2014 ACS Central Regional Meeting

MATERIALS ENERGY HEALTH

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BRIDGING CHEMISTRY AND INNOVATION
CERM 2014

THE 45TH CENTRAL REGIONAL MEETING

OCT. 29 – NOV. 1, 2014

DOUBLETREE BY HILTON
PITTSBURGH - GREEN TREE

PROGRAM BOOK

ACS Chemistry for Life®

The American Chemical Society Celebrates

National Historic Chemical Landmarks

Chemists and Chemistry that Transformed Our Lives

National Historic Chemical Landmarks

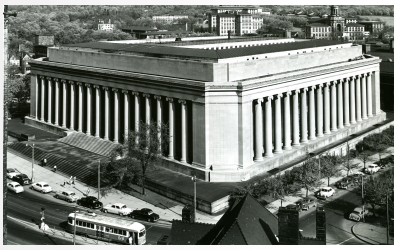
Commemorated within the ACS Pittsburgh Section

The Legacy of Rachel Carson's *Silent Spring*

Rachel Carson's Silent Spring, *published in 1962, was a landmark in the development of the modern environmental movement. The legacy of* Silent Spring *continues today in the chemistry community's increased focus on green practices and the public's support for sustainability.*

Chatham University, 1 Woodland Avenue (Science Complex student lounge)

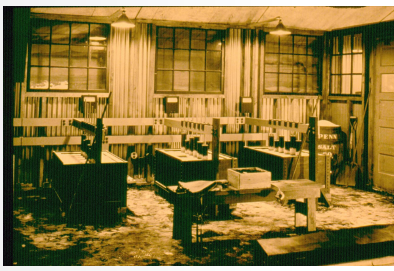
Mellon Institute of Industrial Research



Prior to its merger with the Carnegie Institute of Technology, the Mellon Institute provided research services for industry and trained hundreds of scientists. Research performed here launched companies such as Dow Corning and the chemical division of Union Carbide.

Carnegie Mellon University, 4400 Fifth Avenue (Fifth Avenue entrance)

Commercialization of Aluminum



In 1886, Charles Martin Hall invented an economical electrochemical process to release aluminum metal from its ore. Pittsburgh investors supported the commercialization of Hall's process and founded the Pittsburgh Reduction Company, now known as Alcoa.

Alcoa Inc., 201 Isabella Street (Corporate Center Hall of Fame)

First Commercial Oil Refinery

In the 1850s, Samuel Kier constructed a distillation unit for refining crude oil into kerosene. Kier's still touched off the search for dependable sources of crude oil and led to the nation's first oil boom, centered around the western Pennsylvania town of Titusville.

U.S. Steel Tower, Seventh Avenue and Grant Street (sidewalk level)

More information about these and other National Historic Chemical Landmark subjects is available online.

ACS National Historic Chemical Landmarks | 202-872-6214 | landmarks@acs.org | www.acs.org/landmarks

45th American Chemical Society Central Regional Meeting

TABLE OF CONTENTS

2014 CENTRAL REGIONAL MEETING COMMITTEE MEMBERS

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General co-Chair: Heather Juzwa, Shimadzu Scientific Instruments, Inc.
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Program co-Chair: Dr. Michelle Ward, University of Pittsburgh
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Activities/Events co-Chair: Karen Johnson, Bidwell Training Center
Career Workshop Chair: Dr. Joseph Jolson, Custom Client Solutions
Exhibition co-Chair: Eli Absey, Waters Corporation
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Information Technology co-Chair: Dr. Tamika Madison, University of Pittsburgh
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The CERM 2014 Organizing Committee thanks Waynesburg undergraduates Tara Fagioli and Nick Frazee for their part in the Undergraduate Programming Organization and Traci Johnsen for her contribution to the Final Program Book.

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The CERM 2014 organizing committee extends a sincere thank you Jeremy Sunseri and the Art Institute of Pittsburgh, for designing a logo that embodies the theme of our meeting.

BRIDGING CHEMISTRY AND INNOVATION
CERM 2014

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Phone 202-872-4461
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October 29, 2014

Dear Central Regional Meeting Participants,

On behalf of the more than 161,000 members of the American Chemical Society, I am delighted to extend my warm personal greetings to all of you attending the 45th Central Regional Meeting (CERM 2014) in lovely Pittsburg, Pennsylvania.

Planned technical program span a diverse array of chemistry topics, including green chemistry, proteomics, chemistry education, materials characterization, nucleic-acid-based materials, and energy-related research. There will also be a symposium on diversity in the chemical sciences and four poster sessions throughout the meeting.

Make sure to take advantage of the outing to learn about rum production and distillation, and take advantage of the many luncheons hosted by various committees including the Younger Chemists Committee, the Women Chemists Committee, Project SEED, and an Undergraduate Network & Résumé Luncheon.

I encourage everyone to attend the Awards Reception honoring the recipients of the ACS Pittsburgh Section's 2014 Distinguished Service Award and 2014 Pittsburgh Award winners. Awards being presented will include the ACS Division of Chemical Education Regional Award for Excellence in High School Teaching, the E. Ann Nalley Regional Award for Volunteer Service to ACS, and the Stanley C. Israel Regional Award for Advancing Diversity in the Chemical Sciences.

