulsion polymerization in the presence of commercially avaliable hydrophobized TiO_2 nanoparticles. **E.S. Adurahim, M.A. Bahattab, A. Schoth, K. Landfester, R. Munoz-Espi**

10:50 PMSE **542.** Cutinase paradigm: Sustainable biocatalysis for polymer surface modifications and plastic recycling. **A. Shirke**, D. Basore, A. Su, S. Holton, G. Butterfoss, C. Bystroff, R.A. Gross

11:10 PMSE **543.** Chain mobility and penetrant transport in poly(ethylene furanoate) compared to poly(ethylene terephthalate). **S.K. Burgess**, R.M. Kriegel, W.J. Koros

11:30 PMSE **544.** Proton conduction in a cephalopod structural protein. **D.D. Ordinario**, L. Phan, W.G. Walkup, J. Jocson, E. Karshalev, N. Hüsken, A.A. Gorodetsky

Next Generation Smart Materials

Smart Nanomaterials, Composites, and Gels

Sponsored by POLY, Cosponsored by PMSE‡

Innovations in Macromolecular Network Chemistry

Medical: Hydrogels and Particles

Sponsored by POLY, Cosponsored by PMSE

PROF

Division of Professional Relations

R. D. Libby, *Program Chair*

BUSINESS MEETINGS:

PROF Division Business Meeting, 3:00 PM: Tue

SUNDAY MORNING

Section A

Hyatt Regency Denver at Colorado Convention Center

Capitol Ballroom 6

Native American Women Chemists of Color

Cosponsored by CMA and WCC

L. M. Watkins, *Organizer*

N. B. Jackson, G. Thomas, *Presiding*

8:30 Introductory Remarks.

8:40 PROF **1.** Otakuye Conroy-Ben: University of Utah. **O. Conroy-Ben**

8:50 PROF **2.** Robyn Hannigan, University of Massachusetts Boston. **R. Hannigan**

9:00 PROF **3.** Joslynn Lee, University of Minnesota Medical School. **J. Lee**

9:10 PROF **4.** Naomi Lee, National Institutes of Health. **N. Lee**

9:20 PROF **5.** Amy Paris, Kimberly-Clark Corporation. **A.K. Paris**

9:30 Panel Discussion.

10:30 Intermission.

10:45 Questions and Answers.

11:45 Concluding Remarks.

Growing Opportunities for Research Abroad: An Undergraduate Perspective of International Research Experiences

Sponsored by IAC, Cosponsored by CHED, PROF and YCC

SUNDAY AFTERNOON

Section A

Hyatt Regency Denver at Colorado Convention Center

Capitol Ballroom 6

Earning ACS Awards: An Interactive Symposium on Constructing Successful Award Nominations

Cosponsored by BMGT, SCHB and WCC

J. L. Bryant, *Organizer, Presiding*

A. S. Hinkle, *Presiding*

1:00 Introductory Remarks.

1:15 Moderated Panel I.

2:00 Hands-On Working Sessions.

2:45 Report Out from Working Groups.

3:00 Intermission.

3:15 Introductory Remarks.

3:20 Moderated Panel II.

4:00 Hands-On Working Sessions.

4:45 Report Out from Working Groups.

4:55 Concluding Remarks.

Growing Opportunities for Research Abroad: An Undergraduate Perspective of International Research Experiences

Sponsored by IAC, Cosponsored by CHED, PROF and YCC

Starting a Successful Research Program at a Predominantly Undergraduate Institution

Sponsored by YCC, Cosponsored by PROF

MONDAY MORNING

Section A

Hyatt Regency Denver at Colorado Convention Center

Capitol Ballroom 6

ACS Award for Encouraging Women into Careers in the Chemical Sciences: Symposium in Honor of E. Ann Nalley

Championing the Empowerment of Women in Chemistry

Cosponsored by WCC

Z. M. Lerman, *Organizer*

F. K. Wood-Black, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 PROF **6.** Ann Nalley: A teacher — a colleague — a legacy. **D.G. McGuire**

9:00 PROF **7.** The importance of mentoring in developing female leaders. **M. Jeffries-El**

9:25 PROF **8.** Inspiration for generations. **K. Galindo**

9:50 PROF **9.** Paying it forward: Small actions and encouragement result in a grand legacy. **F.K. Wood-Black**

10:15 PROF **10.** Chain reaction-the smallest things have the biggest impact: A window into how Ann Nalley changed my life. **C.J. Siddons**

10:40 Intermission.

10:50 PROF **11.** Ann Nalley: Consummate and tireless teacher, friend, mentor, scholar, and international leader in promoting women in science. **T. Conley**

11:15 PROF **12.** NanoExplorers: A high school summer science academy and applied mathematics and aerospace engineering summer academy for middle school girls. **J.L. Gesell, E.A. Nalley, M. Polson**

11:40 PROF **13.** How to get buy in the: Woodall Nalley theory. **R.A. Woodall**

12:05 Concluding Remarks.

Diversifying STEM: Uniting through our Differences for a Brighter Scientific Future

Sponsored by CMA, Cosponsored by CHED and PROF

Excellence in Graduate Polymer Research

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

MONDAY AFTERNOON

Section A

Hyatt Regency Denver at Colorado Convention Center

Capitol Ballroom 6

Chemical Angel Network: Chemists Investing in Chemical Companies

Cosponsored by SCHB

J. L. Bryant, M. Vreeke, *Organizers*

S. S. White, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 PROF **14.** News and updates from the Chemical Angel Network (CaN). **M. Vreeke**, S.S. White, J.C. Giordan

2:00 PROF **15.** Angel Investing 101. **J.C. Giordan**

2:30 Company Presentations.

3:30 Investment Discussion.

4:00 Open Forum.

4:30 Concluding Remarks.

Excellence in Graduate Polymer Research

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

TUESDAY MORNING

Section A

Hyatt Regency Denver at Colorado Convention Center

Capitol Ballroom 6

ACS Award for Encouraging Women into Careers in the Chemical Sciences: Symposium in Honor of E. Ann Nalley

Championing the Empowerment of Women in Chemistry

Cosponsored by WCC

F. K. Wood-Black, *Organizer*

Z. M. Lerman, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 PROF **16.** Ann Nalley, the female trailblazer. **A. Pavlath**

9:00 PROF **17.** Experiences with Ann Nalley Spanning 30 years. **D.J. Nelson**

9:25 PROF **18.** Honoring Ann Nalley, a friend, mentor, and champion for women in science. **M.P. Wu**

9:50 Intermission.

10:00 PROF **19.** Woman of valor: More precious than pearls. **Z.M. Lerman**

10:25 PROF **20.** The Legacy of Dr. E. Ann Nalley. **O.D. Nelson**

10:50 PROF **21.** What women can do (WWCD©): The future is really up to us. **J.C. Giordan**

11:15 PROF **22. Award Address** (ACS Award for Encouraging Women into Careers in the Chemical Sciences sponsored by the Camille and Henry Dreyfus Foundation). Inspiring women in chemistry: Leading by example. **E.A. Nalley**

11:40 Concluding Remarks.

TUESDAY AFTERNOON

Section A

Hyatt Regency Denver at Colorado Convention Center

Capitol Ballroom 6

Proposing and Administering a Successful REU Program

L. M. Watkins, *Organizer*

G. Thomas, *Presiding*

1:00 Introductory Remarks.

1:05 PROF **23.** REU site focusing on regional 2-yr community college students. **W. Jang, A.D. Headley, S.D. Starnes**

1:30 PROF **24.** Hosting an REU at a PUI: Benefits and challenges. **S.B. Braun-Sand**, A.M. Schoffstall

1:55 PROF **25.** Description of an inaugural Research Experiences for Undergraduates (REU) program. **A.M. Powe**

2:20 PROF **26.** Chemistry REU program at the University of Kansas. **D.R. Benson**

2:45 PROF **27.** CheMIE REU chemistry research community with a focus on molecular innovation and entrepreneurship. **W.M. David, W.J. Brittain**

3:10 Intermission.

3:25 PROF **28.** Exploring the unknown with the REU program at the University of Oregon. **G.L. Richmond**

3:50 PROF **29.** Mentoring experience behind successful iREU participants. **R. Duran, D. Spivak, G. Thomas**

4:15 PROF **30.** International multisite REU program. **T.A. Nile**

4:40 Panel Discussion.

5:20 Concluding Remarks.

WEDNESDAY AFTERNOON

Section A

Hyatt Regency Denver at Colorado Convention Center

Capitol Ballroom 6

Hands-on STEM Enrichment Programs for Persons with Disabilities

A. A. Hill, C. A. Supalo, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 PROF **31.** Enriching the discourse of equity in the globalized knowledge economy. **J. Bhattacharya**

1:55 PROF **32.** Hands-on laboratory experiences for the visually impaired. **A.A. Hill**

2:15 PROF **33.** 2014 "Summer Science Spectacular": A model for successful partnerships between the NFB and post-secondary institutions. **C.A. Supalo**

2:35 PROF **34.** Summer research experience for undergraduate students with disabilities at the University of Delaware. **K.S. Booksh**

2:55 Intermission.

3:10 PROF **35.** Exemplars of summer enrichment programs for students with disabilities hosted around the world. **H. Wohlers**

3:30 PROF **36.** Cal Poly laboratory chemistry workshops for blind and visually impaired high school students. **D.M. Fantin**

3:50 PROF **37.** Outreach and educational programs for deaf and hard-of-hearing students in the sciences. **A.D. Ross, S.B. Smith, T. Pagano**

4:10 PROF **38.** Research and cooperative work experiences for deaf and hard-of-hearing undergraduate students in the sciences. **T. Pagano, A.D. Ross, S.B. Smith**

4:30 Concluding Remarks.

‡ *Cooperative Cosponsorship*

RUBB

Rubber Division

T. R. DeLapa, *Program Chair*

MONDAY EVENING

STRETCH Your Students' Polymer Knowledge by Putting Some BOUNCE into Your Curriculum

Polymer Science Education and the NGSS

Sponsored by CHED, Cosponsored by PMSE, POLY, RUBB and SCC‡

SCHB

Division of Small Chemical Businesses

J. Sabol, *Program Chair*

OTHER SYMPOSIA OF INTEREST:

Water Our Most Critical Resource *(see AGFD, Wed, Thu)*

Colorado Biotechnology: The Science of Colorado's Craft Beer, Wine & Spirits Industries *(see BIOT, Sun)*

Citizens First: Communicating Climate Science to the Public *(see CHED, Tue)*

Transitioning between Academic Research into Practical Use: Solar-Energy and Advanced Materials *(see COMSCI, Mon)*

Microalgae: A Renewable Energy Source and a Sustainable Solution for the Environment *(see ENVR, Wed)*

Hydraulic Fracturing Impacts on Water, Soil and Air Quality *(see ENVR, Mon, Tue)*

SOCIAL EVENTS:

Breakfast, 7:30 AM: Sun

Luncheon, 12:00 PM: Sun

SCHB Hach Award Luncheon, 12:00 PM: Mon

SCHB Hach Award Reception, 5:30 PM: Mon

Social Hour, 5:30 PM: Mon

BUSINESS MEETINGS:

SCHB Division Executive Committee Meeting, 8:30 AM: Sun

SCHB Division Business Meeting, 1:15 PM: Sun

SUNDAY AFTERNOON

Section A

Embassy Suites Denver–Downtown Convention Center

Cripple Creek Ballroom 2

SCHB Entrepreneurs' Poster Session

Cosponsored by YCC

G. Ruger, *Organizer, Presiding*

1:30 - 3:30

SCHB **1.** Thirty-five years and going strong: SCHB offers resources and networking opportunities for small and growing chemical businesses. **M. Chorghade**, A. Rahman, S.S. Seelig, P. Kearney, D.J. Deutsch, S.V. Vercellotti, J.E. Sabol, J.L. Maclachlan, C.A. Burton, K. Hylton-Rodic, J. Lee, G. Ruger, N.A. Vaidya

SCHB **2.** Chemical Angel Network chemists investing in chemical businesses. **S. White**, M. Vreeke, J.C. Giordan

Section A

Embassy Suites Denver–Downtown Convention Center

Cripple Creek Ballroom 2

Best Practices for Success with SBIR & STTR Grants

Cosponsored by PROF and YCC

P. Kearney, *Organizer, Presiding*

2:00 Introductory Remarks.

2:05 SCHB **3.** ThruPore Technologies LLC: Experiences in NSF's I-Corps and SBIR programs. **M.G. Bakker**, F.M. Sayler

2:30 SCHB **4.** Chemical entrepreneur's first time NIH SBIR grant application submission. **P.C. Kearney**

2:55 Panel Discussion.

Earning ACS Awards: An Interactive Symposium on Constructing Successful Award Nominations

Sponsored by PROF, Cosponsored by BMGT, SCHB and WCC

MONDAY MORNING

Section A

Embassy Suites Denver–Downtown Convention Center

Cripple Creek Ballroom 2

Kathryn C. Hach Award for Entrepreneurial Success: Symposium in Honor of Terry L. Brewer

Cosponsored by PROF and YCC

P. Kearney, *Organizer*

J. E. Sabol, *Organizer, Presiding*

8:00 Coffee & Networking.

8:30 Introductory Remarks.

8:50 SCHB **5.** Entrepreneurs: Locally born to accept the global challenges. **S. Moles**

9:20 SCHB **6.** Innovation and entrepreneurship: Advantages of private companies. **J. Mooney**

9:50 Intermission.

10:20 SCHB **7.** Small business in a big industry. **K. Savala**

10:50 SCHB **8. Award Address** (Kathryn C. Hach Award for Entrepreneurial Success sponsored by the Kathryn C. Hach Award Fund). Small business (chemistry) in a big world (technology). **T.L. Brewer**

MONDAY AFTERNOON

Section A

Embassy Suites Denver–Downtown Convention Center

Cripple Creek Ballroom 2

Water is the Next Oil: Small Businesses Percolating to the Top

Cosponsored by YCC

A. Boal, *Organizer, Presiding*

2:00 Introductory Remarks.

2:05 SCHB **9.** Surface-modified carbon electrodes for long-life capacitive deionization processes. **J.R. Landon**, C. Lippert

2:35 SCHB **10.** Innovating water treatment with on-demand chemistry. **A.K. Boal**

3:05 SCHB **11.** Evolution of Hach Chemical Company to Hach Lange: Success and growth through customer focus. **C.C. Johnson**

3:35 Concluding Remarks.

Chemical Angel Network: Chemists Investing in Chemical Companies

Sponsored by PROF, Cosponsored by SCHB

MONDAY EVENING

Section A

Colorado Convention Center

Halls C/D

Sci-Mix

J. Sabol, *Organizer*

8:00 - 10:00

1-2, 9. See previous listings.

CCS

Committee on Chemical Safety

E. Howson, *Program Chair*

SUNDAY AFTERNOON

Nanotechnology: Delivering on the Promise

Research & Development

Sponsored by PRES, Cosponsored by AGFD, AGRO, ANYL, CARB, CCPA, CCS, CHAS, COLL, COMSCI, CORP, ENFL, HIST, I&EC, IAC, MPPG, PMSE, POLY, SCHB and SOCED

MONDAY MORNING

Nanotechnology: Delivering on the Promise

Opportunities and Challenges for Health, Safety and the Environment

Sponsored by PRES, Cosponsored by AGFD, AGRO, ANYL, CARB, CCPA, CCS, CHAS, COLL, COMSCI, CORP, ENFL, HIST, I&EC, IAC, MPPG, PMSE, POLY, SCHB and SOCED

MONDAY AFTERNOON

Nanotechnology: Delivering on the Promise

Bridging the Gap to a Thriving US Marketplace

Sponsored by PRES, Cosponsored by AGFD, AGRO, ANYL, CARB, CCPA, CCS, CHAS, COLL, COMSCI, CORP, ENFL, HIST, I&EC, IAC, MPPG, PMSE, POLY, SCHB and SOCED

Legalized Marijuana & Health & Safety

Sponsored by CHAS, Cosponsored by CCS

TUESDAY MORNING

Ask Dr. Safety: EH&S Support of Nanotechnology R&D

Sponsored by CHAS, Cosponsored by AGFD, CCS and PRES

TUESDAY AFTERNOON

Safety in Undergraduate Teaching

Sponsored by CHAS, Cosponsored by CCS

CCPA

Committee on Chemistry and Public Affairs

S. Butts, *Program Chair*

SUNDAY AFTERNOON

Nanotechnology: Delivering on the Promise

Research & Development

Sponsored by PRES, Cosponsored by AGFD, AGRO, ANYL, CARB, CCPA, CCS, CHAS, COLL, COMSCI, CORP, ENFL, HIST, I&EC, IAC, MPPG, PMSE, POLY, SCHB and SOCED

MONDAY MORNING

Nanotechnology: Delivering on the Promise

Opportunities and Challenges for Health, Safety and the Environment

Sponsored by PRES, Cosponsored by AGFD, AGRO, ANYL, CARB, CCPA, CCS, CHAS, COLL, COMSCI, CORP, ENFL, HIST, I&EC, IAC, MPPG, PMSE, POLY, SCHB and SOCED

MONDAY AFTERNOON

Nanotechnology: Delivering on the Promise

Bridging the Gap to a Thriving US Marketplace

Sponsored by PRES, Cosponsored by AGFD, AGRO, ANYL, CARB, CCPA, CCS, CHAS, COLL, COMSCI, CORP, ENFL, HIST, I&EC, IAC, MPPG, PMSE, POLY, SCHB and SOCED

TUESDAY MORNING

DOE Nanoscience Research Centers

National Resources for the Nanoscience Community

Sponsored by PRES, Cosponsored by ANYL, CCPA, CEI, ENFL and MPPG

CORP

Committee on Corporation Associates

D. Mason, *Program Chair*

SUNDAY AFTERNOON

Nanotechnology: Delivering on the Promise

Research & Development

Sponsored by PRES, Cosponsored by AGFD, AGRO, ANYL, CARB, CCPA, CCS, CHAS, COLL, COMSCI, CORP, ENFL, HIST, I&EC, IAC, MPPG, PMSE, POLY, SCHB and SOCED

MONDAY MORNING

Nanotechnology: Delivering on the Promise

Opportunities and Challenges for Health, Safety and the Environment

Sponsored by PRES, Cosponsored by AGFD, AGRO, ANYL, CARB, CCPA, CCS, CHAS, COLL, COMSCI, CORP, ENFL, HIST, I&EC, IAC, MPPG, PMSE, POLY, SCHB and SOCED

MONDAY AFTERNOON

Nanotechnology: Delivering on the Promise

Bridging the Gap to a Thriving US Marketplace

Sponsored by PRES, Cosponsored by AGFD, AGRO, ANYL, CARB, CCPA, CCS, CHAS, COLL, COMSCI, CORP, ENFL, HIST, I&EC, IAC, MPPG, PMSE, POLY, SCHB and SOCED

DAC

Committee on Divisional Activities

M. J. Morello, *Program Chair*

MONDAY MORNING

Frontiers in Glycoscience

Synthesis and Functions

Sponsored by CELL, Cosponsored by CARB‡ and DAC‡

MONDAY AFTERNOON

Frontiers in Glycoscience

Control of Sequence and Regiochemistry

Sponsored by CELL, Cosponsored by CARB‡ and DAC‡

TUESDAY MORNING

Frontiers in Glycoscience

Characterization and Applications

Sponsored by CELL, Cosponsored by CARB‡ and DAC‡

TECHNICAL PROGRAM

TUESDAY AFTERNOON

Frontiers in Glycoscience

Medicine

Sponsored by CELL, Cosponsored by DAC‡

CEI

Committee on Environmental Improvement

C. Middlecamp, *Program Chair*

SUNDAY MORNING

Green Chemistry and the Environment

Sponsored by ENVR, Cosponsored by CEI, MPPG‡ and NUCL

Uranium in Seawater

The Chemistry

Sponsored by I&EC, Cosponsored by CEI and MPPG‡

Assessing Toxicity of Environmental Contaminants

Sponsored by ENVR, Cosponsored by AGRO, CEI and MPPG‡

SUNDAY AFTERNOON

Green Chemistry and the Environment

Sponsored by ENVR, Cosponsored by CEI and MPPG

Assessing Toxicity of Environmental Contaminants

Sponsored by ENVR, Cosponsored by AGRO, CEI and MPPG‡

Uranium in Seawater

The Sorbents

Sponsored by I&EC, Cosponsored by CEI, MPPG‡ and NUCL

MONDAY MORNING

Green Chemistry and the Environment

Sponsored by ENVR, Cosponsored by CEI

Uranium in Seawater

Sorbents and Analysis

Sponsored by I&EC, Cosponsored by CEI, MPPG‡ and NUCL

MONDAY AFTERNOON

Uranium in Seawater

Analysis and Toxicity/Cost

Sponsored by I&EC, Cosponsored by CEI, MPPG‡ and NUCL

TUESDAY MORNING

DOE Nanoscience Research Centers

National Resources for the Nanoscience Community

Sponsored by PRES, Cosponsored by ANYL, CCPA, CEI, ENFL and MPPG

ACS-CEI Award for Incorporating Sustainability into Chemistry Education

Sponsored by CHED, Cosponsored by CEI

Technical program information known at press time. The official technical program for the 249th ACS National Meeting is available at: www.acs.org/denver2015

‡ *Cooperative Cosponsorship*

Citizens First: Communicating Climate Science to the Public

Sponsored by CHED, Cosponsored by CEI‡

WEDNESDAY MORNING

Green Chemistry: Theory and Practice

Sponsored by CHED, Cosponsored by CEI‡

Water Sustainability in Oil and Gas Exploration: Treatment Issues

Sponsored by ENVR, Cosponsored by CEI and MPPG‡

WEDNESDAY AFTERNOON

Green Chemistry: Theory and Practice

Sponsored by CHED, Cosponsored by CEI‡

Water Sustainability in Oil and Gas Exploration: Treatment Issues

Sponsored by ENVR, Cosponsored by CEI and MPPG‡

WEDNESDAY EVENING

Water Sustainability in Oil and Gas Exploration: Treatment Issues

Sponsored by ENVR, Cosponsored by CEI and MPPG‡

CMA

Committee on Minority Affairs

J. Sarquis, *Program Chair*

OTHER SYMPOSIA OF INTEREST:

ACS Award for Encouraging Disadvantaged Students in Chemistry: Symposium in Honor of Catherine H. Middlecamp *(see CHED, Mon)*

SOCIAL EVENTS:

Diversity Reception, 5:00 pm: Sun

CMA Luncheon *(Tickets Required)***,** 11:30 AM: Mon

BUSINESS MEETINGS:

CMA Open Meeting, 12:00 PM: Sun

SUNDAY MORNING

Native American Women Chemists of Color

Sponsored by PROF, Cosponsored by CMA and WCC

MONDAY MORNING

Section A

Hyatt Regency Denver at Colorado Convention Center

Mineral Hall F

Diversifying STEM: Uniting through our Differences for a Brighter Scientific Future

Cosponsored by CHED and PROF

C. P. Frazier, S. A. Lopez, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 CMA **1.** Peer-led activities in STEM based on values affirmation. **L.M. Campos**

8:30 CMA **2.** Alliance for Diversity in Science and Engineering: A graduate-student centered approach to diversify STEM. **S.A. Lopez**

8:55 CMA **3.** NSF AGEP California Alliance: A community of practice to increase diversity in the physical sciences and engineering. **R.L. Garrell**

9:20 CMA **4.** Future faculty workshop. **T.M. Swager**

9:45 Intermission.

9:55 CMA **5.** Chancellor's Science Scholars program: Adapting the Meyerhoff model to UNC-Chapel Hill. **J.L. Templeton**, M. Peifer, A. Panter, W. Marzluff, M. Patil

10:20 CMA **6.** STEM Posse: Recruiting and retaining underrepresented students in the STEM disciplines. **I.R. Epstein**

10:45 CMA **7.** Building a STEM community for the next generation. **E. Patridge**

11:10 Panel Discussion.

11:40 Concluding Remarks.

MONDAY AFTERNOON

ACS Award for Encouraging Disadvantaged Students in Chemistry: Symposium in Honor of Catherine H. Middlecamp

Four-Part Harmony (or Disharmony)

Sponsored by CHED, Cosponsored by CMA and WCC

CPRC

Committee on Public Relations and Communications

D. Gottfried, *Program Chair*

TUESDAY MORNING

The Interface of Chemical and Biological Sciences International Disarmament Efforts

Sponsored by IAC, Cosponsored by ANYL, CHAL, CPRC and PRES

TUESDAY AFTERNOON

The Interface of Chemical and Biological Sciences International Disarmament Efforts

Sponsored by IAC, Cosponsored by ANYL, CHAL, CPRC and PRES

COMSCI

Committee on Science

D. Crans, *Program Chair*

SUNDAY MORNING

The Transnational Practice of Chemistry and Allied Sciences and Engineering: Study, Research and Careers without Borders

Sponsored by PRES, Cosponsored by BMGT, COMSCI, IAC and SOCED

SUNDAY AFTERNOON

Nanotechnology: Delivering on the Promise

Research & Development

Sponsored by PRES, Cosponsored by AGFD, AGRO, ANYL, CARB, CCPA, CCS, CHAS, COLL, COMSCI, CORP, ENFL, HIST, I&EC, IAC, MPPG, PMSE, POLY, SCHB and SOCED

MONDAY MORNING

Section A

Colorado Convention Center

Room 301

Transitioning between Academic Research into Practical Use: Solar-Energy and Advanced Materials

Cosponsored by MPPG‡ and PRES

D. C. Crans, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 COMSCI **1.** Will solar-driven water splitting devices see the light of day? **H.B. Gray**

9:05 Discussion.

9:15 COMSCI **2.** Solar water splitting and the hydrogen economy. **J. Turner**

9:45 Discussion.

9:55 COMSCI **3.** Revolutionizing CdTe photovoltaics through industrial research. **A. Duggal**

10:25 Discussion.

10:35 Intermission.

10:50 COMSCI **4.** If it works, will it matter? **C.A. Martin**

11:20 Discussion.

11:30 COMSCI **5.** Postdoc's perspective on use-inspired academic research. **J. McKone**

11:50 Discussion.

12:00 Panel Discussion.

Nanotechnology: Delivering on the Promise

Opportunities and Challenges for Health, Safety and the Environment

Sponsored by PRES, Cosponsored by AGFD, AGRO, ANYL, CARB, CCPA, CCS, CHAS, COLL, COMSCI, CORP, ENFL, HIST, I&EC, IAC, MPPG, PMSE, POLY, SCHB and SOCED

MONDAY AFTERNOON

Nanotechnology: Delivering on the Promise

Bridging the Gap to a Thriving US Marketplace

Sponsored by PRES, Cosponsored by AGFD, AGRO, ANYL, CARB, CCPA, CCS, CHAS, COLL, COMSCI, CORP, ENFL, HIST, I&EC, IAC, MPPG, PMSE, POLY, SCHB and SOCED

IAC

International Activities Committee

H.N. Cheng, *Program Chair*

SUNDAY MORNING

Section A

Hyatt Regency Denver at Colorado Convention Center

Mineral Hall D

Growing Opportunities for Research Abroad: An Undergraduate Perspective of International Research Experiences

Cosponsored by CHED, PROF and YCC

H. Cheng, *Organizer*

S. Hill, *Organizer, Presiding*

9:00 Introductory Remarks.

9:10 IAC **1.** Exploring electrochemistry in Düsseldorf, Germany. **B. Ferguson, J. Grote, K. Mayrhofer**

9:30 IAC **2.** Undergraduate research in Jülich, Germany: Fuel cell systems studies as a catalyst for personal growth and cultural exploration. **K. Fong, D. Krekel**

9:50 IAC **3.** A summer in Freiburg: Materials chemistry research in Germany. **G. Ruehl, M. Benkler**

10:10 IAC **4.** My ACS-IREU experience: Science and exploration in Europe. **J. Ford, M. Schwilk, H. Werner**

10:30 Intermission.

10:40 IAC **5.** Research along the Ruhr: A chemical and personal excursion in west Germany. **T.J. Myers, M. Ulbricht**

11:00 IAC **6.** Highlights of an international research experience in Berlin, Germany. **L. Hristov, A. Senf**

11:20 IAC **7.** Hybrid polymer studies in Germany: Synthesis, surface chemistry, and soccer. **D. Brauer**

11:40 IAC **8.** ACS international research experience for undergraduates: Kiel, Germany. **A. Kim**

The Transnational Practice of Chemistry and Allied Sciences and Engineering: Study, Research and Careers without Borders

Sponsored by PRES, Cosponsored by BMGT, COMSCI, IAC and SOCED

SUNDAY AFTERNOON

Section A

Hyatt Regency Denver at Colorado Convention Center

Mineral Hall D

Growing Opportunities for Research Abroad: An Undergraduate Perspective of International Research Experiences

Cosponsored by CHED, PROF and YCC

H. Cheng, *Organizer*

S. Hill, *Organizer, Presiding*

1:30 IAC **9.** Organic solar cell active layer synthesis and synopsis of time abroad. **T. Range, C. Ping Sen, S. Valiyaveettil**

1:50 IAC **10.** Electrochemistry in Singapore: Going into the sea lion's den and returning out a more well-versed chemist. **G. Panetti**

2:10 IAC **11.** Reflections on a summer research experience at the National University of Singapore. **S.J. Faucher**

2:30 Intermission.

2:40 IAC **12.** My inorganic materials chemistry IREU experience in Italy. **C.M. Gentle**

3:00 IAC **13.** Italian inquiry into alternative energy. **S. Barnett**

3:20 IAC **14.** Italian research experience: Development of a sustainable and efficient protocol for palladium-catalyzed Sonogashira cross-coupling reactions. **M.F. McLaughlin, L. Vaccaro**

3:40 Intermission.

3:50 IAC **15.** Summer research in the UK: Unique chemistry in a unique environment. **D.G. Mackanic, S. Mabbott, D. Graham**

4:10 IAC **16.** Investigations into the stability of photosynthetic proteins in Glasgow, Scotland. **E.K. Reagan, N. Javid, S.K. Nalluri, R. Ulijn**

4:30 IAC **17.** Solar power in Scotland: Examining new materials for organic photovoltaic devices. **L.R. Savagian**

TUESDAY MORNING

Section A

Hyatt Regency Denver at Colorado Convention Center

Mineral Hall D

The Interface of Chemical and Biological Sciences International Disarmament Efforts

Cosponsored by ANYL, CHAL, CPRC and PRES

L. Brown, *Organizer*

D. J. Phillips, *Presiding*

9:00 Introductory Remarks.

9:15 IAC **18.** Finding the needle in the haystack: The development of analytical capabilities at the OPCW and partner laboratories in support of verification of the Chemical Weapons Convention. **M. Blum**

9:45 IAC **19.** Chemical Issues in context: The role of intent in nonproliferation and disarmament policy. **K. Rodda**

10:15 IAC **20.** Chemistry, international disarmament and policy in a technologically evolving world. **J. Forman**

10:45 Intermission.

11:00 IAC **21.** Eradication techniques for chemical and biological weapons. **R. Holmes**

11:30 IAC **22.** Emerging technologies and diffusion of innovation: Security challenges for the 21st century. **M. Kosal**

12:00 IAC **23.** Finding better therapeutics for chemical poisonings: The NIH Countermeasures against Chemical Threats (CounterACT) program. **D. Jett**

TUESDAY AFTERNOON

Section A

Hyatt Regency Denver at Colorado Convention Center

Mineral Hall D

The Interface of Chemical and Biological Sciences International Disarmament Efforts

Cosponsored by ANYL, CHAL, CPRC and PRES

L. Brown, *Organizer*

D. J. Phillips, *Presiding*

2:00 IAC **24.** Education and outreach relevant to the Organisation for the Prohibition of Chemical Weapons Chemical Weapons Convention. **A. Suárez**

2:30 IAC **25.** Not in my backyard: Outreach efforts by the Program Executive Office, Assembled Weapons Alternatives (PEO-ACWA) on chemical weapons destruction. **G.B. Mohrman**

3:00 IAC **26.** U.S. Department of State's Chemical Security Program: Challenges, successes, and expanding international disarmament/nonproliferation efforts. **D. Verdugo**

3:30 Intermission.

3:45 Panel Discussion.

4:30 Concluding Remarks.

SCC

Senior Chemists Committee

G. Heinze, *Program Chair*

MONDAY EVENING

STRETCH Your Students' Polymer Knowledge by Putting Some BOUNCE into Your Curriculum

Polymer Science Education and the NGSS

Sponsored by CHED, Cosponsored by PMSE, POLY, RUBB and SCC‡

SOCED

Society Committee on Education

D. Swartling, *Program Chair*

SOCIAL EVENTS:

Networking Social with Graduate School and Research Opportunity Representatives, 1:00 PM: Sun

ACS Student Chapter Awards Ceremony, 7:00 PM: Sun

Undergraduate Social, 8:30 PM: Sun

Undergraduate Speed Networking with Chemistry Professionals, 3:45 PM: Mon

Chemistry and the Environment Film Series, 12:00 PM: Tue

SUNDAY MORNING

The Transnational Practice of Chemistry and Allied Sciences and Engineering: Study, Research and Careers without Borders

Sponsored by PRES, Cosponsored by BMGT, COMSCI, IAC and SOCED

High School Program

Sponsored by CHED, Cosponsored by SOCED

Undergraduate Research Papers

Organic Chemistry

Sponsored by CHED, Cosponsored by SOCED

SUNDAY AFTERNOON

Nanotechnology: Delivering on the Promise

Research & Development

Sponsored by PRES, Cosponsored by AGFD, AGRO, ANYL, CARB, CCPA, CCS, CHAS, COLL, COMSCI, CORP, ENFL, HIST, I&EC, IAC, MPPG, PMSE, POLY, SCHB and SOCED

High School Program

Sponsored by CHED, Cosponsored by SOCED

Undergraduate Research Papers

Analytical and Environmental Chemistry

Sponsored by CHED, Cosponsored by SOCED

MONDAY MORNING

Section A

Sheraton Denver Downtown Hotel

Grand Ballroom 1

Biomass to Fuel and Products

Cosponsored by CELL, ENFL and MPPG

D. J. Swartling, *Organizer, Presiding*

9:00 SOCED **1.** Current state of biofuels in the USA and world. **T. Foust**

Section A

Sheraton Denver Downtown Hotel

Grand Ballroom 1

Forensic Toxicology of Marijuana

Cosponsored by BMGT and TOXI

D. J. Swartling, *Organizer, Presiding*

10:45 SOCED **2.** Forensic toxicology of marijuana. **K.M. Allen, D. Wallace Duckworth**

Nanotechnology: Delivering on the Promise

Opportunities and Challenges for Health, Safety and the Environment

Sponsored by PRES, Cosponsored by AGFD, AGRO, ANYL, CARB, CCPA, CCS, CHAS, COLL, COMSCI, CORP, ENFL, HIST, I&EC, IAC, MPPG, PMSE, POLY, SCHB and SOCED

Excellence in Graduate Polymer Research

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

Undergraduate Research Papers

Computational, Physical and Inorganic Chemistry

Sponsored by CHED, Cosponsored by SOCED

MONDAY AFTERNOON

Section A

Sheraton Denver Downtown Hotel

Grand Ballroom 1

Sustainability in the 21st Century: Optimizing Complex Interdependent Systems

Cosponsored by CELL and ENFL

D. J. Swartling, *Organizer, Presiding*

2:30 SOCED **3.** Eminent Scientist Lecture: Sustainability in the 21st century: Optimizing complex interdependent systems. **H.T. Kohlbrand**

Nanotechnology: Delivering on the Promise

Bridging the Gap to a Thriving US Marketplace

Sponsored by PRES, Cosponsored by AGFD, AGRO, ANYL, CARB, CCPA, CCS, CHAS, COLL, COMSCI, CORP, ENFL, HIST, I&EC, IAC, MPPG, PMSE, POLY, SCHB and SOCED

Undergraduate Research Posters

Agricultural and Food Chemistry

Sponsored by CHED, Cosponsored by AGFD, ANYL, BIOL, BIOT, COMP, ENVR, GEOC, INOR, MEDI, PMSE, POLY and SOCED

Excellence in Graduate Polymer Research

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

Undergraduate Research Papers

Biochemistry and Chemical Education

Sponsored by CHED, Cosponsored by SOCED

TUESDAY EVENING

Excellence in Graduate Polymer Research

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

WCC

Women Chemists Committee

K. Woznack and A. Debaillie, *Program Chairs*

SOCIAL EVENTS:

WCC Breakfast, 7:30 AM: Mon

WCC Just Cocktails, 3:30 PM: Mon

WCC/Eli Lilly Travel Award Poster Session, 11:00 AM: Tue

WCC Luncheon, 12:00 PM: Tue

BUSINESS MEETINGS:

WCC Division Business Meeting, 5:30 PM: Fri

WCC Division Business Meeting, 7:30 AM: Sat

SUNDAY MORNING

ACS Award for Creative Work in Fluorine Chemistry: Symposium in Honor of Véronique Gouverneur

Sponsored by FLUO, Cosponsored by WCC

Native American Women Chemists of Color

Sponsored by PROF, Cosponsored by CMA and WCC

Harry Gray Award for Creative Work in Inorganic Chemistry by a Young Investigator: Symposium in Honor of Emily A. Weiss

Sponsored by INOR, Cosponsored by WCC

SUNDAY AFTERNOON

ACS Award for Creative Work in Fluorine Chemistry: Symposium in Honor of Véronique Gouverneur

Sponsored by FLUO, Cosponsored by WCC

Earning ACS Awards: An Interactive Symposium on Constructing Successful Award Nominations

Sponsored by PROF, Cosponsored by BMGT, SCHB and WCC

Harry Gray Award for Creative Work in Inorganic Chemistry by a Young Investigator: Symposium in Honor of Emily A. Weiss

Sponsored by INOR, Cosponsored by WCC

SUNDAY EVENING

ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry: Symposium in Honor of Kim R. Dunbar

Sponsored by INOR, Cosponsored by WCC

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TECHNICAL PROGRAM

MONDAY MORNING

Section A

Colorado Convention Center
Room 105

WCC Rising Stars Awards Symposium
Cosponsored by BIOT, COLL, GEOC, INOR, ORGN, PHYS, PMSE and PROF

S. Azad, M. A. Kane, *Organizers, Presiding*

9:20 Introductory Remarks.

9:30 WCC **1.** Making science and education gel: Building a career in technical research and pursuing a passion for STEM education outreach. **J.L. Curtis-Fisk**

9:50 WCC **2.** Redox-active ligands for the f-block: Promoting multi-electron chemistry at low-valent uranium centers. **S.C. Bart**

10:10 Intermission.

10:25 WCC **3.** Tale of two journeys: Protein misfolding in light chain amyloidosis and the career path of a protein biochemist. **M. Ramirez Alvarado**

10:45 WCC **4.** Chemical research with fun in new materials design and application. **C. Liu**

11:05 WCC **5.** Engineering next-generation porous materials for energy and environmental applications. **K.S. Walton**

ACS Award for Achievement in Research for the Teaching and Learning of Chemistry: Symposium in Honor of Vickie M. Williamson
Sponsored by CHED, Cosponsored by WCC

ACS Award for Encouraging Women into Careers in the Chemical Sciences: Symposium in Honor of E. Ann Nalley

Championing the Empowerment of Women in Chemistry
Sponsored by PROF, Cosponsored by WCC

MONDAY AFTERNOON

Section A

Colorado Convention Center
Room 710

WCC Rising Stars Awards Symposium
Cosponsored by BIOT, COLL, GEOC, INOR, ORGN, PHYS, PMSE and PROF

S. Azad, M. A. Kane, *Organizers, Presiding*

1:20 WCC **6.** Art and Industry: Science takes an artsy turn. **M.H. Keefe**

1:40 WCC **7.** Phase-selective synthesis and surface passivation of binary and ternary copper sulfide nanoparticles. **K. Plass**, N. Freymeyer, C. Kim, Z. Georgieva

2:00 WCC **8.** Nuclear waste management: Where geology meets nuclear science. **F.N. Smith**

2:20 Intermission.