Last but not least, I want to express my special thanks to the CERM 2014 Co-Chairs, Heather Juzwa and Jay Auses, Co-Program Chairs, Michelle Ward and Adrian Michael, and the many organizers and volunteers, especially the members of the Pittsburgh Local Section and the 24 other participating Central region local sections of the American Chemical Society – representing more than 14,400 members in the region – for their hard work and dedication to create an intellectually stimulating experience here in Pittsburg.

Best wishes for a most successful CERM 2014!

Sincerely,

Tom Barton
President
American Chemical Society

CITY OF PITTSBURGH

OFFICE OF THE MAYOR

A Proclamation

AMERICAN CHEMICAL SOCIETY CENTRAL REGIONAL MEETING 2014

October 29 – November 1, 2014

***WHEREAS**, the American Chemical Society (ACS), founded at New York University in 1876, is a non-profit organization that supports scientific inquiry in the field of chemistry; and*

***WHEREAS**, ACS has more than 161,000 members at all degree levels and in all fields of chemistry, chemical engineering and related fields; and*

***WHEREAS**, ACS is recognized as the world's largest scientific society and one of the leading sources of authoritative scientific information; and*

***WHEREAS**, the 45th ACS Central Regional Meeting, organized by the Pittsburgh Section of the ACS, will be held in Pittsburgh from October 29 through November 1, 2014 .*

***NOW THEREFORE BE IT RESOLVED** that I, William Peduto, Mayor of the City of Pittsburgh, do hereby commend the American Chemical Society for its commitment to scientific inquiry here in our most livable City of Pittsburgh.*

WILLIAM PEDUTO

Mayor

COUNCIL 84 AFSCME UNION LABEL

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BRIDGING CHEMISTRY AND INNOVATION
CERM 2014

A MESSAGE FROM THE GENERAL CO-CHAIRS

On behalf of the Organizing Committee, it is our pleasure to welcome you to CERM 2014 in the "Most Livable City" of Pittsburgh. We have worked diligently over several years to make this an exciting and valuable conference for all. To make the most of your experience, we encourage you to take advantage of all the symposia and activities you can.

CERM 2014 should enable attendees to Bridge Chemistry and Innovation. The Technical Program represents the many disciplines the Central Region has to offer. Likewise, the symposia exemplify the collaboration between health, energy, and materials fields. Our plenary speakers are true leaders in their respective fields.

We understand the importance of investing in our future, so we are offering unique programming days for both High School Teachers and Undergraduates. Your peers will explain how they created an award winning student affiliate chapter, and you will learn how Project SEED sculpted the lives of some rising stars.

The Career Workshop and Resume Review is an excellent opportunity for career advancement. We invite you to focus on your professional development by attending the two Leadership Institute Courses. Celebrate with the 2014 Award Winners at the Awards Banquet.

While we have assembled an outstanding science program, make sure to take advantage of this meeting's unique networking opportunities. We have scheduled special luncheons for the YCC and WCC to maximize quality interactions between attendees.

This meeting would not be possible without the support of our sponsors and exhibitors—thank you all! Please show your gratitude by visiting the Junior Ballroom and thanking our exhibitors for their support.

What better place to Bridge Chemistry and Innovation than in the City of Bridges? Not only does Pittsburgh offer beautiful scenery, there are many fun things to do with family and friends. We are hosting a Welcome Reception, Wine, Wii, and 'Wiches on Wednesday night where you can challenge the exhibitors in a Wii tournament and sample some of Pittsburgh's finest foods. You can also see Pittsburgh from Mount Washington after riding the iconic Duquesne Incline and seeing a behind the scenes tour of how it works. And, to top off the evening, learn about Rum Science with tastings!

We hope *yinz* are ready for a great meeting!

Jay Auses

Heather Juzwa

PLENARY LECTURES

Bradley D. Smith, Ph.D.
University of Notre Dame

Wednesday, October 29
Salons D, E - 9:00 am – 10:00 am

SMART MOLECULES FOR IMAGING, THERAPY, AND HEALTH

Bradley D. Smith earned a B. S. degree from the University of Melbourne and Ph.D. from Pennsylvania State University. He conducted postdoctoral research at Oxford University, UK and then at Columbia University before joining the faculty at the University of Notre Dame in 1991. He is currently the Emil T. Hofman Professor of Chemistry and Biochemistry and Director of the Notre Dame Integrated Imaging Facility. He and his coworkers develop molecular imaging technologies for detecting cancer and microbial infections in living subjects. Dr Smith has also invented a series of interlocked dye molecules and converted them into imaging probes for a wide range of applications in biomedical science, biotechnology, and nanotechnology. A more detailed description of Smith's research program can be found at http://www.nd.edu/~bsmith3.

Vicki H. Wysocki, Ph.D.
The Ohio State University

Thursday, October 30
Salons D, E - 1:00 pm – 2:00 pm

CHARACTERIZATION AND NUCLEOPROTEIN COMPLEXES BY ION MOBILITY MASS SPECTROMETRY

Vicki Hopper Wysocki received her B.S. from Western Kentucky University and Ph.D. from Purdue University. She is Professor and Ohio Eminent Scholar of Macromolecular Structure and Function at Ohio State University, Columbus, OH, where she also serves as Director of the Campus Chemical Instrument Center. Prior to moving to OSU, Dr. Wysocki was a Professor and Department Chair of Chemistry and Biochemistry at the University of Arizona, Tucson, AZ. Her research interests include development of new instrumentation for mass spectrometry of protein complexes, fragmentation mechanisms of peptides, proteomics biomarker identification for development of disease diagnostics, IR spectroscopic characterization of small peptide fragments, and ion-surface chemistry. She currently serves on editorial or advisory boards for Chemical and Engineering News, Analyst, Mass Spectrometry Reviews, and International Journal of Mass Spectrometry. Dr. Wysocki has been the recipient of several awards including the 2009 ASMS Distinguished Contribution in Mass Spectrometry Award.