2:35 WCC **9.** Magnetic quantum dots for biomedical applications. **J.O. Winter**

2:55 WCC **10.** Overview of the discovery of a potent *Septoria tritici* fungicide. **B.A. Lorsbach**

3:15 Concluding Remarks.

ACS Award for Achievement in Research for the Teaching and Learning of Chemistry: Symposium in Honor of Vickie M. Williamson
Sponsored by CHED, Cosponsored by WCC

ACS Award for Encouraging Disadvantaged Students in Chemistry: Symposium in Honor of Catherine H. Middlecamp

Four-Part Harmony (or Disharmony)
Sponsored by CHED, Cosponsored by CMA and WCC

ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry: Symposium in Honor of Kim R. Dunbar
Sponsored by INOR, Cosponsored by WCC

F. Albert Cotton Award in Synthetic Inorganic Chemistry: Symposium in Honor of Jaqueline L. Kiplinger
Sponsored by INOR, Cosponsored by WCC

TUESDAY MORNING

ACS Award for Encouraging Women into Careers in the Chemical Sciences: Symposium in Honor of E. Ann Nalley

Championing the Empowerment of Women in Chemistry
Sponsored by PROF, Cosponsored by WCC

E. B. Hershberg Award for Important Discoveries in Medicinally Active Substances: Symposium in Honor of Ruth R. Wexler
Sponsored by MEDI, Cosponsored by WCC

ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry: Symposium in Honor of Kim R. Dunbar
Sponsored by INOR, Cosponsored by WCC

F. Albert Cotton Award in Synthetic Inorganic Chemistry: Symposium in Honor of Jaqueline L. Kiplinger
Sponsored by INOR, Cosponsored by WCC

TUESDAY AFTERNOON

ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry: Symposium in Honor of Kim R. Dunbar
Sponsored by INOR, Cosponsored by WCC

F. Albert Cotton Award in Synthetic Inorganic Chemistry: Symposium in Honor of Jaqueline L. Kiplinger
Sponsored by INOR, Cosponsored by WCC

WEDNESDAY MORNING

National Fresenius Award: Symposium in Honor of Abigail G. Doyle
Sponsored by ORGN, Cosponsored by WCC

ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry: Symposium in Honor of Kim R. Dunbar
Sponsored by INOR, Cosponsored by WCC

WEDNESDAY AFTERNOON

Frank H. Field and Joe L. Franklin Award for Outstanding Achievement in Mass Spectrometry: Symposium in Honor of Hilkka I. Kenttämaa
Sponsored by ANYL, Cosponsored by WCC

YCC

Younger Chemists Committee

T. Matos and A. Gavrilenko, *Program Chairs*

SUNDAY MORNING

Growing Opportunities for Research Abroad: An Undergraduate Perspective of International Research Experiences
Sponsored by IAC, Cosponsored by CHED, PROF and YCC

SUNDAY AFTERNOON

Section A

Hyatt Regency Denver at Colorado Convention Center
Agate B/C

Starting a Successful Research Program at a Predominantly Undergraduate Institution
Cosponsored by PROF

A. V. Gavrilenko, T. D. Matos, *Organizers*
M. Druelinger, *Organizer, Presiding*

1:00 Introductory Remarks.

1:15 YCC **1.** What is undergraduate research and why do research at a predominantly undergraduate institution? **T.J. Wenzel**

1:25 YCC **2.** Collaborative research with undergraduates: research project and research group design. **G. Van Hecke**

1:45 YCC **3.** Balancing teaching, research, service, and life in the context of primarily undergraduate institutions (PUIs). **B.L. Gourley**

2:05 YCC **4.** Art and necessity of gaining internal support from institutional administrators. **M. Druelinger**

2:25 Intermission.

2:35 YCC **5.** Undergraduate new investigator grants at the ACS Petroleum Research Fund. **B. Lee**

3:00 YCC **6.** Funding opportunities at the National Science Foundation of particular interest to faculty at primarily undergraduate institutions (PUIs). **M. Bushey**

3:30 YCC **7.** Writing more competitive grant proposals. **T.J. Wenzel**

3:50 Panel Discussion.

SCHB Entrepreneurs' Poster Session
Sponsored by SCHB, Cosponsored by YCC

Growing Opportunities for Research Abroad: An Undergraduate Perspective of International Research Experiences
Sponsored by IAC, Cosponsored by CHED, PROF and YCC

Best Practices for Success with SBIR & STTR Grants
Sponsored by SCHB, Cosponsored by PROF and YCC

Young Investigator in Medicinal Chemistry
Sponsored by MEDI, Cosponsored by YCC

MONDAY MORNING

Kathryn C. Hach Award for Entrepreneurial Success: Symposium in Honor of Terry L. Brewer
Sponsored by SCHB, Cosponsored by PROF and YCC

Excellence in Graduate Polymer Research
Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

MONDAY AFTERNOON

Water is the Next Oil: Small Businesses Percolating to the Top
Sponsored by SCHB, Cosponsored by YCC

Excellence in Graduate Polymer Research
Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

TUESDAY MORNING

Section A

Hyatt Regency Denver at Colorado Convention Center
Centennial H

Chemical Tales of Success: Helpful Tips for Younger Chemists
Cosponsored by NUCL and SCHB

J. C. Braley, *Organizer, Presiding*

8:30 YCC **8.** What I wish I had known: You can learn from my mistakes. **L.M. Balbes**

9:00 YCC **9.** Professional skills for chemists. **R.M. Richards**

9:40 YCC **10.** Balancing entrepreneurship with academic life. **A.L. Prieto**

10:10 Intermission.

10:30 YCC **11.** Tales from the home stretch. **K.M. Schulz**

11:00 YCC **12.** Tales from the dark side: Alternative careers in administration. **P.K. Dorhout**

TUESDAY EVENING

Excellence in Graduate Polymer Research
Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

WEDNESDAY EVENING

Environmental Chemistry: Pedagogical Models and Practices
Sponsored by ENVR, Cosponsored by CHED, MPPG‡ and YCC

THURSDAY MORNING

Environmental Chemistry: Pedagogical Models and Practices
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UNDERGRADUATE PROGRAM

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SUNDAY, MARCH 22

Undergraduate Hospitality Center
Sheraton Denver Downtown, Majestic Ballroom
8:00 AM–5:00 PM

Undergraduate Research Oral Session
Sheraton Denver Downtown, Denver Room
8:30 AM–5:00 PM

Making the Most of Your First National Meeting
Sheraton Denver Downtown, Majestic Ballroom
9:00–9:45 AM

Graduate School Reality Check: Getting In
Sheraton Denver Downtown, Plaza Ballrooms A&B
10:00–11:15 AM
Cosponsored by the ACS Younger Chemists Committee

Chem Demo Exchange
Colorado Convention Center, Hall B2
11:00 AM–12:30 PM

Graduate School Reality Check: You're In – Now What?
Sheraton Denver Downtown, Plaza Ballrooms A&B
11:15 AM–12:30 PM
Cosponsored by the ACS Younger Chemists Committee

How to Be a Successful ACS Student Chapter
Sheraton Denver Downtown, Plaza Ballrooms D&E
1:00–2:30 PM

Networking Social with Graduate School and Research Opportunity Representatives
Sheraton Denver Downtown, Grand Ballroom
1:00–5:00 PM

Symposium: Can You Have a Life and Career?
Sheraton Denver Downtown, Plaza Ballrooms D&E
2:45–4:00 PM
Cosponsored by the ACS Women Chemists Committee

Workshop: Improving Scientific Communication Skills
Sheraton Denver Downtown, Plaza Ballroms A&B
4:00–5:30 PM

Workshop: Careers in Teaching Chemistry
Sheraton Denver Downtown, Plaza Ballrooms D&E
4:00–5:30 PM

Student Chapter Awards Ceremony
Colorado Convention Center, Bellco Theatre
7:00–8:30 PM

Undergraduate Social
Colorado Convention Center, Four Seasons Ballroom
8:30–11:00 PM
Hosted by the Colorado School of Mines and the University of Colorado at Boulder

MONDAY, MARCH 23

Undergraduate Hospitality Center
Sheraton Denver Downtown, Majestic Ballroom
8:00 AM–5:00 PM

Undergraduate Research Oral Session
Sheraton Denver Downtown, Denver Room
8:30 AM–5:00 PM

Symposium: Biomass to Fuel & Products
Sheraton Denver Downtown, Grand Ballroom I
9:00–10:30 AM
Cosponsored by the ACS Cellulose and Renewable Materials Division and the ACS Division of Energy & Fuels

Workshop: Networking 101
Colorado Convention Center, Rooms 601/603
9:45–11:00 AM

Workshop: Chemists Celebrate Earth Day
Sheraton Denver Downtown, Grand Ballroom II
9:45–11:45 AM
Cosponsored by the ACS Committee on Community Activities

Symposium: Forensic Toxicology of Marijuana
Sheraton Denver Downtown, Grand Ballroom I
10:45–11:45 AM
Cosponsored by the ACS Divisions of Chemical Toxicology and Business Development & Management

Undergraduate Research Poster Session
Colorado Convention Center, Hall C
12:00 NOON–2:00 PM
Cosponsored by the ACS Divisions of Agricultural and Food Chemistry, Analytical, Environmental, Inorganic, Medicinal, Physical, and Polymer Chemistry, Biological Chemistry, and Geochemistry

Eminent Scientist Lecture
"Sustainability in the 21st Century: Optimizing Complex Interdependent Systems", with Henry Kohlbrand, Dow Chemical Company
Sheraton Denver Downtown, Grand Ballroom I
2:30–3:30 PM
Cosponsored by the ACS Cellulose and Renewable Materials Division and the ACS Division of Energy & Fuels

Speed Networking with Chemistry Professionals
Hyatt Regency Denver at Colorado Convention Center, Centennial D
3:45–5:15 PM
Cosponsored by ACS Corporation Associates and the ACS Senior Chemists Committee

Kavli Lectures
Colorado Convention Center, Bellco Theatre
4:00–6:30 PM

Sci-Mix/Successful Student Chapter Posters
Colorado Convention Center, Hall C
8:00–10:00 PM

TUESDAY, MARCH 24

Chemistry and the Environment Film Series
Sheraton Denver Downtown, Grand Ballroom I
12:00 NOON–2:00 PM
Cosponsored by the ACS Committee on Environmental Improvement

Program format and times are subject to change. Please consult the final program.

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EXPOSITION HIGHLIGHTS

SEE WHAT'S NEW INSIDE THE EXPOSITION. Visit the ACS National Exposition at the Colorado Convention Center, Halls A/F, from Sunday, March 22, through Tuesday, March 24. The show hours will be Sunday, 6:00 to 8:30 PM, and Monday and Tuesday, 9:00 AM to 5:00 PM.

Companies will showcase services, instruments, books, computer hardware, scientific software, and an array of chromatographic, lab, and safety equipment. Technical personnel will give demonstrations, answer questions, and discuss your needs and interests. You can also visit the ACS Career Fair Recruiters Row inside the exposition, where employers will showcase their products and services. Also, join us at the ACS Booth in the middle of the exposition floor, where ACS staff members will present the many benefits, services, products, and merchandise offered by ACS.

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Free Exhibitor Workshops. Free workshops will be hosted by exhibitors on the exposition floor and in private rooms inside the Moscone Center. These workshops will introduce new products and services, build skills with specific tools and techniques, and highlight innovative applications that may improve your productivity. Preregister at www.acs.org/denver2015 to reserve your seat.

Presentations, Prizes & Special Events. Visit the Daily Prize Raffle area (#339) from Sunday through Tuesday for a chance to win a prize. Also, don't forget to join us on Sunday from 6:00 to 8:30 PM for the Attendee Welcome Reception. Take a break, and visit the exposition on Monday and Tuesday from 1:00 to 3:00 PM for treats in the Town Center. Stop by the Town Center on Tuesday, from 2:00 to 4:00 PM to view the Division of Energy and Fuels poster session.

Internet & Technology. Use free Internet access, and leave messages for one another at the Meeting Mail terminals located throughout the exposition and Moscone Center. Also, enjoy free Wi-Fi service at designated areas in the Moscone Center.

Admission Requirements & Expo-Only Registration. Exposition admission is complimentary for all national meeting registrants; however, you are required to wear your badge. Individuals who want to visit the exhibits without registering for the technical component of the national meeting can obtain an expo-only badge for $50. Students with school identification can obtain an expo-only badge for $25. Registration can be handled online or in person at ACS Attendee Registration in the Moscone Center, North Lobby.

ACS Exposition

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Scios/Teneo

Formulaction USA
Booth # 532
Micro Rheology Instrument
Film Formation Analyzer

FRITSCH Milling and Sizing
Booth # 1217
Pulverisette 7 premium line Planetary Ball Mill
Analysette 28 Image Analyzer
Pulverisette 1 premium line Jaw Crusher
Pulverisette 14 premium line Rotor Speed Mill

Gamry Instruments
Booth # 1009
Interface 5000 Potentiostat

Gaussian
Booth # 400
Gaussian
GaussView

Hands-On Learning
Booth # 304
LabBridge
Labpaq
STEMpaq

HE Chemical
Booth # 1206
6-Amino-2-fluoronicotinic acid
3-Fluoro-4-(trifluoromethyl)picolinic acid
6-Bromo-2-fluoronicotinic acid
6-Chloro-2-fluoronicotinic acid
3-Bromo-2-mercapto-4-(trifluoromethyl)pyridine

Hiden Analytical Inc.
Booth # 511
Compact SIMS
QGA
Catlab
HPR-20

Indofine Chemical Co.
Booth # 1318
Gossypin
Piperlongumine
Ferulic acid
Acetosyringone
Vanillic acid

InfoChem GmbH
Booth # 809
ICsynth
SPRESImobile
Chemisches Zentralblatt
Patent Database
ICcartridge

Instec, Inc.
Booth 326
Automatic Liquid Crystal Physical Properties Teste
HCS402 Hot & Cold Microscope Stage

ISS Incorporated
Booth # 1406
Tempo

Japan Analytical Industry Co. Ltd.
Booth # 241
Recycling Preparative HPLC
Portable Curie Point Pyrolyzer
Outgas Collector

J-KEM Scientific
Booth # 424
Automated Reaction Controller and Logger
Precision Vacuum Controller
Precision Temperature Controller
Custom Robotic Systems
Precision Syringe Pumps

JEOL USA, Inc.
Booth # 1101
EDXRF System

Keysight Technologies (formerly Agilent LSCA)
Booth # 503
7500 Atomic Force Microscope
8500B FE-SEM with EDS

Kimble Chase LLC
Booth # 1215
Hydrometer
Raysorb NMR
GL45 Flask

Knauer
Booth # 1110
AZURA Educational System
AZURA Bio LC
AZURA Analytical
Contichrom
Columns

KNF Neuberger
Booth # 225
RC 900 Rotary Evaporator
SIMDOS 10 RC Plus Liquid Dosing Pumps
12V Field Filtration Pump

Nat'l Res. Council/ Nat'l Academies
Booth # 504
Fellowships
Graduate Research
Postdoctoral Research
Senior Research

Neaspec GmbH
Booth # 927
NeaSNOM
nano-FTIR

NT-MDT Co.
Booth # 1000
NTEGRA Spectra
Spectrum
Titianium
Next

Oakwood Products Inc.
Booth # 600
(R)-BCNG (1639014-43-9
(S)-BCNG (1639014-40-6
N-Nitrosomethylurea
Phosphorous (V) oxybromide solution in Xylene
Tin (IV) Chloride

Parr Instrument Co.
Booth # 1001
6050 Compensated Calorimeter

PASCO scientific
Booth # 219
Spectrometer

PharmAgra Labs, Inc.
Booth # 509
FIGLU

PIKE Technologies
Booth # 415
UV/VIS Peltier Cuvette Accessories
Temperature Controlled Microscope Statge
IR Short Path Gas Cells

PSS USA, Inc.
Booth # 235
Pullulan ReadyCal Kit
HT GPC ReadyCal Kit
Micro-RI detector
Micro-Viscometer
WinGPC 8.2

Pure Chemistry Scientific Inc.
Booth # 306
Stannanes
Vitamin D
Boronic Acids/Esters
PEG items
Intermidiate

Quantachrome Corp.
Booth # 430
Autosorb iQ Series
New Nova Touch Series
Porometer 3G Series
Quadrasord
Pycnometers

Restek Corp.
Booth # 506
ARC-18
RXI
SKY Liners
Raptor
QuEChERS

Richman Chemical Inc.
Booth # 405
Trimethylene Carbonate

Rieke Metals, LLC
Booth # 336
2-Propylzinc bromide
Cyclobutylzinc bromide
2-Pyridylmagnesium bromide
4-Bromobenzylmagnesium bromide
Poly(3-hexylthiophene-2,5-diyl), regioregular

Schrödinger, Inc.
Booth # 608
Materials Science Suite

SCIENCE/AAAS
Booth # 829
Science
Science Signaling
Science Translational Medicine

Semichem
Booth # 404
Semichem
AMPAC
Codessa

Sigma-Aldrich
Booth # 1216
Phenofluor
TFCS-Na
ESF
COGenerator
Stahl Aerobic Oxidation Kit

SofTA Corporation
Booth # 1404
ELSD Model 2300
ELSD Model 1300
ELSD Model 300S
Evaporative Light Scattering Detector

Sorbent Technologies
Booth # 914
SorbaDex
SorbaRes

StellarNet Inc.
Booth # 1125
Portable and Laboratory Raman Systems
Teaching Lab UV-VIS Specials
NIR Chemical Analyzers

Strem Chemicals
Booth # 813
Buchwald Precatalysts and Ligands
CVD and ALD Precursors
Electropolished Stainless steel CVD bubblers and A
Metal Nanoparticles
Phosphine Ligands and Metathesis Catalysts

Struchem Co., LTD
Booth # 931
D-Bicuculline
methyl 4-amino-3-methoxy-5-nitrobenzoate
4-AMINO-2-HYDROXYBENZENESULFO NAMIDE
2-PROPYL-5-THIAZOLECARBOXYLIC ACID
1-(4-(trifluoromethyl)phenyl)propan-2-one

Symphotic Tii
Booth # 1408
CMS 8400

Synquest Laboratories, Inc.
Booth # 513
Triflic acid
Triflic anhydride
Difluoroacetaldehyde ethyl hemiacetal
Hexafluoroisopropanol
1H,1H,5H-Octafluoropentyl methacrylate

Thermo Scientific
Booth # 1014,1015
Vanquish

Tosoh Bioscience LLC
Booth # 501
CaPure-HA(TM) hydroxyapatite resin

University of Illinois - Nano Plasmonics
Booth # 239
Computational Plasmonics
Arbitrary Geometry
Large Scale Computing
Online Simulation
University of Illinois Funded by NSF

University Science Books
Booth # 605
X-Ray Crystallography
Physical Chemistry for the Chemical Sciences
Principles of NMR

Vacuum Technology Inc.
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ViridisChem, Inc.
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Green Pocketbook
Green Analyzer
GreenSynth
Integrated Planner
ChiroSolve

Wavefunction, Inc.
Booth # 508
Spartan'14 Parallel Suite
Spartan'14
Spartan Student Version 6
Odyssey Version 5
iSpartan

Weihai CY Dendrimer Technology Co.,Ltd.
Booth # 243,1319
Denditic polymers
PAMAM
Dendrimer
CYD-150A
CYD-160A

Wyatt Technology Corp.
Booth # 1010
DynaPro Plate Reader
DAWN
Mobius
Eclipse
NanoStar

Xenocs
Booth # 941
Xeuss 2.0
Nano-inXider

Yamazen Science, Inc.
Booth # 1304
ELSD
WPrep Dual Channel MPLC
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TLC Reader
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249th American Chemical Society National Exposition