Sara E. Skrabalak, Ph.D.
Indiana University - Bloomington

Friday, October 31
Salons D, E - 1:00 pm – 2:00 pm

FROM SYNTHESIS TO MATERIALS DESIGN: NEW NANOSTRUCTURES AND NEW CATALYSTS

Dr. Sara E. Skrabalak received her B.A. degree in chemistry from Washington University in St. Louis in 2002 where she conducted research with Professor William E. Buhro. She completed her Ph.D. degree in chemistry from the University of Illinois at Urbana-Champaign in fall of 2006 under the tutelage of Professor Kenneth S. Suslick. She then conducted postdoctoral research at the University of Washington – Seattle with Professors Younan Xia and Xingde Li. She is an Assistant Professor of Chemistry at Indiana University – Bloomington and a recipient of both an NSF CAREER Award and DOE Early Career Award. She is a 2012 Research Corporation Cottrell Scholar, a 2013 Sloan Research Fellow, and was recently selected for the 2014 ACS Award in Pure Chemistry. This award is sponsored by Alpha Chi Sigma and recognizes young scholars who have "accomplished research of unusual merit for an individual on the threshold of her or his career" in pure chemistry. Her research group focuses on nanomaterial design and synthesis (http://www.indiana.edu/~skrablab/).

Greater Pittsburgh WCC Award for Encouraging Women into the Chemical Sciences
Tara Meyers, Ph.D.

Tara received her B.A. from Grinnell College in 1991 and her Ph.D. from the University of Iowa in 1991. She carried out postdoctoral work at both the University of Iowa (1991-2) and at the University of California, Berkeley (1992-4). Dr. Meyer joined the faculty at the University of Pittsburgh, Department of Chemistry in 1994. Dr. Meyer's research focuses on synthesis and structure/function studies on repeating sequence copolymers and on the design of stimuli responsive materials. Dr. Meyer serves on her Department's Diversity Committee and is active in the local WCC and NOBCCHE

Greater Pittsburgh WCC Award for Career Excellence in the Chemical Sciences
Anna C. Balzs, Ph.D.

Anna is the Distinguished Professor of Chemical Engineering and the Robert von der Luft Professor at the University of Pittsburgh. She received her B.A. in physics from Bryn Mawr College and her Ph.D. in Materials Science from the Massachusetts Institute of Technology. After postdoctoral work in the Polymer Science Department at the University of Massachusetts, Amherst, she joined the faculty at the University of Pittsburgh in 1987. Her research involves developing theoretical and computational models to capture the behavior of polymeric materials, nanocomposites and multi-component fluids in confined geometries.

Distinguished Service Award
Robert Baudoux

Bob attended Portage Township Schools until March, 1945, when he enlisted in the U.S. Navy at 17, rising to petty officer Third Class. Bob graduated from the University of Pittsburgh on June 14, 1950 with a B.S. In 1968 Bob became active with the Pittsburgh Conference, SSP and SACP, becoming Chairman of the SACP in 1978-79 and Pittsburgh Conference President in 1982. He worked at USS Research in XRD until June 1985. In December 1985 Bob ran the exposition of HPLC '88 in Washington, DC. From 1988-2011, Bob managed the Eastern Analytical Symposium. From 1968-2011, Bob worked with the Pittsburgh Conference, SACP, SSP, and the Pittsburgh Section-ACS, including Advertising Manager of The Crucible newsletter from 1991-2004. Bob also managed the exposition of CERM 1993 and 2003 in Pittsburgh.

Distinguished Service Award
Heather Juzwa

Heather is a Senior Field Sales Engineer at Shimadzu. Heather's service to chemistry began as an undergraduate in 1997 and has continued throughout her career. She served as the Secretary of the ACS Student Affiliates as a senior at the University of Pittsburgh in 2000. In 2008, she was Treasurer of the newly formed Pittsburgh YCC, and she served as Chair of the Pittsburgh Section in 2011. As Chair, Heather designed the new Pittsburgh Section website and has remained the Webmaster ever since. She is also entering her third year on the National ACS Award in Chromatography Committee. Heather feels honored to use her talents to help the section succeed and enjoys being a part of the team.

Pittsburgh Award
Jeffry Madura, Ph.D.

Jeffry is the Lambert F. Minucci Endowed Chair in Engineering and Computational Sciences and Professor in the Department of Chemistry and Biochemistry at Duquesne University. He earned a B.A. from Thiel College, a Ph.D. in Physical Chemistry from Purdue University and was a postdoctoral fellow at the University of Houston. He has published 100+ papers in physical chemistry and received over $6M in external research funding. He was a recipient of a Dreyfus Teacher-Scholar Award, was the chair of the ACS COMP Division and is an ACS Fellow. He is co-author to a textbook titled "General Chemistry: Principles and Modern Applications" as well as a co-author to a physical chemistry solutions manual. He received the Bayer School of Natural and Environmental Sciences and the Duquesne University Presidential Award for Excellence in Scholarship in 2007 and the Bayer School of Natural and Environmental Sciences Award for Excellence in Service in 2004. He is currently co-editor to the Journal of Molecular Graphics and Modelling.

CERM 2014 **Regional Award Recipients**

Congratulations to our recipients. The CERM 2014 Awards Committee is proud to recognize the following deserving individuals for their accomplishments and contributions.

E. Ann Nalley Award for Volunteer Service to the American Chemical Society

Patrick B. Smith, Ph.D.

Patrick received a Ph.D. in Physical Chemistry from Michigan State University and then joined the Dow Chemical Company, where he spent 32 years retiring in 2007 as a Fellow. He served with Cargill Dow Polymers between the years of 1998 and 2000, which commercialized poly(lactic acid). He joined Archer Daniels Midland in 2007 as the team leader for their Metabolix joint venture to commercialize poly(hydroxyalkanoates) and worked on other biobased projects at ADM. He joined the Michigan Molecular Institute in November of 2010. He is a Fellow of the American Chemical Society and has received the Midland Chapter Sigma Xi Award for the Outstanding Research Publication in 1987 and the Midland Chapter ACS Award for Outstanding Achievement and Promotion of the Chemical Sciences in 1998. He is also the recipient of Dow Analytical Science's V. A. Stenger Award in 1984 (Analytical Sciences highest award) and the Dow Michigan R&D Scientists' Award in 1994 for excellence in scientific contribution (Dow Chemical Scientists' highest award).

Regional Award for Excellence in High School Teaching

Erica Posthuma-Adams

Erica has been an educator for fourteen years. She is an active member of the American Chemical Society Division of Chemical Education and is a Lead Contributor for the JCE's ChemEd Xchange. Currently teaching at University High School of Indiana, Erica is an experienced user of the Chemistry Modeling Curriculum, saying that Modeling Instruction provides her with the tools necessary to empower her students and become the teacher she has always wanted to be. Erica recently published an article in the Journal of Chemical Education special AP issue on the topic of using Modeling Instruction to engage students in the practice of science.

Stanley C. Israel Regional Award for Advancing Diversity in the Chemical Sciences

Amanda C Bryant-Friedrich, Ph.D.

Amanda has been an Associate Professor of Medicinal and Biological Chemistry at the University of Toledo in the College of Pharmacy and Pharmaceutical Sciences (CPPS) since 2007. She received her B.S. in Chemistry from North Carolina Central University and a M.S in Chemistry from Duke University. She then left the United States and obtained her Dr. rer. Nat. (PhD) from the Ruprecht Karls Universität, Heidelberg, Germany followed by a Postdoctoral Fellowship in the laboratory of Prof. Bernd Giese at the Universität Basel, Basel, Switzerland. She ultimately became a tenured Associate Professor of Chemistry at Oakland University in Rochester, Michigan before joining the faculty at the University of Toledo where she is also the Director for International Graduate Student Retention and Recruitment for the CPPS.

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45TH CENTRAL REGIONAL MEETING

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Dr. Paul Johnson, Duquesne University – in Memory of Dr. Kurt C. Schreiber

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Toledo Section – a Celebration of Project SEED Luncheon

AB Sciex – At the Forefront of Proteomics Technical Session

ACS Division of Analytical Chemistry

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ACS Division of Chemical Education

ACS Division of Organic Chemistry – COPE Symposium

ACS Small Chemical Business Division (SCHB)

American Elements – Periodic Table Magnets

Duquesne University – Undergraduate Programming

Gentech Scientific – Wine, Wii, and 'Wiches Hors d'oeuvres

Jasco – Undergraduate Network and Resume Luncheon

Perkin Elmer – CERM 2014 Award Banquet Hors d'oeuvres

Shimadzu Scientific Instruments, Inc. – Transportation

St. Francis University – Undergraduate Programming

Waynesburg University – Undergraduate Programming

Waters Corporation – Molecular Recognition of and by Nucleic Acids Technical Session

Society for Analytical Chemists of Pittsburgh

Promoting Science Education in Pittsburgh and Nationwide

The SACP is dedicated to the education of the membership, of the community, and of the future scientists in our schools through:

- Monthly technical talks and meetings
- Workshops and symposia for professionals and community members
- Internships, scholarships, and grants to scientists from the undergraduate level to assistant professors
- Science fairs and competitions for middle and high school students
- Participating in and funding science outreach events around the region

Visit our booth at the CERM 2014 Exposition or our website, www.sacp.org, for more information on our awards, grants, and programing.

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Dedicated to the Promotion of Science Education

Spectroscopy Society of Pittsburgh

The SSP is a nonprofit, professional organization dedicated to educating members of the scientific community, students and teachers about spectroscopy and science.