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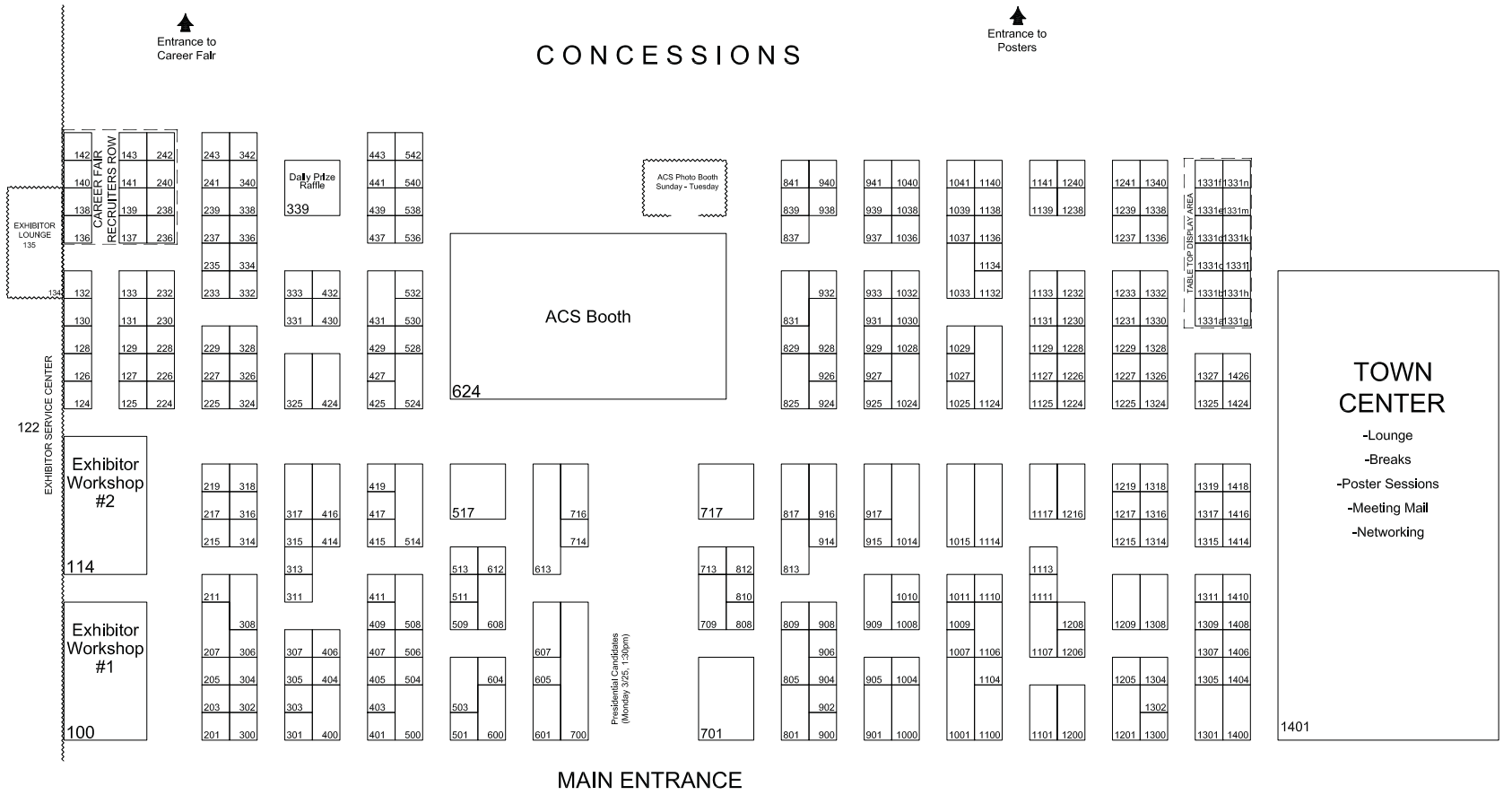
March 22-24, 2015

Colorado Convention Center - Exhibit Halls A&F
Denver, CO



ACS Members are ROCKSTARS of CHEMISTRY

ACS members who joined in the last 12 months are invited to attend our ROCKSTARS RECEPTION.

ACS looks forward to welcoming you to this very special event, Monday, March 23, from 3:00 p.m. to 4:00 p.m. in the Colorado Convention Center Room 601. New members will network with other Rockstars of Chemistry, such as award winners, published authors, and notable scientists. Light refreshments will be served. Guests will receive reserved seating for the Kavli Lecture Series.

Not a member yet?
Join today for your ticket to the Rockstars Reception. Go to **www.acs.org/ROCKSTAR**

Been a member for years?
Stop by the ACS Booth and take a commemorative ACS Rockstars photo at the open air photo booth!

Learn about your benefits at the *Membership Rocks* presentation in the ACS Theater on Monday at 10:30 a.m. and 11 a.m. or Tuesday at 11 a.m. and 11:30 a.m.

American Chemical Society

PRESIDENTIAL SYMPOSIA AND EVENTS

Sponsored and Recommended by the ACS President

Photo: Peter Cutts Photography

Diane Grob Schmidt, Ph.D.
ACS President

Saturday, March 21, 2015
10:00 AM-2:00 PM
Presidential Outreach Event: Exploring Our World Through Chemistry
(Cosponsored by CCA)
Denver Zoo, 2300 Steele Street

Sunday, March 22, 2015
8:00 AM-12:00 PM
Chemistry Without Borders: The Transnational Practice of Chemistry and Allied Sciences and Engineering
(Cosponsored by IAC, COMSCI, BMGT & SOCED)
Colorado Convention Center, Mile High Ballroom 3A (Lower Level)

Sunday, March 22, 2015
1:30-5:30 PM

Monday, March 23, 2015
8:30 AM-4:45 PM
Nanotechnology: Delivering on the Promise
(Cosponsored by the following ACS Divisions and Committees and other scientific societies AGFD, AGRO, ANYL, CARB, CHAS, COLL, ENFL, HIST, I&EC, PMSE, POLY, SCHB, MPPG, CA, CCS, CCPA, COMSCI, DAC, IAC, SOCED; American Institute of Chemical Engineers, Gordon Research Conferences, Materials Research Society & National Academy of Engineering)
Colorado Convention Center, Mile High Ballroom 3A (Lower Level)

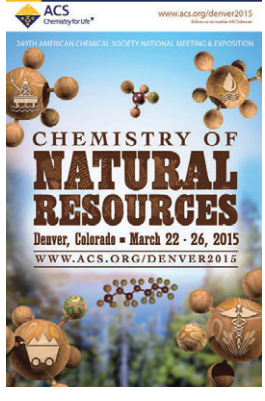
Tuesday, March 24, 2015
8:30-11:30 AM
DOE Nanoscience Research Centers: National Resources for the Nanoscience Community
(Cosponsored ANYL, ENFL, CCPA, CEI & MPPG)
Colorado Convention Center, Rooms 506-507 (Street Level)

OTHER SYMPOSIA RECOMMENDED BY THE PRESIDENT

Excellence in Graduate Polymer Research
(Sponsored by POLY and cosponsored by PRES)
Sheraton Denver Downtown Hotel

GSSPC: Designed by Nature, Developed by Science: Interdisciplinary Perspectives on Biocatalysis
(Sponsored by CHED and cosponsored by PRES, ANYL, BIOL, CATL, ENVR, I&EC, MEDI, & ORGN)
Sheraton Denver Downtown Hotel

Department, University and National Models for Faculty Development to Support Adoption of Evidence-Based Teaching
(Sponsored by CHED and cosponsored by PRES, INOR & ORGN)
Sheraton Denver Downtown Hotel



The Interface of Chemical and Biological Sciences International Disarmament Efforts
(Sponsored by IAC and cosponsored by PRES, ANYL, CHAL & CPRC)
Hyatt Regency Denver at Colorado Convention Center

Transitioning between Academic Research into Practical Use: Solar-Energy and Advanced Materials?
(Sponsored by COMSCI and cosponsored by PRES & MPPG)
Colorado Convention Center

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- Come to the Membership Benefits kiosk to receive a gift in thanks for your ACS membership
- Enter contests and receive giveaways, including tablets, gift cards, photos and more!

Whether looking for educational resources, powerful research tools, ACS Member Insurance, C&EN, future meeting dates and locations, mole dolls or other ACS merchandise, WE HAVE IT ALL FOR YOU. There is something for every member of the chemistry community at the ACS booth.

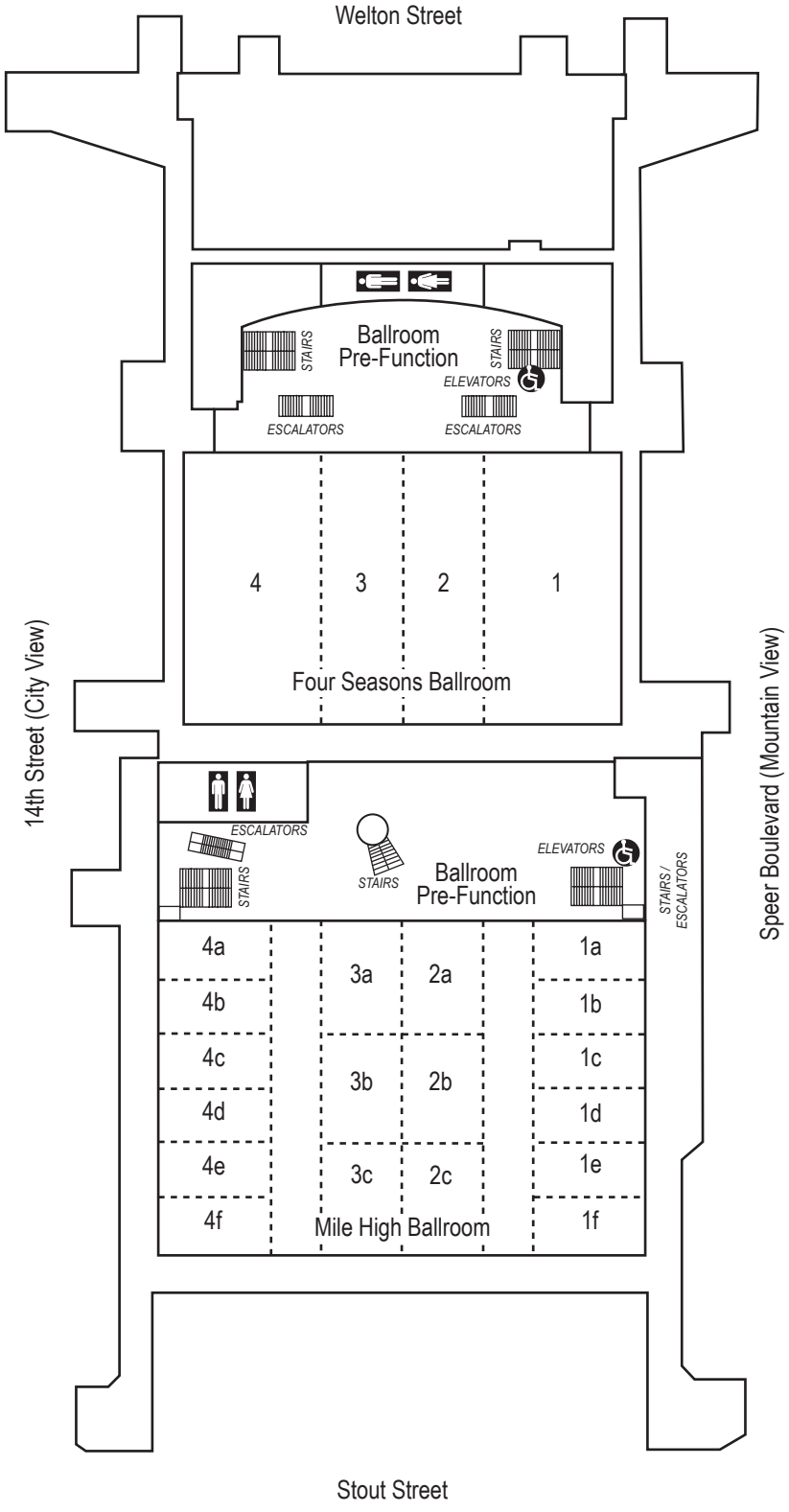
Exhibit Hours:

Sunday, March 22	Monday, March 23	Tuesday, March 24
6:00pm -8:30pm	9:00am – 5:00 pm	9:00am – 5:00pm