We achieve this goal by:

- Hosting workshops, symposia, and monthly technical meetings
- Participating in science festivals
- Financially supporting community related activities and affiliated societies
- Awarding grants, scholarships, and endowments

To learn more about our awards, grants, and programs - or how to become a member – visit our booth in the CERM 2014 exposition or our website at www.ssp-pgh.org

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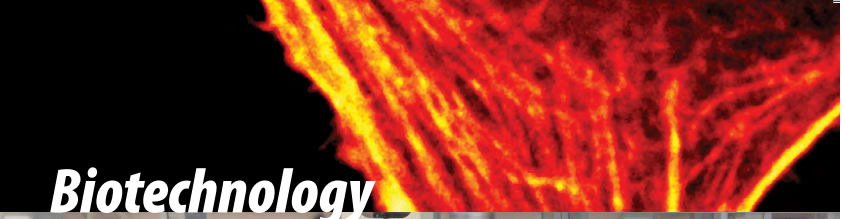

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*The Economist, 2014

COFFEE BREAKS	TECHNICAL PROGRAM	WORKSHOPS	LUNCHEONS	EXHIBITION	GRADUATE SCHOOL AND RECRUITMENT FAIR	SPECIAL EVENTS

WEDNESDAY, OCTOBER 29	8:00 am–12:00 pm	9:00 am–10:00 am	9:00 am–5:00 pm	10:20 am-12:00 pm	12:00 pm-1:20 pm	1:30 pm-5:00 pm	3:00 pm-3:30 pm	5:00 pm-7:00 pm	7:00 pm-9:00 pm	7:30 pm-9:15 pm
Allegheny						**CERM009:** Solid-State Materials (Part I)				
Carnegie						**CERM040:** Fresh Faces in (Bio)Inorganic Chemistry				
Interstate						**CERM001:** Electronic Materials for Device Applications: Energy Transfer, Charge Separation, and Morphology				
Junior Ballroom	Coffee		Vendor Exhibition	**CERM035a:** Kickoff Poster (Hallway)					Wine, Wii, and 'Wiches	
Monongahela						**CERM003:** Electricity: Generation, Storage, and Transmission				
Offsite/Other							Coffee Break (Foyer 2 and outside Westinghouse and Foster)			Rum Science – Pittsburgh Style
Ohio						**CERM013:** Synthetic Organic Methods and Total Synthesis				
PPG						**CERM006**: Surface Chemistry: Polymer Science and Biointerfaces				
Salk						**CERM004**: At the Forefront of Proteomics				
Salons D, E		Plenary - Smith						**CERM035b:** Sci-Mix Poster 1		
Starzl						**CERM042:** General Session				
Thompson					YCC Luncheon					
Westinghouse	ACS Career: Finding your Pathway					ACS Career: Resume Review				

THURSDAY, OCTOBER 30	8:00am–12:00pm	8:30am–11:30am	9:00 am – 5:00 pm	9:30 am-11:30 am	9:40 am – 10:00 am	10:00 am – 3:00 pm	11:40 am – 12:50 pm	1:00 pm – 2:00 pm	1:00 pm – 5:00 pm	2:20 pm – 3:20 pm	3:30 pm – 3:50 pm	2:20 pm – 5:00 pm	4:00 pm-5:00 pm	4:00 pm – 6:00 pm	5:00 pm – 9:00 pm
Allegheny		**CERM009b:** Solid-State Materials (Part II)										**CERM009c:** Solid-State Materials (Part III)			
Duquesne							WCC Luncheon								
Foster		**CERM011:** Diversity in the Chemical Sciences (Part I)										**CERM011b:** Diversity in the Chemical Sciences (Part II)			
Frick		**CERM015:** Green Chemistry Success Stories										**CERM018:** Careers Related to Chemical Education			
Interstate		**CERM042b:** General Session (Part II)										**CERM042c:** General Session (Part III)			
Junior Ballroom			Vendor Exhibition											Sci-Mix Poster 2 (Hallway)	
Linc				Waters Corporation Workshop						Gateway Analytical Workshop			Jasco, Inc. Workshop		

meeting at-a-glance

COFFEE BREAKS	TECHNICAL PROGRAM	WORKSHOPS	LUNCHEONS	EXHIBITION	GRADUATE SCHOOL AND RECRUITMENT FAIR	SPECIAL EVENTS

THURSDAY, OCTOBER 30	8:00am–12:00pm	8:30am–11:30am	9:00 am – 5:00 pm	9:30 am-11:30 am	9:40 am – 10:00 am	10:00 am – 3:00 pm	11:40 am – 12:50 pm	1:00 pm – 2:00 pm	1:00 pm – 5:00 pm	2:20 pm – 3:20 pm	3:30 pm – 3:50 pm	2:20 pm – 5:00 pm	4:00 pm-5:00 pm	4:00 pm – 6:00 pm	5:00 pm – 9:00 pm
Monongahela		**CERM010:** Oil, Gas, and chemical from Shale Formations (Part I)										**CERM010b:** Oil, Gas, and chemical from Shale Formations (Part II)			
Offsite/Other					Coffee Break (Foyer 2 and outside Westinghouse and Foster)	MEET-U Energy Truck (East Parking Lot)					Coffee Break (Foyer 2 and outside Westinghouse and Foster)				
Ohio		**CERM008:** Computational Modeling in Energy Research										**CERM005:** Cope Symposium in Honor of Jeff Johnston			
PPG		**CERM007:** Nucleic Acid Based Materials (Part I)										**CERM007b:** Nucleic Acid Based Materials (Part II)			
Salk		**CERM012:** Organic Process Research and Development: Utilization and Recovery of Precious Metal Catalysts													
Salons D, E								Plenary Wysocki							CERM 2014 Awards Banquet
Westinghouse	ACS Leadership: Fostering Innovation								ACS Leadership: Leading Change						

FRIDAY, OCTOBER 31	8:30am–11:30am	9:00am–5:00pm	9:40am–10:00am	10:00am–11:30am	11:30am–12:50pm	12:00pm–1:30pm	1:00pm– 2:00pm	2:00pm– 3:00pm	2:00pm-3:30pm	2:20pm–5:00pm	3:30 pm–3:50pm	5:30pm–7:30pm	5:30pm-10:20pm
Allegheny	**CERM009d:** Solid-State Materials (Part IV)									**CERM033:** Culinary Chemistry: Bridging Innovations in Food and Science			
Duquesne					Undergraduate Network and Resume Luncheon				Undergraduate Workshop: How to be an Award Winning Student Section				
Foster	**CERM026:** Entrepreneurs' Tool Kit: Resources and True Stories (Part I)									**CERM031:** Entrepreneurs' Tool Kit: Resources and True Stories (Part II)			
Interstate	**CERM025:** Innovations in Undergraduate Chemistry Education									**CERM030:** Beyond the Cookbook: Moving Undergraduate Laboratory Courses Forward			

COFFEE BREAKS	TECHNICAL PROGRAM	WORKSHOPS	LUNCHEONS	EXHIBITION	GRADUATE SCHOOL AND RECRUITMENT FAIR	SPECIAL EVENTS

FRIDAY, OCTOBER 31	8:30am–11:30am	9:00am–5:00pm	9:40am–10:00am	10:00am–11:30am	11:30am–12:50pm	12:00pm–1:30pm	1:00pm– 2:00pm	2:00pm– 3:00pm	2:00pm-3:30pm	2:20pm–5:00pm	3:30 pm–3:50pm	5:30pm–7:30pm	5:30pm-10:20pm
Junior Ballroom		Graduate School and Recruitment Fair						Ice Cream Social with ACS Governance					
Monongahela	**CERM023:** The Science of CO2 Capture in Energy Production (Part I)									**CERM023b:** The Science of CO2 Capture in Energy Production (Part II)			
Offsite/Other			Coffee Break (Foyer 2 and outside Westinghouse and Foster)								Coffee Break (Foyer 2 and outside Westinghouse and Foster)	Undergraduate Member Social Hour and Tailgate (Courtyard), Duquesne Room if inclement weather)	Rum Science – Pittsburgh Style and a View
Ohio	**CERM027:** Analytical Chemistry in the Central Region (Part I)									**CERM027b:** Analytical Chemistry in the Central Region (Part II)			
PPG	**CERM022:** Molecular Recognition of and by Nucleic Acids									**CERM032:** Spectroscopic Studies of Protein Structure and (Mal)Function			
Salk	**CERM042d:** General Session (Part IV)												
Salons D, E				Undergraduate Poster Session			Plenary Skrabalak						
Thompson						ACS Steering Committee Luncheon (by invitation only)							
Westinghouse	**CERM021:** Surface and Microscopic Characterization of Manufactured Nanomaterlals (Part I)									**CERM021b:** Surface and Microscopic Characterization of Manufactured Nanomaterlals (Part II)			

SATURDAY, NOVEMBER 1	7:15 am-8:15 am	8:30 am–9:20am	9:20am–9:50am	9:50am-10:00am	10:00am–11:30am	10:00 am	10:30 am	11:30am–1:30pm	1:30pm–2:30pm	1:30 pm	2:30 pm–3:00pm	3:00pm–3:10pm	3:10pm–5:10 pm
Salon 2	~~Teacher Breakfast (by invitation only)~~												
Offsite/Other				Coffee Break (outside Salons 3, 4)		Carrie Blast Furnace Tour	'Burgh, Bits & Bites Food Tour			'Burgh, Bits & Bites Food Tour		Coffee Break (outside Salons 3, 4)	
Salon A		Teacher Programming	Vernier Software & Technology Workshop		Teacher Programming			Celebration of Project SEED Poster Session & Luncheon	Teacher Programming		Vernier Software & Technology Workshop		Teacher Programming

GOVERNANCE AT CERM 2014

Welcome to our esteemed guests.

George Bodner
Director. District II

George Bodner is the Arthur E. Kelly Distinguished Professor of Chemistry, Education and Engineering at Purdue University. He earned his Bachelors Degree at the State University of New York, Buffalo in 1969 and his Ph.D. at Indiana University in 1972. He has been a member of the American Chemical Society since 1969.

Bill Carroll
Director-At-Large

Bill Carroll is a vice president of Occidental Chemical Corp. He earned a Bachelors degree at DePauw University in 1973, Masters Degree from Tulane University in 1975, and Ph.D. from Indiana University in 1978. He has been a member of the American Chemical Society since 1973.

Thomas Gilbert
Director, District I

Tom Gilbert is a chemistry professor at Northeastern University where he also served as Academic Director of Graduate Programs in Biotechnology and as Acting Dean of the School of Education. He received his B.S. from Clarkson College of Technology (now Clarkson University) in 1968, and his Ph.D. from MIT in 1971. He joined the Northeastern faculty in 1981 after 10 years with the Research Department of the New England Aquarium in Boston. He has been an ACS member since 1968 and an ACS Councilor since 1990.

STEERING COMMITTEE LUNCHEON

The Central Regional Meeting Steering Committee will have a business luncheon on Friday, October 31, 2014 in the Thompson Room from 12:00 pm – 1:30 pm.

This luncheon is reserved for members of the steering committee and their invited guests only.