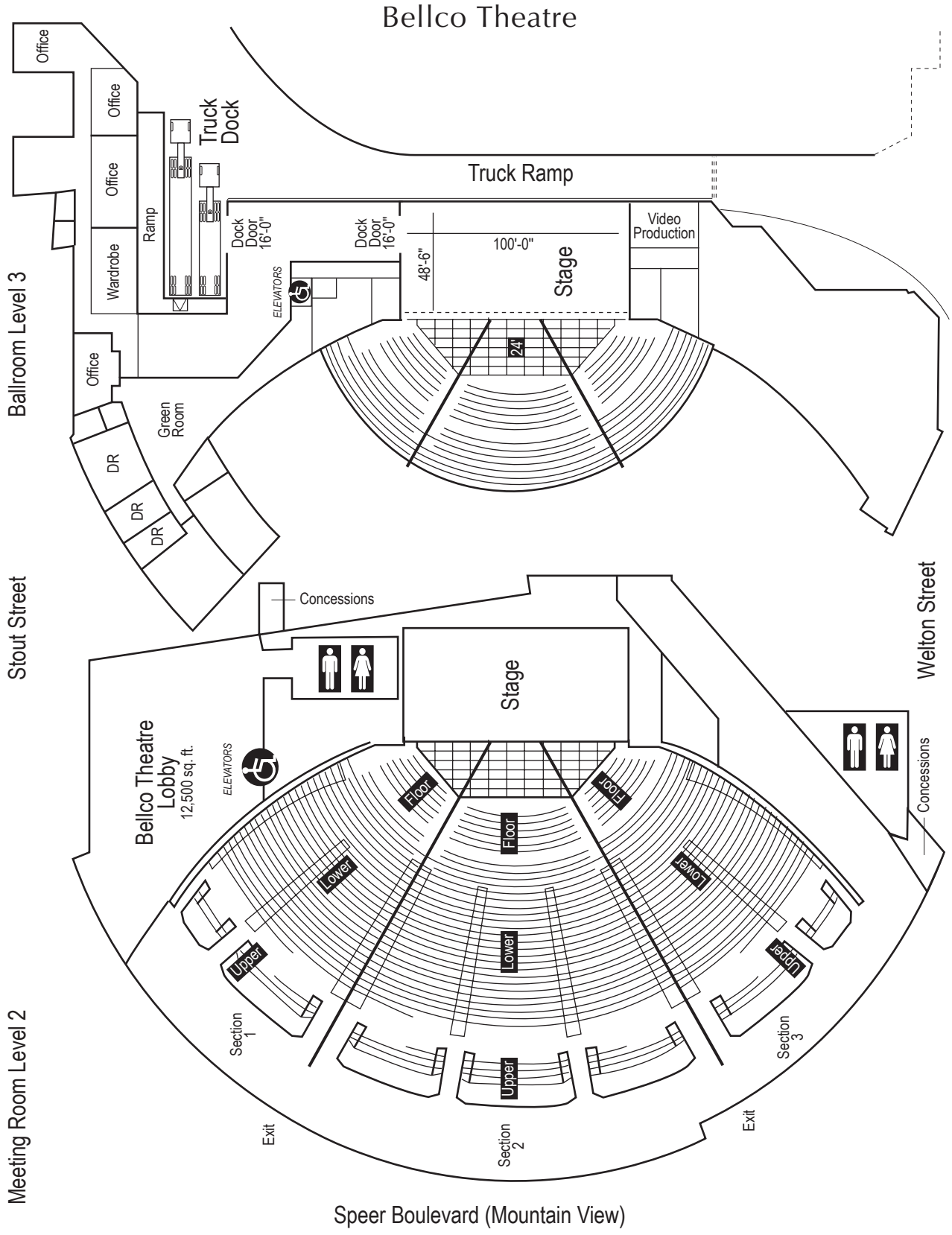
American Chemical Society

COLORADO CONVENTION CENTER

Ballroom Level

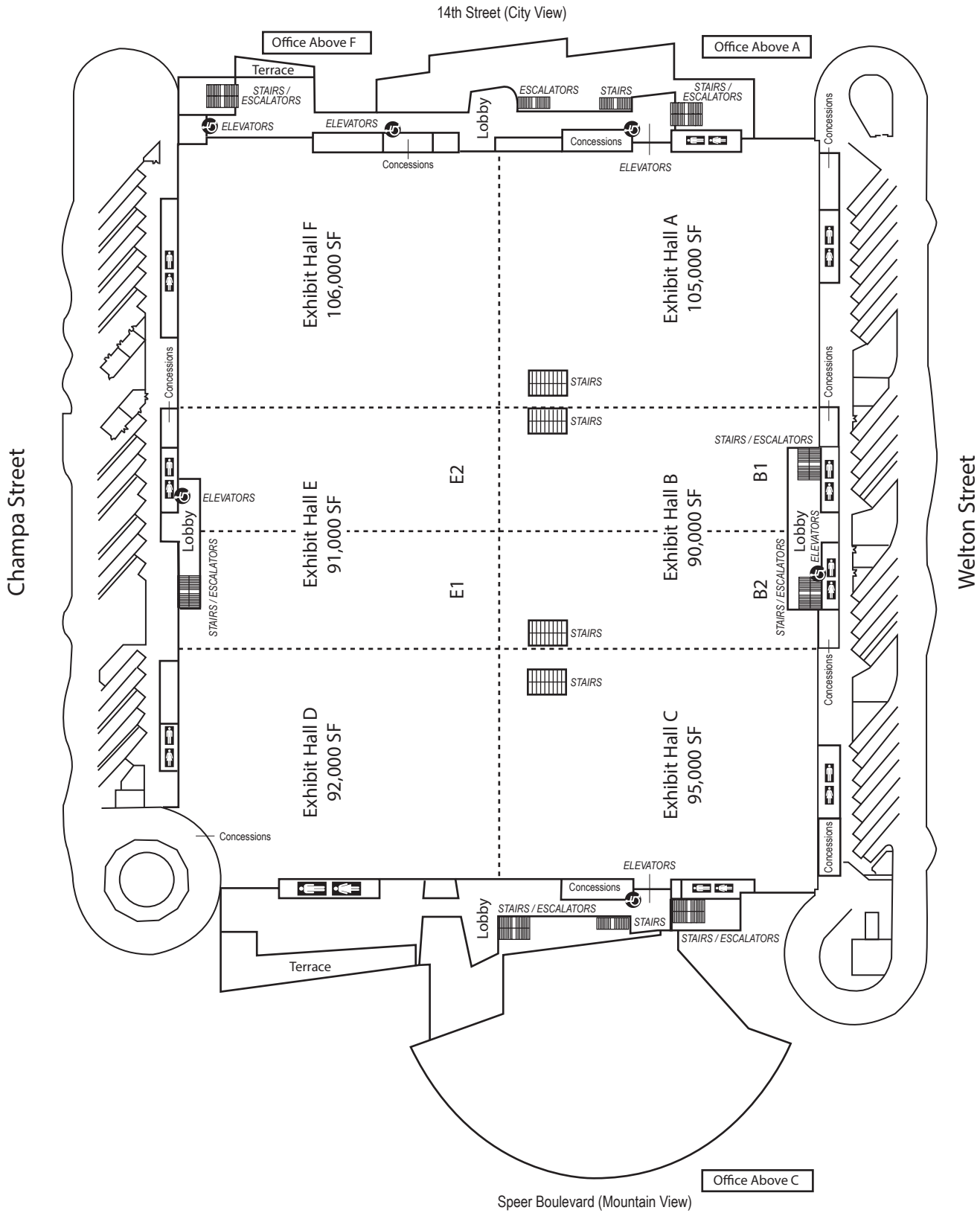


COLORADO CONVENTION CENTER



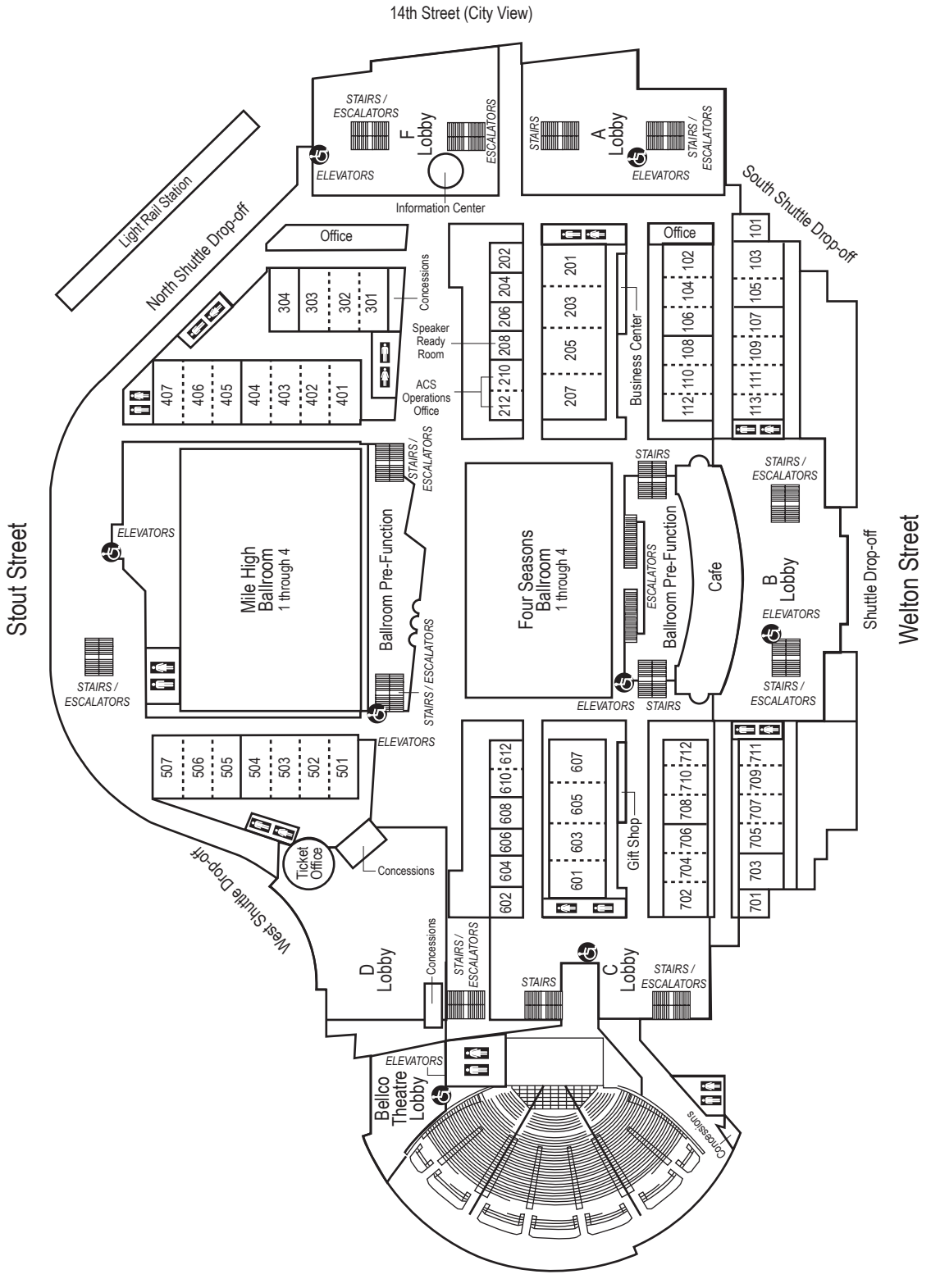
COLORADO CONVENTION CENTER

Exhibit Level



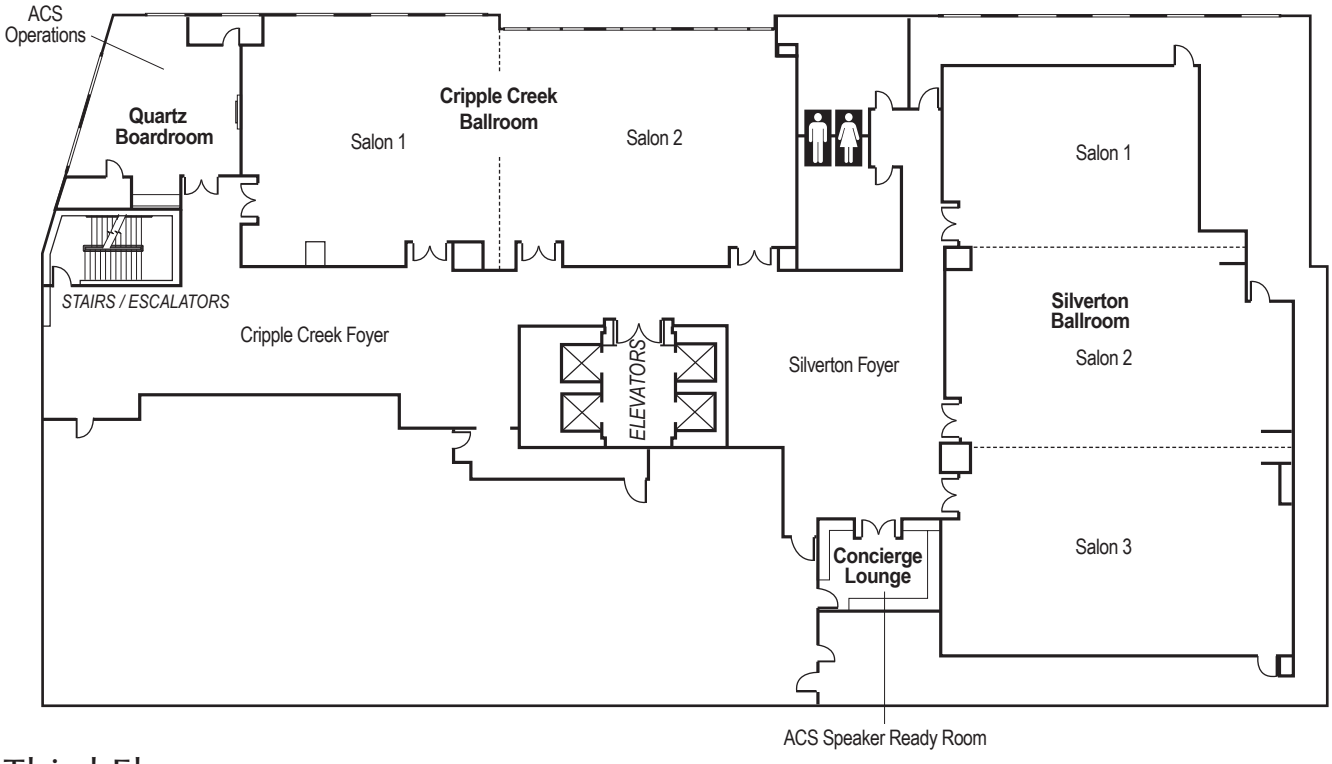
COLORADO CONVENTION CENTER

Meeting Room Level

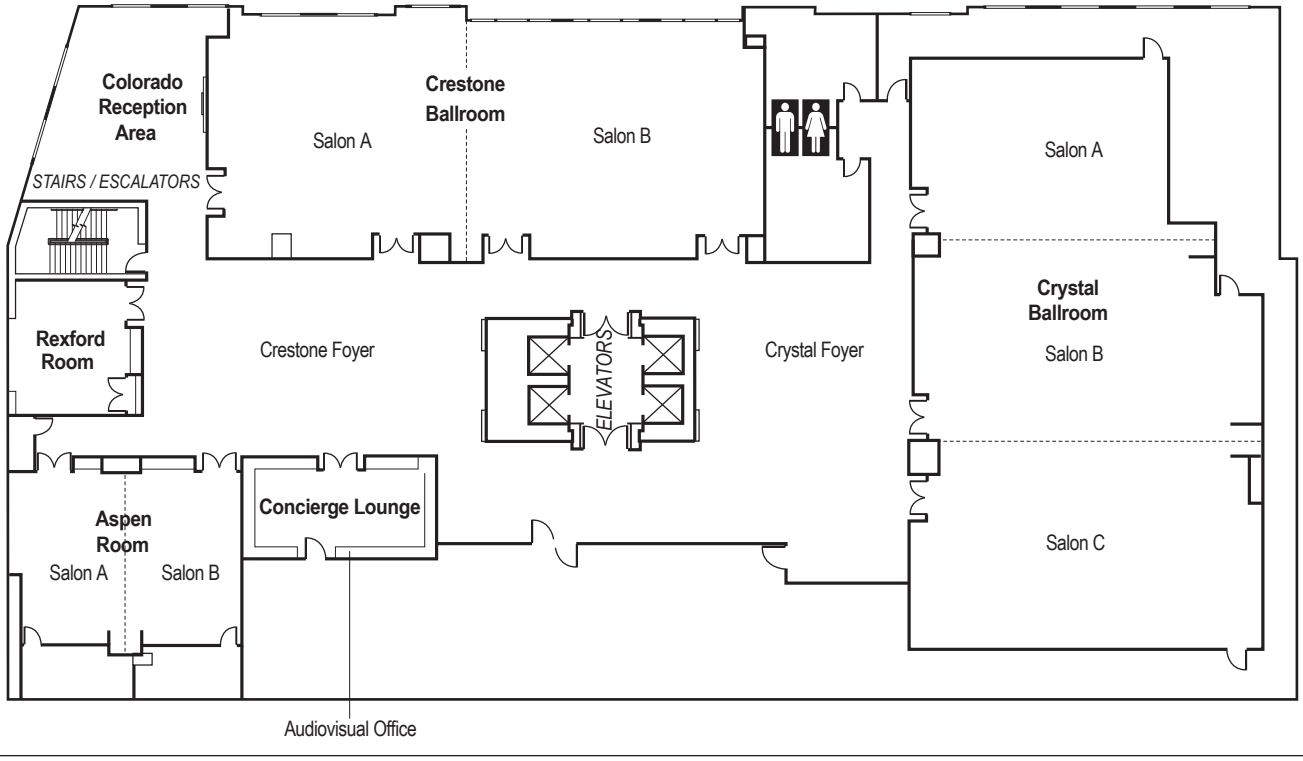


EMBASSY SUITES DENVER DOWNTOWN CONVENTION CENTER

Second Floor



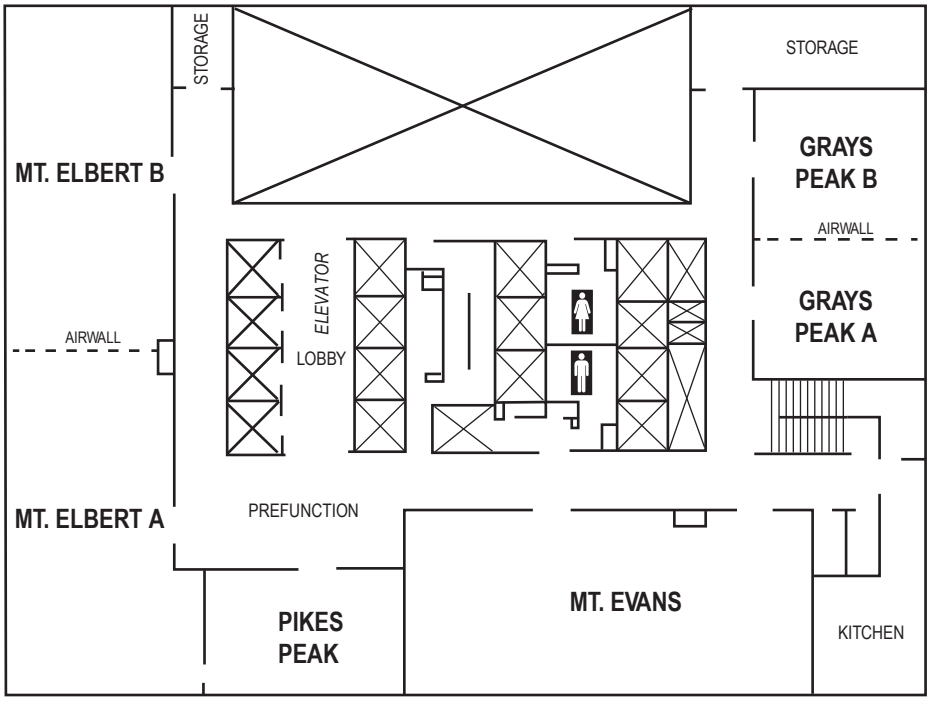
Third Floor



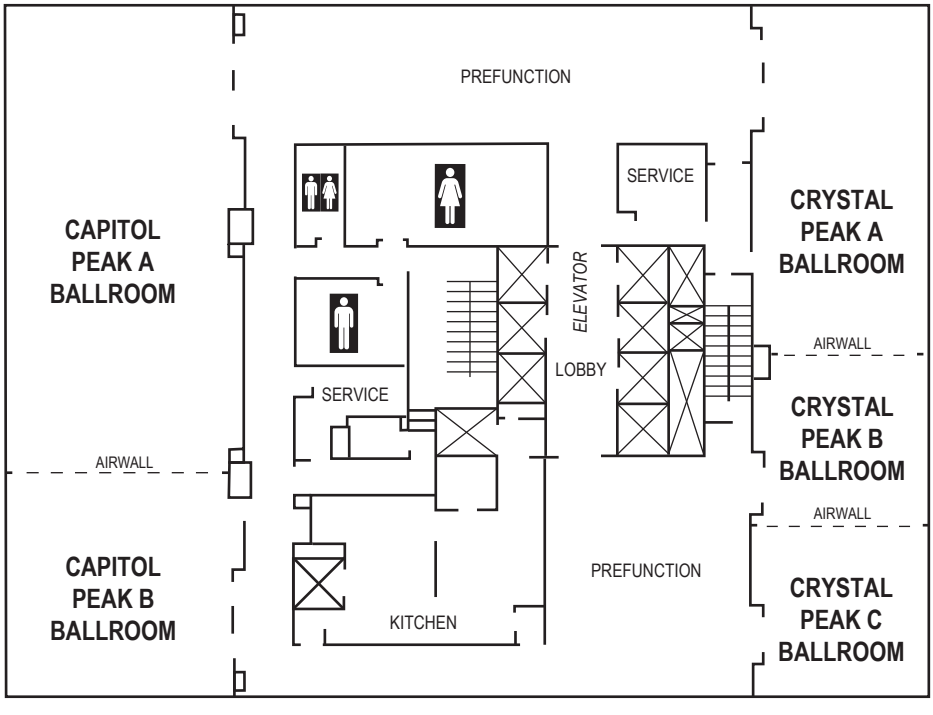
GRAND HYATT CONFERENCE CENTER

Atrium Tower

Second Floor

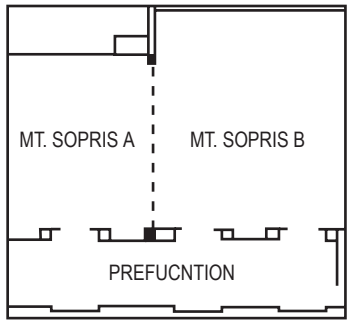


Pinnacle Club—38th Floor

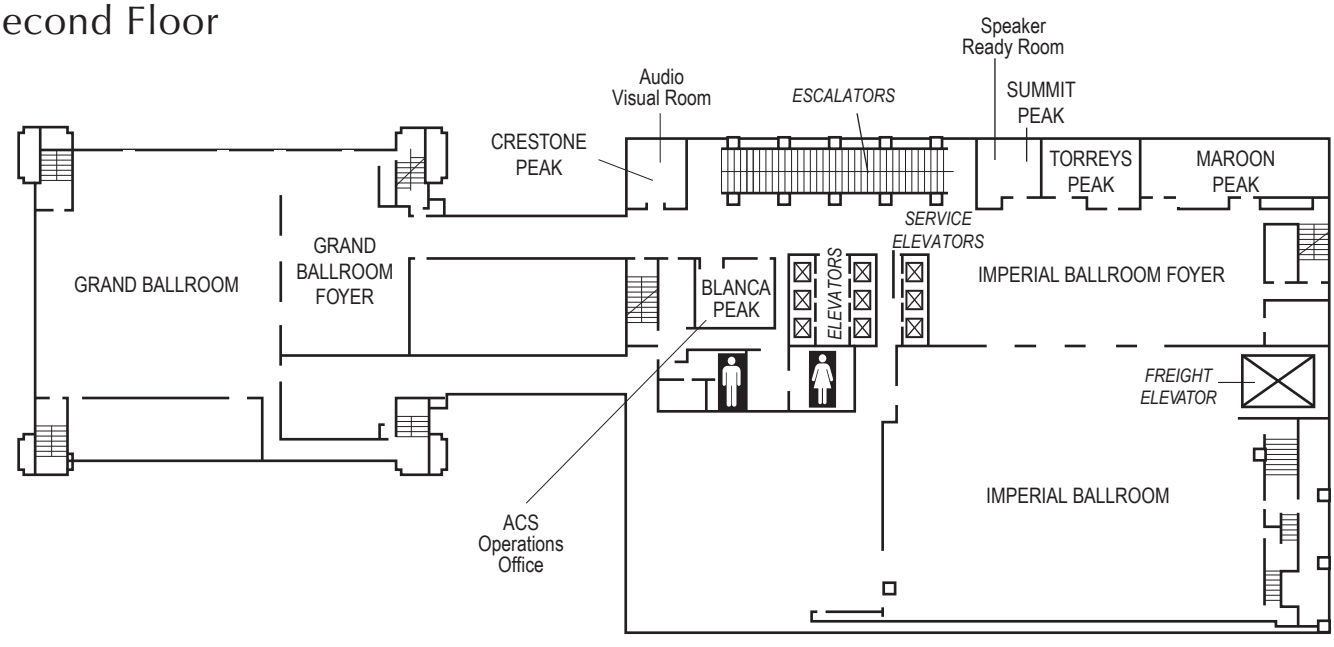


GRAND HYATT DENVER

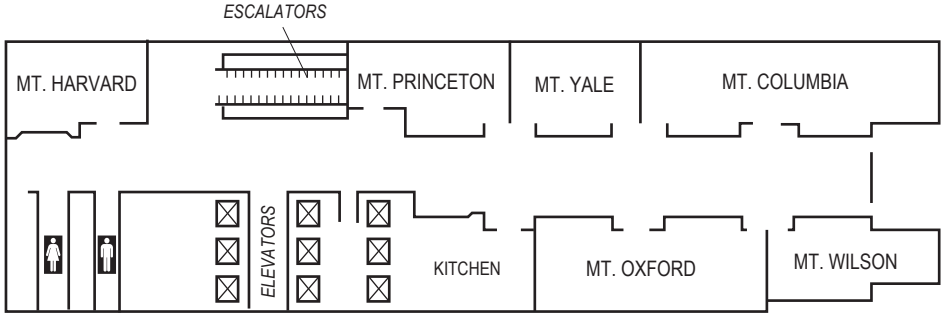
Lobby Level



Second Floor

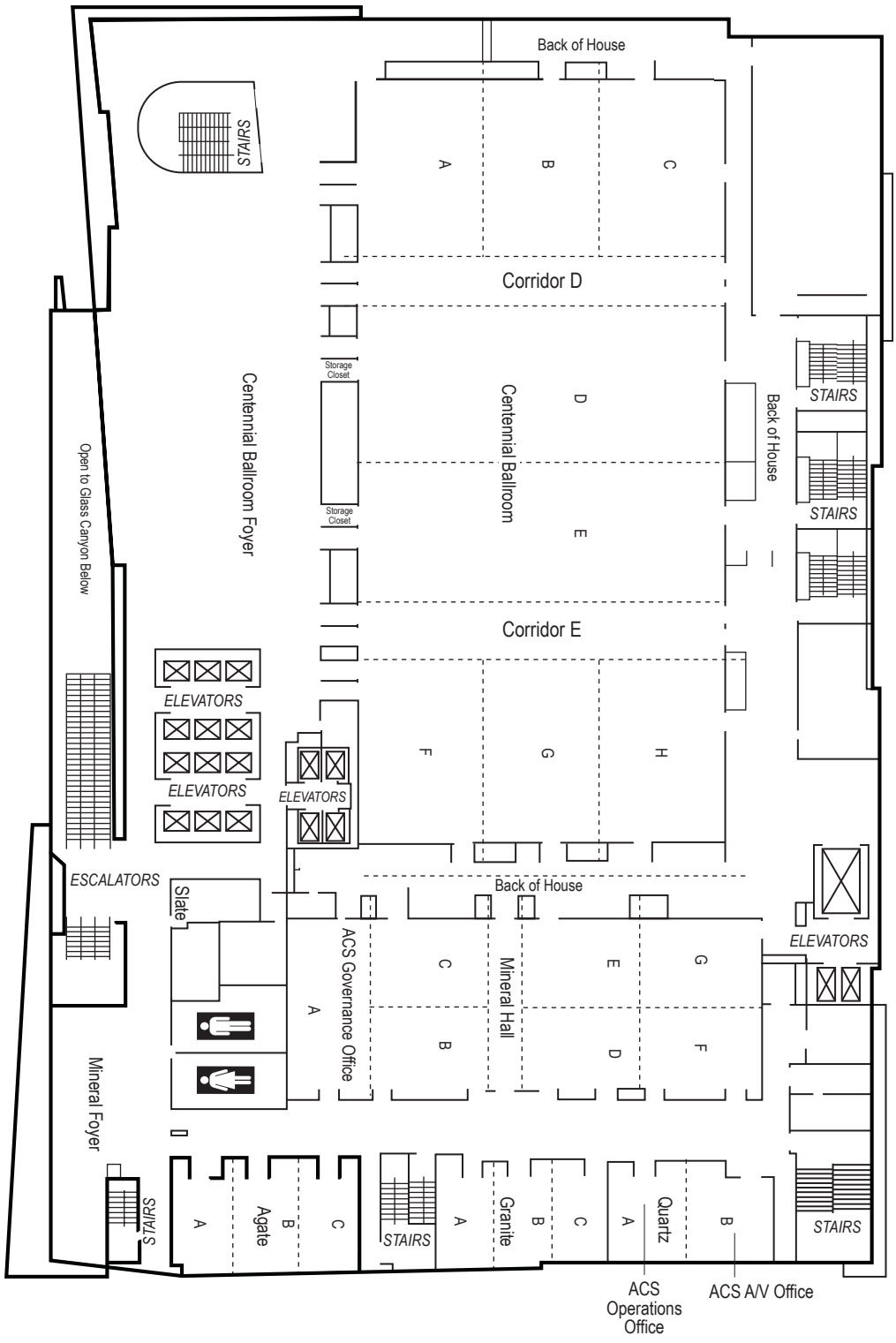


Third Floor



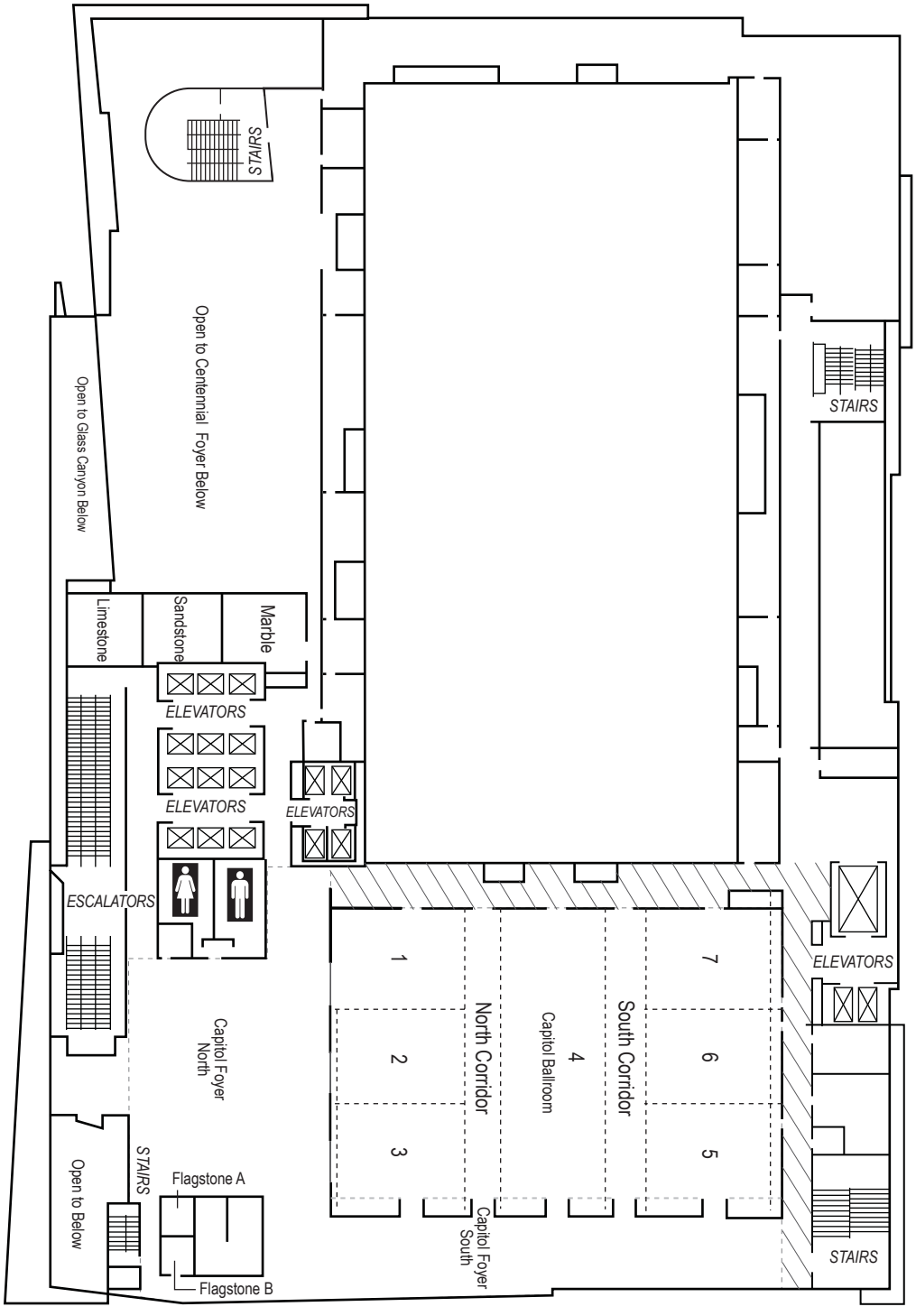
HYATT

Level Three



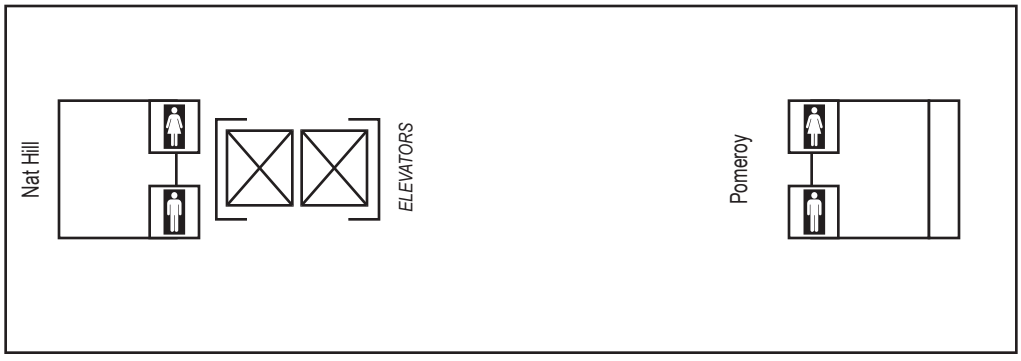
HYATT

Level Four

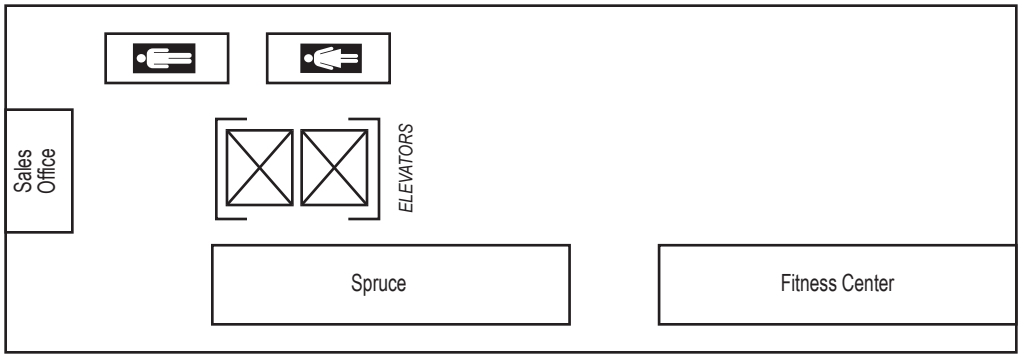


MARRIOTT CITY CENTER

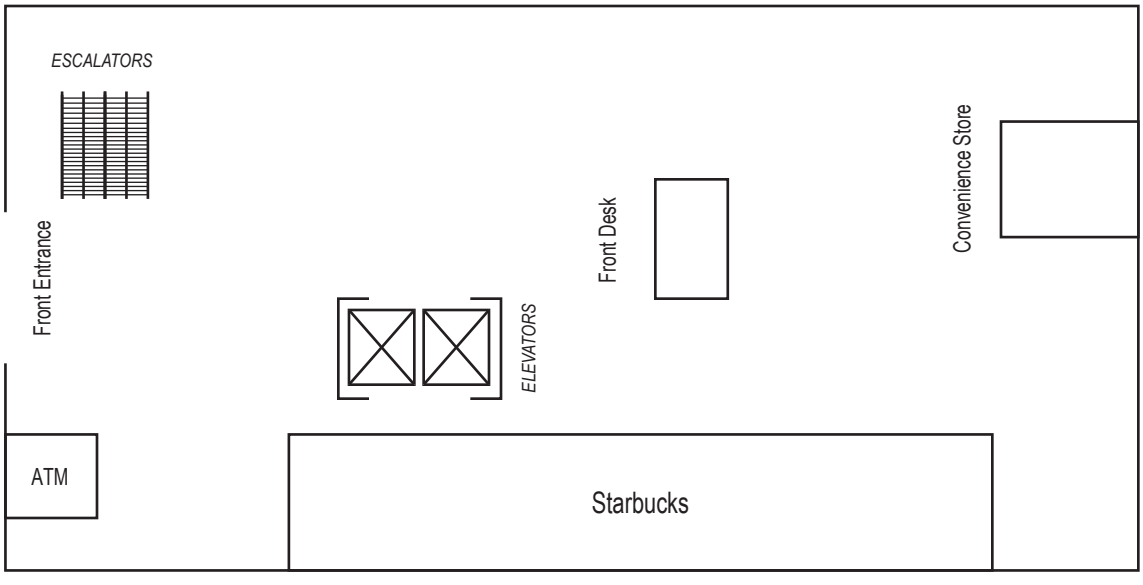
3rd Floor



2nd Floor

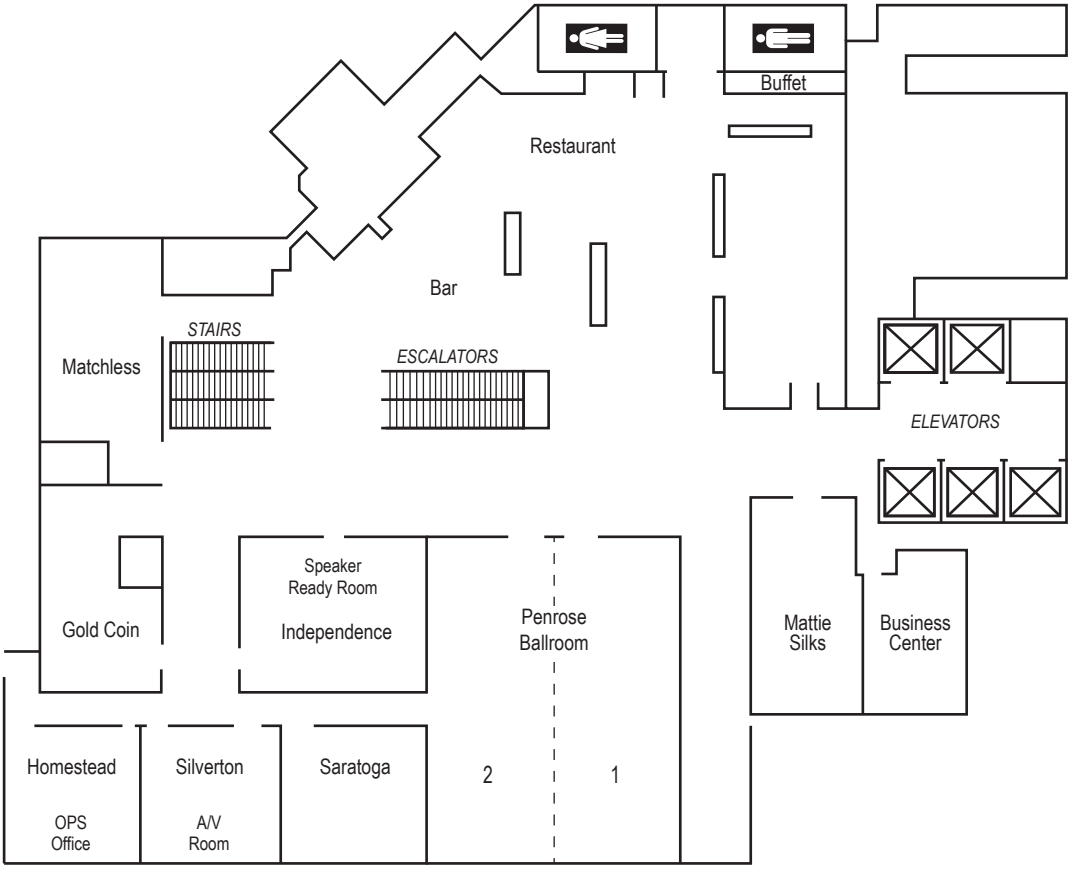


Lobby Level

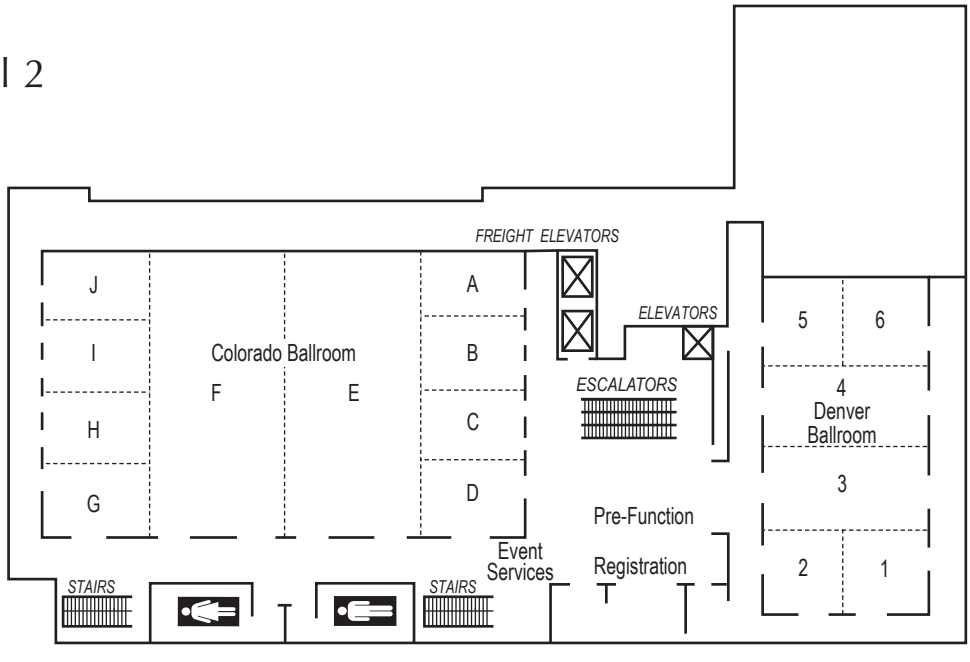


MARRIOTT CITY CENTER

Lower Level 1

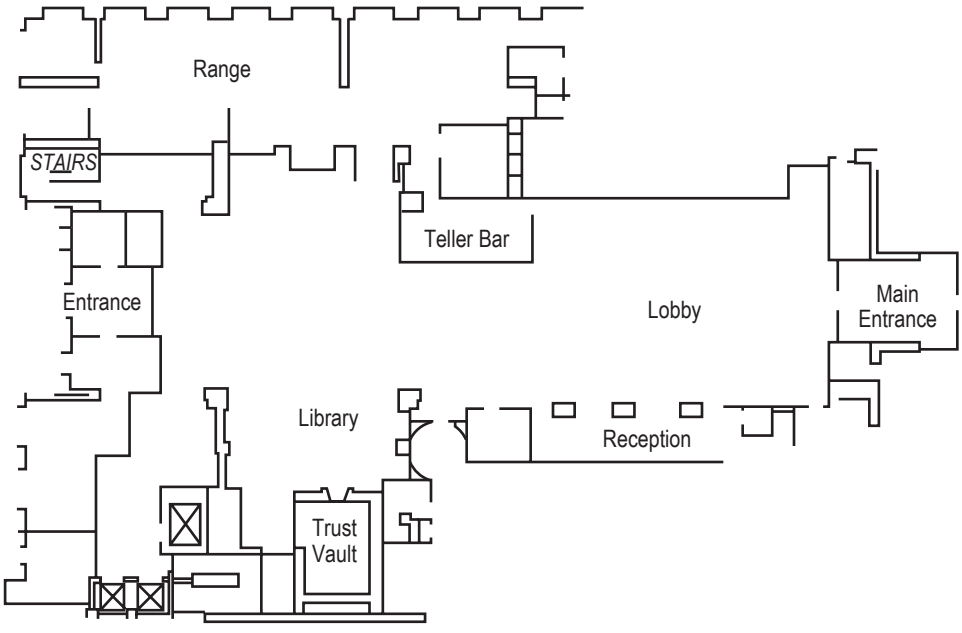


Lower Level 2

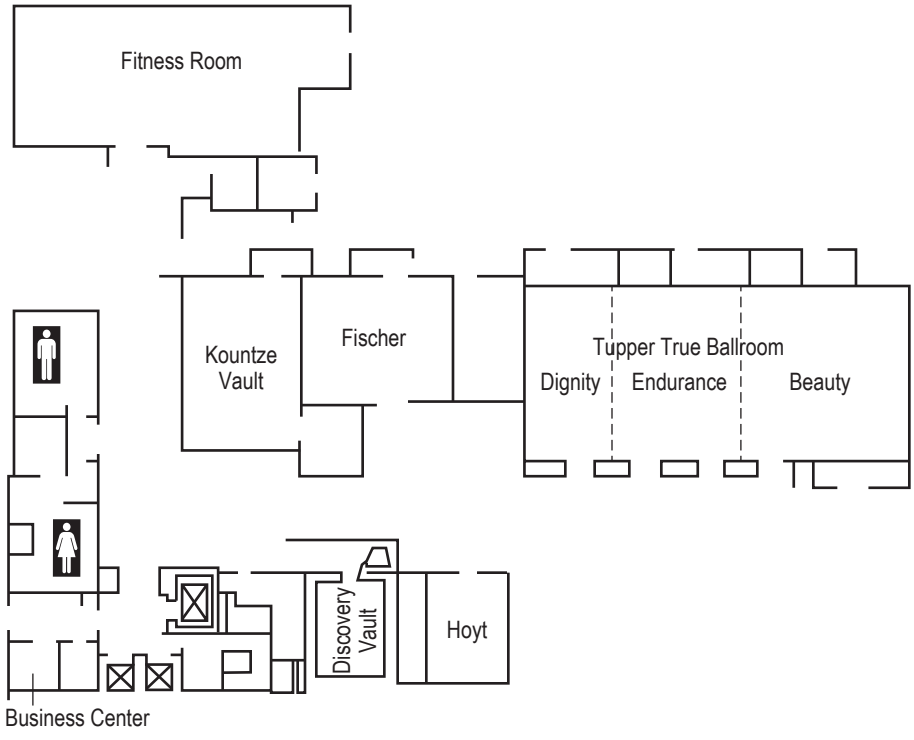


RENAISSANCE DENVER DOWNTOWN

Lobby Level

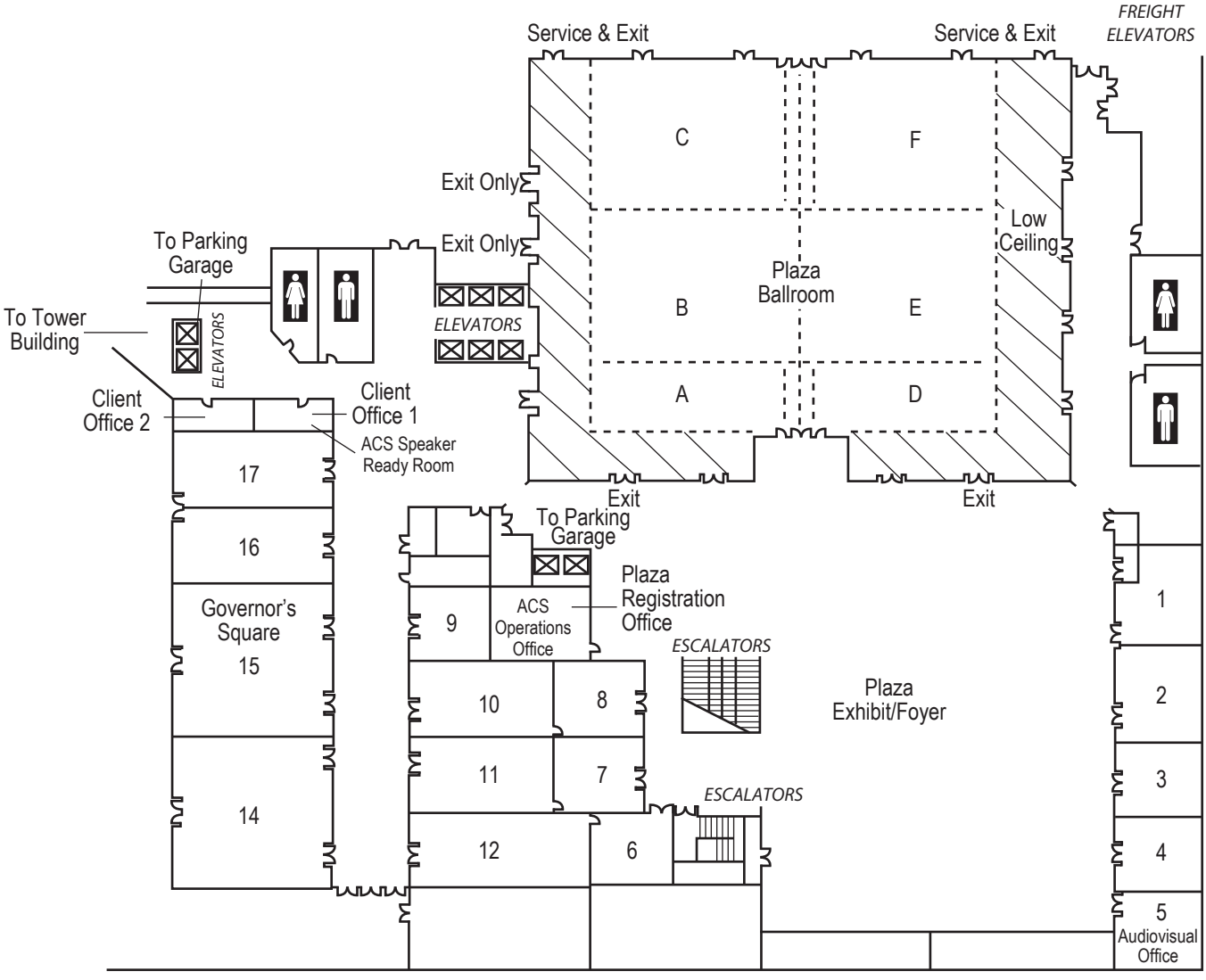


Lower Level



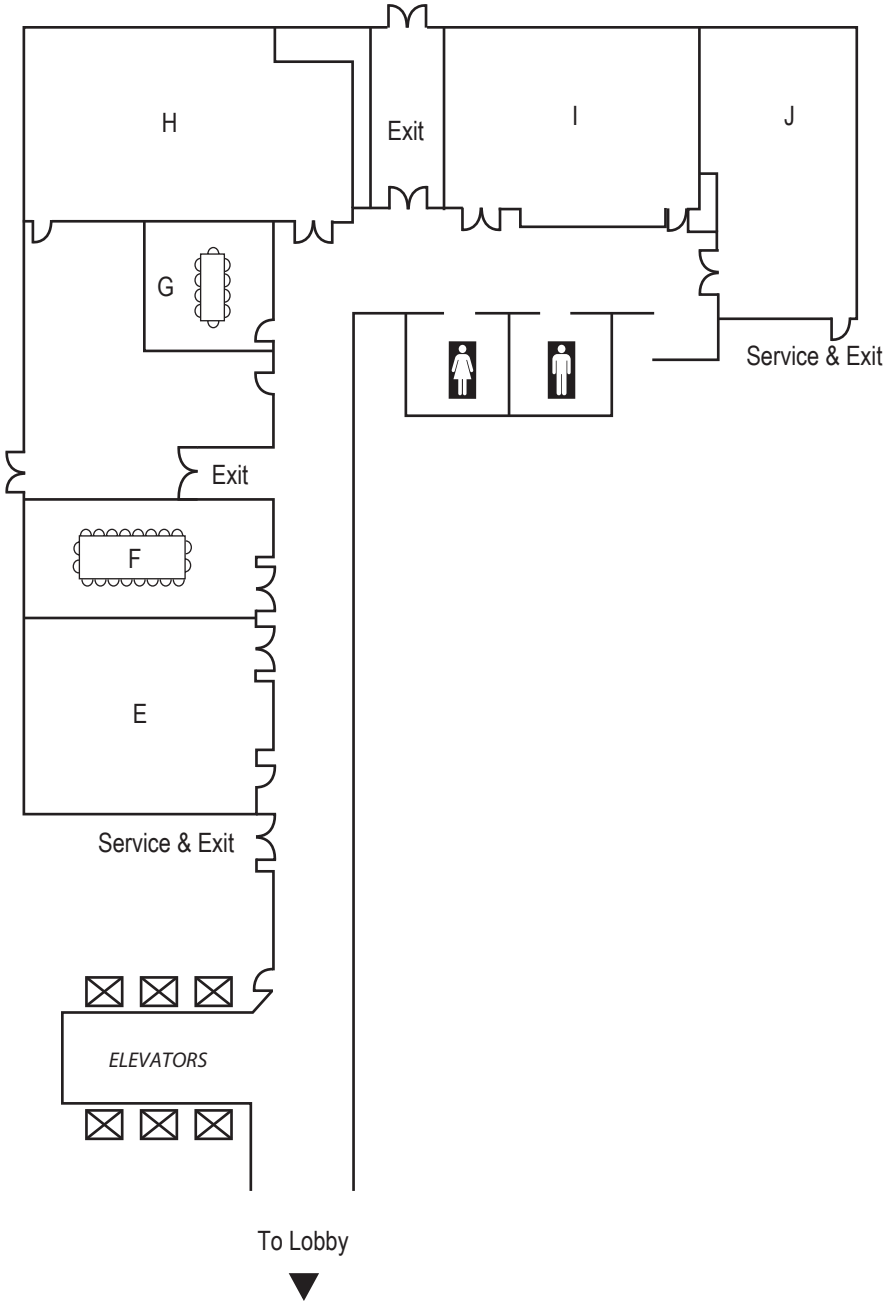
SHERATON DENVER DOWNTOWN