Ice Cream Social with ACS Governance

MEET the members of the ACS Governance in attendance about the state of the society and its views.

NETWORK with your peers and our exhibiting institutions.

INDULGE in delicious ice cream and candy.

Friday, October 31, 2014
2:00 pm – 3:00 pm
Junior Ballroom

GOVERNANCE AT CERM 2014 >>>

Welcome to our esteemed guests.

Rigoberto Hernandez
Director, District IV

Rigoberto Hernandez is a Professor in the School of Chemistry and Biochemistry at Georgia Institute of Technology. He earned his B.S.E. degree in chemical engineering and mathematics at Princeton University in 1989, and his Ph.D. in chemistry at the University of California, Berkeley, in 1993. He has been a member of the American Chemical Society since 1992.

Kathleen Schulz
Director-At-Large

Kathleen M. Schulz is the President of Business Results Inc. She earned her Bachelors degree at Eastern New Mexico University in 1964, and Ph.D. at the University of Missouri in 1973. She has been a member of the American Chemical Society since 1964.

Ice Cream Social with ACS Governance

MEET the members of the ACS Governance in attendance about the state of the society and its views. **NETWORK** with your peers and our exhibiting institutions. **INDULGE** in delicious ice cream and candy.

Friday, October 31, 2014
2:00 pm – 3:00 pm
Junior Ballroom

2014 ACS Central Regional Meeting

www.acscerm2014.org

The 45th Central Regional Meeting

Oct. 29 – Nov. 1, 2014

Doubletree by Hilton
Pittsburgh - Green Tree

Bridging Chemistry and Innovation
CERM 2014

CENTRAL REGIONAL MEETING CAREER WORKSHOPS

Wednesday, October 29 - WESTINGHOUSE ROOM

Finding Your Pathway

8:00 AM – 12:00 PM

Learn about the four main career pathways available to chemical professionals: Higher education, industry, government, and entrepreneurship. To help you choose which one is right for you, you'll learn about the careers, the job market, and the hiring trends in each pathway. This workshop is ideal for recent grads, grad students, and experienced professionals considering a career change. The workshop allows time for you to inventory your own values, interests, background, strengths, and weaknesses so that you can select which career pathway you'd like to explore in detail.

Individual Resume Reviews and Consultation

1:30 PM – 5:00 PM

During your one-on-one personal consultation, have your resume reviewed or ask career related questions. What documents are included in my marketing package? What is the difference between a CV and a resume? When should I use a CV? When should I use a resume? Should I submit a cover letter with my resume? What should I put in my resume? What should I, and what shouldn't I, put in my cover letter? What is the purpose of the interview? What kinds of questions will I be asked during the interview? Should I ask questions during the interview? What should I say if I am asked about salary requirements? Can I negotiate my offer?

FOR MORE INFORMATION CONTACT

Joseph Jolson
ACS Career Workshop Chair
joe@customclientsolutions.net

2014 ACS Central Regional Meeting

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BRIDGING CHEMISTRY AND INNOVATION
CERM 2014

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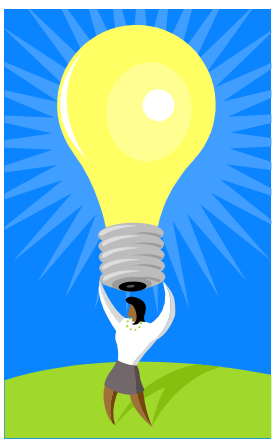
ACS Leadership Institute

Thursday, October 30, 2014, Westinghouse Room

Join us to learn essential skills and strengthen your competitive edge in today's global economy. The first 9 people who register are free with additional scholarships available!



Fostering Innovation

8:00 AM – 12:00 PM

The very basis of Chemistry, your profession, and ACS challenge you to advance your thinking, identify new solutions, and design new approaches continuously. In this four-hour course you will learn that innovation doesn't happen by chance but can be managed. The understanding and tools you gain will help you learn how to tap into your own innovation style as well as learn how to stimulate innovative thinking for different circumstances.

Leading Change

1:00 PM – 5:00 PM

Almost any initiative today in the workplace involves change and can often meet resistance. This four-hour course provides leaders with a step-wise process to lead change and guide volunteers more effectively through the change process to achieve greater results and efficiency. Participants will gain a skill that can be used in many common workplace and professional situations.

For more information contact: Julianne Wolfe, Leadership Development Chair, jwolfe@rjleegroup.com

Waters

THE SCIENCE OF WHAT'S POSSIBLE.™

Recent years have witnessed an exponential increase in the adoption rate of Supercritical Fluid Chromatography (SFC) and Supercritical Fluid Extraction (SFE) in several areas of industry. The intrinsic low viscosity and high diffusivity of supercritical CO_2 renders SFC a faster, higher efficiency form of chromatography. SFC readily lends itself as a complementary alternative to reversed phase LC because of its normal-phase-like separation mechanism. The low viscosity and high diffusivity also play a large role in the ability to extract compounds from a semi-solid to solid matrices in a selective fashion. The use of supercritical CO_2 in both techniques significantly reduces the usage of organic solvents, making each one a less expensive, green technology. In this presentation the fundamentals of supercritical fluids and SFC (both preparative and analytical) as well as an overview of SFE will be illustrated. Several examples of cost reduction, solvent reduction and overall increased efficiency will be reviewed.