Plaza Building Concourse Level



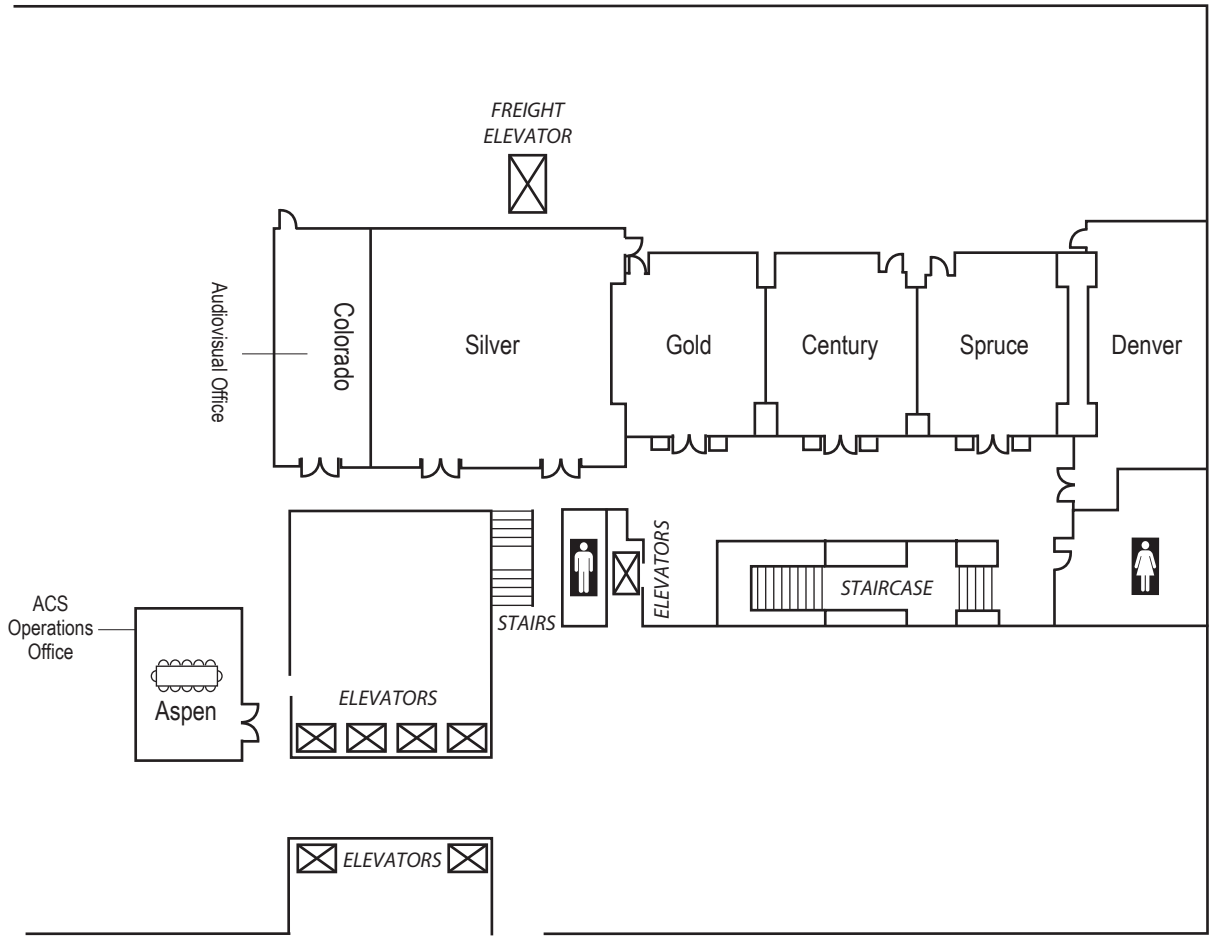
SHERATON DENVER DOWNTOWN

Plaza Building Lobby/Street Level



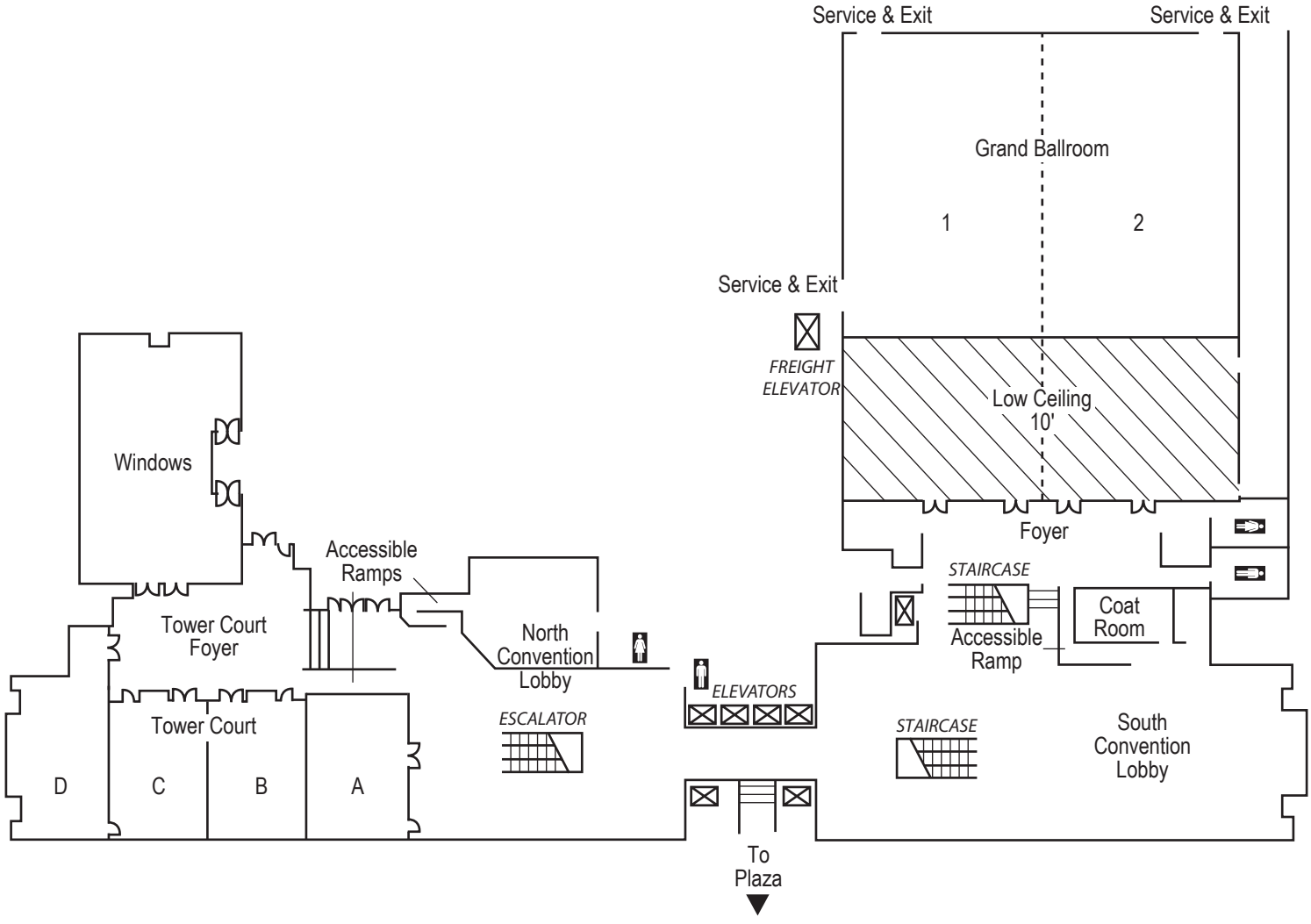
SHERATON DENVER DOWNTOWN

Tower Building Mezzanine Level



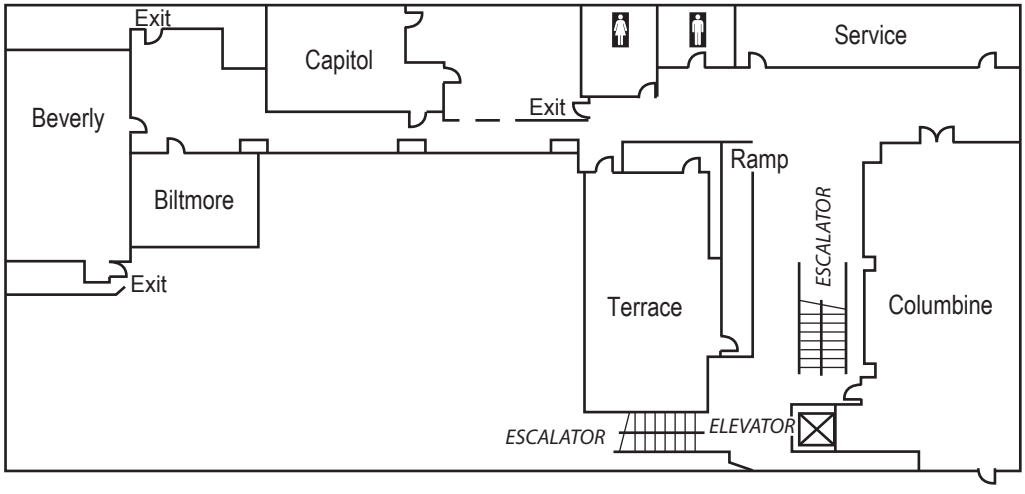
SHERATON DENVER DOWNTOWN

Tower Building Second Level

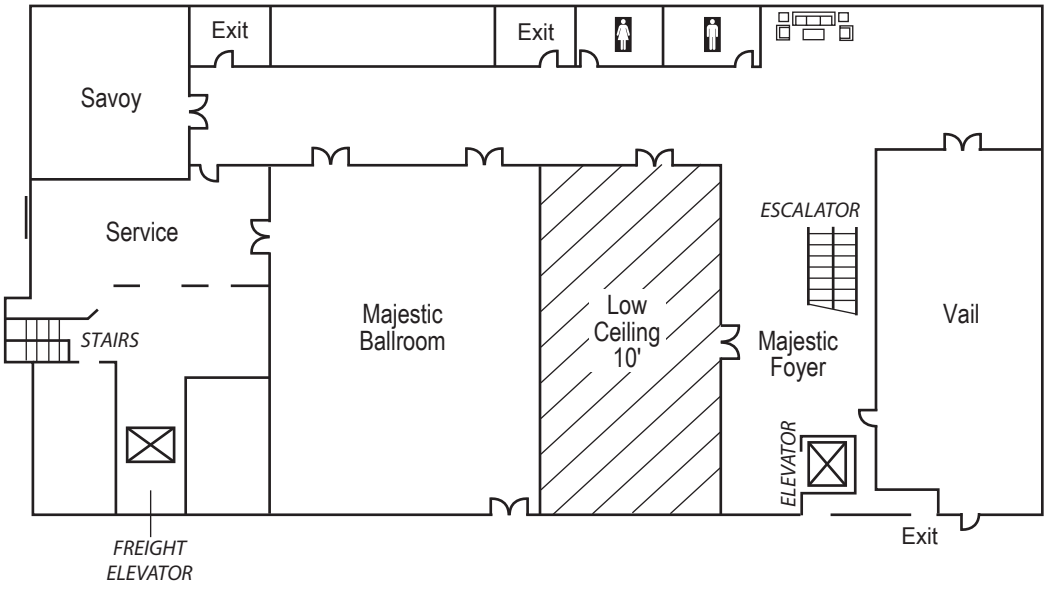


SHERATON DENVER DOWNTOWN

Tower Building Terrace Level

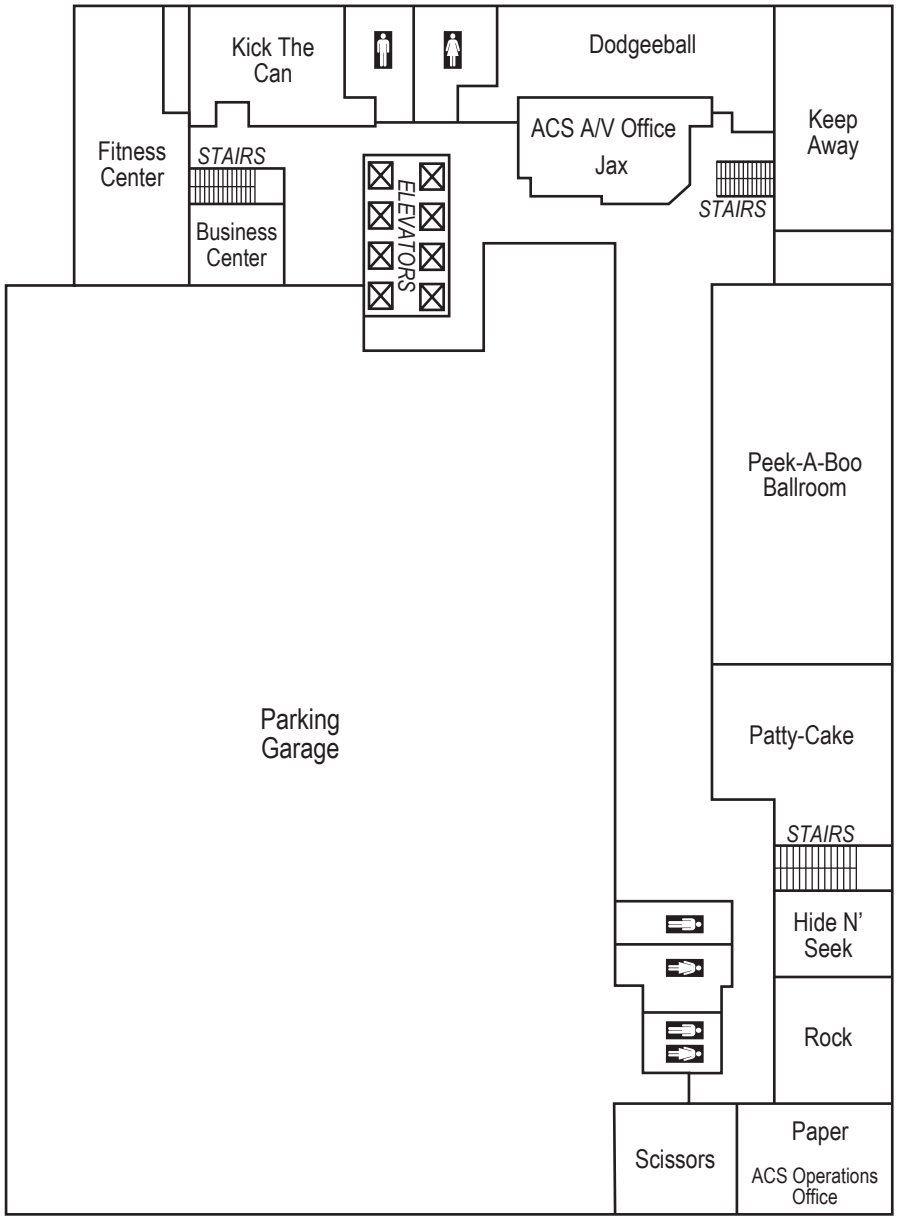


Tower Building Majestic Level



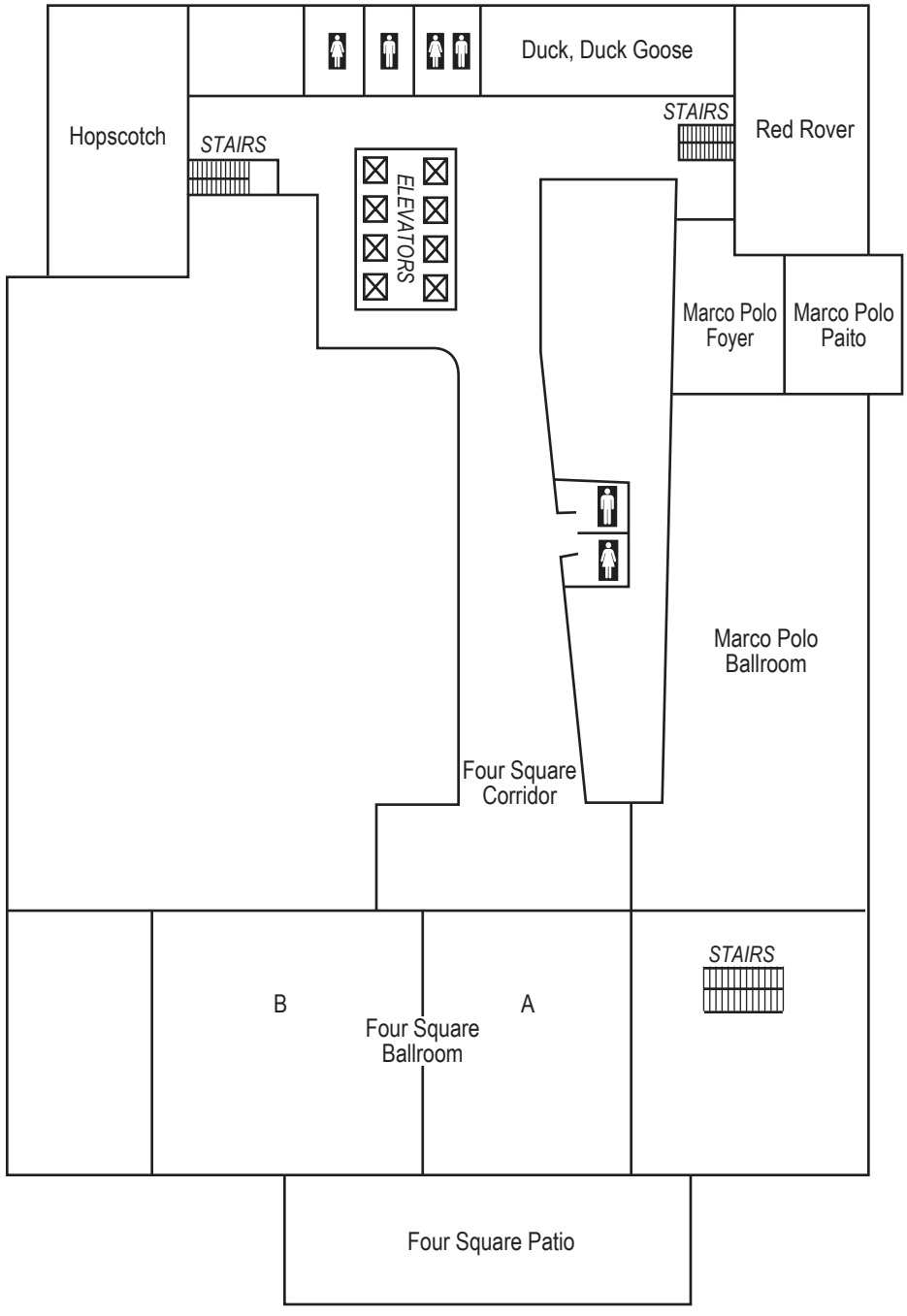
THE CURTIS MEETING SPACE

2nd Floor



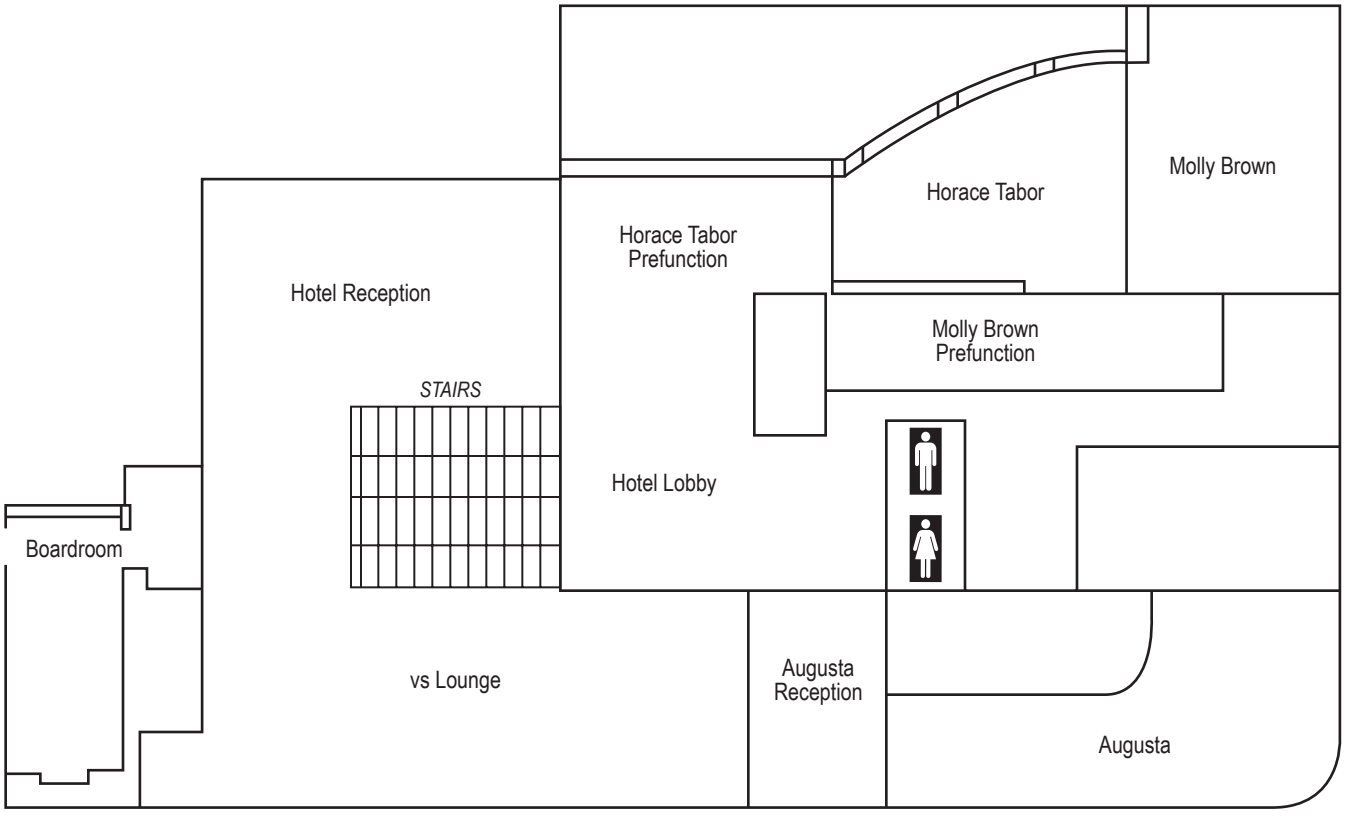
THE CURTIS MEETING SPACE

3rd Floor



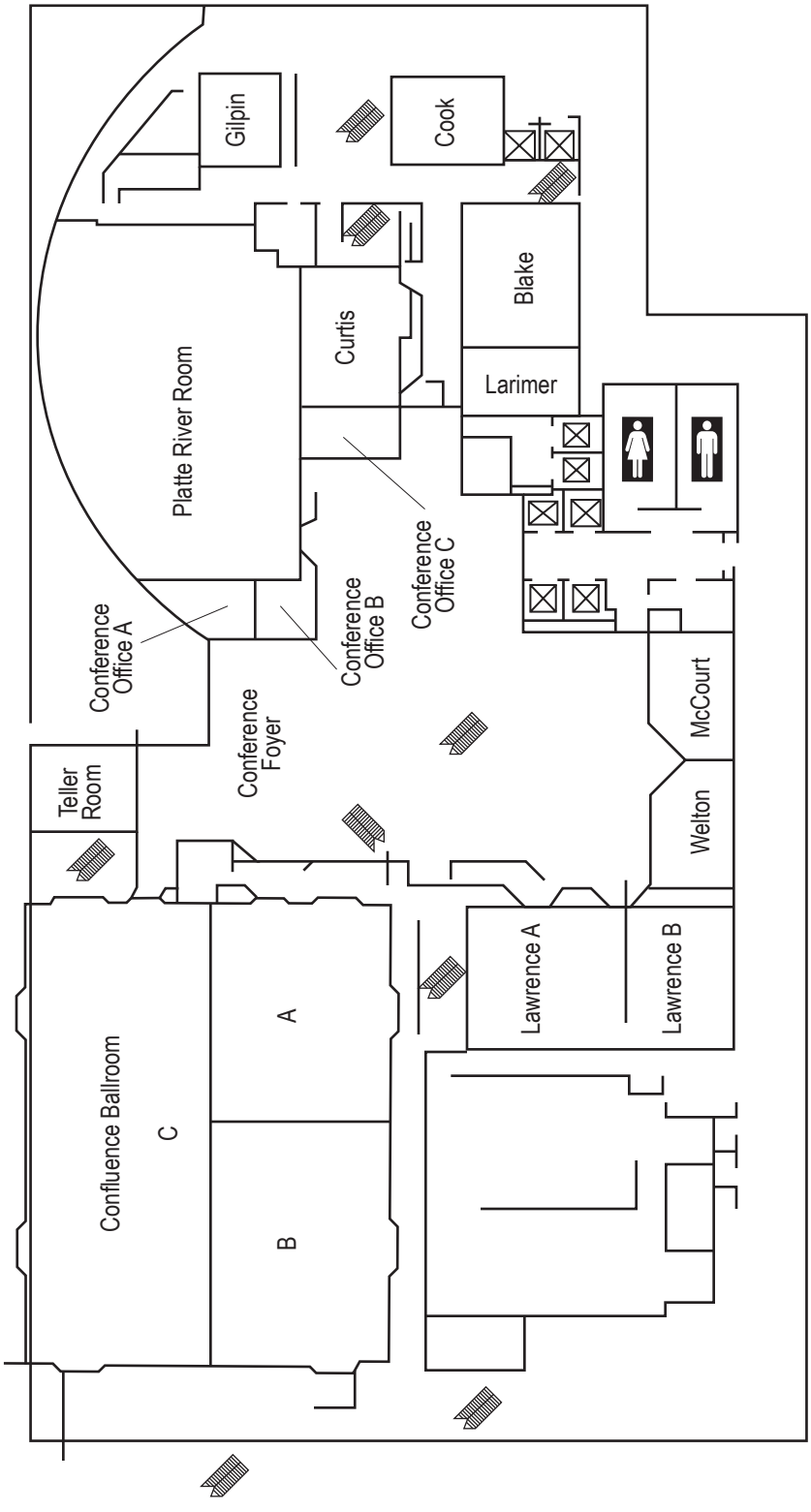
WESTIN DENVER HOTELS

Lobby Level, Second Floor



WESTIN DENVER HOTELS

Lobby Level, Third Floor



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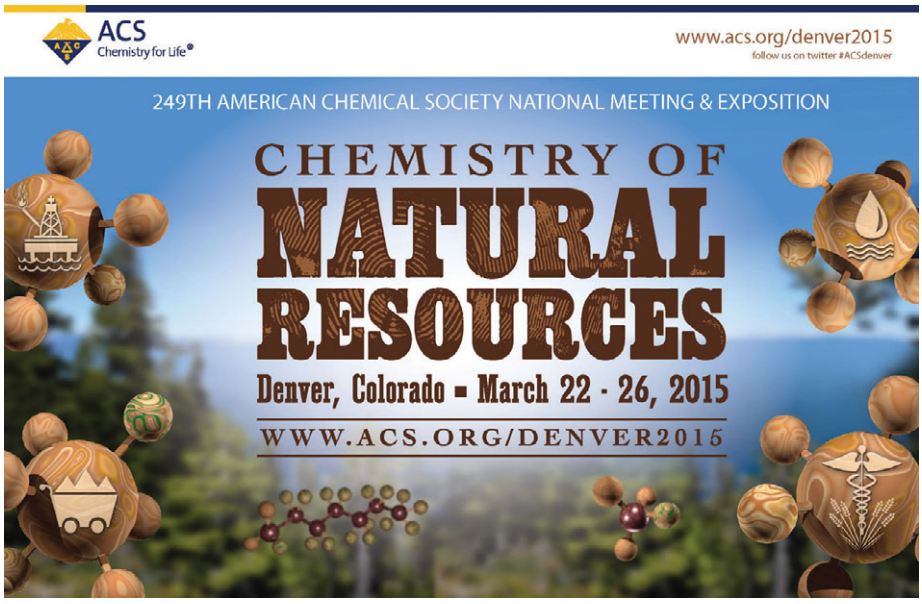

Sunday, March 22, 2015

1:30-5:30 PM

Nanotechnology: Delivering on the Promise

Monday, March 23, 2015

8:30 AM-4:45 PM

Nanotechnology: Delivering on the Promise

(Cosponsored by the following ACS Divisions and Committees and other scientific societies AGFD, AGRO, ANYL, CARB, CHAS, COLL, ENFL, HIST, I&EC, PMSE, POLY, SCHB, MPPG, CA, CCS, CCPA, COMSCI, DAC, IAC, SOCED; American Institute of Chemical Engineers, Gordon Research Conferences, Materials Research Society & National Academy of Engineering)

Colorado Convention Center, Mile High Ballroom 3A (Lower Level)

Tuesday, March 24, 2015

8:30-11:30 AM

DOE Nanoscience Research Centers: National Resources for the Nanoscience Community
(Cosponsored ANYL, ENFL, CCPA, CEI & MPPG)

Colorado Convention Center, Rooms 506-507 (Street Level)

NANO RELATED SYMPOSIA RECOMMENDED BY THE ACS PRESIDENT

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Ask Dr. Safety: EH&S Support of Nanotechnology R&D
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Electrical, Thermal, & Mass Transport in Polymer Nanocomposites & Alloys
(Sponsored by POLY and cosponsored by PRES)

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Visit our website at www.acs.org/denver2015 to view a list of economical hotels.

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Shuttle information

Shuttle Schedule

SUNDAY, MARCH 22
7:00 AM – 10:00 AM ..... 15 minute service
10:00 AM – 4:00 PM ..... 30 minute service
4:00 PM – 7:00 PM ..... 15 minute service
7:00 PM – 11:00 PM ..... 30 minute service

MONDAY, MARCH 23
7:00 AM – 10:00 AM ..... 15 minute service
10:00 AM – 4:00 PM ..... 30 minute service
4:00 PM – 11:00 PM ..... 15 minute service

TUESDAY, MARCH 24
7:00 AM – 10:00 AM ..... 15 minute service
10:00 AM – 4:00 PM ..... 30 minute service
4:00 PM – 11:00 PM ..... 15 minute service

WEDNESDAY, MARCH 25
7:00 AM – 11:00 PM ..... 30 minute service

THURSDAY, MARCH 26
7:00 AM – 6:00 PM..... 60 minute service

Route 1 Route 2 Walk to Convention Center
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Hilton Garden Inn Denver Downtown

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1

Take advantage of linen reuse and other initiatives at your hotel, and always turn the lights off when away from your room. If you are staying at the Westin or Sheraton, enroll in their Make A Green Choice program.

2

Responsibly dispose of recyclable materials (paper, plastic, glass, aluminum) at the convention center and hotels.

3

Download the national meeting mobile app or digital program. Limited quantities of the printed Onsite Program are available.

4

Avoid the use of taxis by walking when safe and possible. Stop by the Greener Meetings Booth for your pedometer (***While supplies last).*** Burn calories, and enjoy the city.

5

Ride the ACS carbon-neutral shuttle service when walking isn't an option between your hotel and the center. Shuttle service will be provided between many ACS contracted properties.

6

Avoid the use of disposable, plastic water bottles. Stop by the ACS Colorado Host Local Section Booth to pick up a free, reusable water bottle (***While supplies last).*** Avoid the cost and waste associated with disposable bottles.

Colorado Convention Center, Lobby A/F

Greener Meetings Booth

Sun., 3 – 6 PM
Mon., 8 – 1PM
Tues., 8 – 1 PM

Colorado Host Local Section Booth

Sat., 3 to 6 PM
Sun., 7:30 AM to 7:30 PM
Mon., 7:30 AM to 9 PM
Tues., 7:30 AM to 5 PM
Wed., 7:30 AM to 4 PM
Thurs., 7:30 AM to 1 PM

ACKNOWLEDGMENTS

Specific ACS Divisions and Committees gratefully acknowledge the financial and other contributions made to their division by the institutions and companies listed below and others who were not known at press time.

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