Gateway® ANALYTICAL

Unknown materials or foreign particulate matter are commonly-encountered nuisances in the chemical/ industrial manufacturing and pharmaceutical industries. These materials can range from commonly encountered fibers which are ubiquitous to the environment to unique materials such as drug/excipient mixtures, thermally degraded materials, complex polymers and metal alloys. Remediation of uch materials requires the use of multi-analytical methods and specialized micro-preparation techniques which can provide unique and often times complimentary elemental and chemical information in the characterization of such materials. For the purpose of this session, common analytical methods which will be discussed including optical and polarized light microscopy, infrared (IR) and Raman spectroscopy, scanning electron microscopy – energy dispersive X-ray spectroscopy (SEM-EDS), laser-induced breakdown spectroscopy (LIBS) and Raman chemical imaging (RCI). Gateway Analytical is a full-service analytical testing laboratory offers a wide array of standard and advanced testing techniques for applications in pharmaceutical testing, product contamination and failure analysis, materials characterization and criminal forensic investigations. This session will provide an overview of each application area and how a multi-analytical approach is essential to fully characterizing unknown materials or foreign particulate matter.

JASCO

Whether one is new to fluorescence or has some practical lab experience, this short tutorial will present an overview of fundamental fluorescence theory to highlight how to best optimize data collection and minimize unwanted interferences. A review of the processes of absorption, emission, and scattering will lay the foundation for identifying key design features of the instrumentation and parameters that can be used for optimization of the fluorescence signal. Scattering and absorption interferences play an important role in the quality of fluorescence data, so recognizing and minimizing Rayleigh and Raman scattering, inner-filtering effects, photobleaching, etc. is critical to obtaining good qualitative and quantitative data with confidence. Practical experimental and instrumental parameter considerations will be discussed in light of how to minimize common mistakes and unwanted interferences and maximize the fluorescence signal.

Vernier

This 30 minute demonstration will focus on the use of the Vernier Mini GC Plus gas chromatograph to investigate a forensics/CSI scenario. We will show how the Mini GC Plus measures and analyzes the components in a mixture of liquids.

Vernier

In this 30 minute presentation, you will have an opportunity to collect data wirelessly with Vernier sensors and the LabQuest 2 data collection interface. We will use Data Share, a free wi-fi browser option, to display collected sensor readings into any smart device. In addition, we will demonstrate wireless data collection with iPads and Vernier sensors.

Vendor Seminars

Waters Corporation
9:30 am – 11:30 am
Linc Room
Tom DePhillipo
The SFC Advantage

Gateway Analytical
2:20 pm – 3:20 pm
Linc Room
Antonio Scatena, Ph.D.
Multi-Analytical Approach to Materials and Foreign Particulate Matter Characterization

Jasco
4:00 pm – 5:00 pm
Linc Room
Sherry Hemmingsen, Ph.D.
Fluorescence Fundamentals and Foibles: Getting the Most Out of Your Data

Vernier Software and Technology
9:20 am – 9:50 am
Salon A
Jack Randall, Ph.D.
Vernier Mini GC Plus Demonstration

Vernier Software and Technology
2:30 pm – 3:00 pm
Salon A
Jack Randall, Ph.D.
Wireless Data Collection with Vernier Sensors

2014 ACS Central Regional Meeting

YCC Luncheon

Oct 29, 2014
12:00-1:20
Thompson Room

During the event you will have the chance to listen to the lecture presented by Dr. M. Mónica Giusti.

Later you can join us for the lunch.

YCC Luncheon is a part of CERM and the lunch is sponsored by YCC

Doubletree by Hilton
Pittsburgh - Green Tree

Visit **pghycc.org** for more details

Keynote Speaker

M. Mónica Giusti

Is an Associate Professor and the Graduate Studies Chair at the Food Science and Technology Department, The Ohio State University, and a visiting faculty of the Facultad de Industrias Alimentarias, Universidad Nacional Agraria, La Molina, Peru. Her research is focused on the chemistry and functionality of flavonoids, with emphasis on anthocyanins. Together with her collaborators, her lab has investigated different aspects of polyphenols including their incidence and concentration in plants, stability and interactions with food matrices, novel analytical procedures, and the bioavailability, bio-transformations and potential bioactivity of these wonderful plant pigments.

For her innovative work on anthocyanins and their food applications, she was named the 2010 Ohio Agricultural Research and Development Center Director's Innovator of the Year, the 2011 TechColumbus Outstanding Woman in Technology, and the 2013 OSU Early Career Innovator of the Year. Dr. Giusti has been granted 2 patents on the chemoprotective effects of anthocyanins and their isolation from plant materials, with 5 additional patents pending. Her patented technology for anthocyanin isolation was the foundation for the start-up company Anthocyantific, LCC.

Dr. Giusti is a member of the American Chemical Society and the Institute of Food Technologists (IFT), where she served in the executive board of the IFT Fruit and Vegetable division and as officer for the Ohio Valley section of the IFT. Before joining The Ohio State University, Dr. Giusti was a faculty member at the Department of Nutrition and Food Science at the University of Maryland. Dr. Giusti, born in Lima, Peru, received a Food Engineer degree from the Universidad Nacional Agraria, La Molina, Peru and Master's and Doctorate degrees in Food Science from Oregon State University, Corvallis, Oregon.

2014 ACS Central Regional Meeting

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BRIDGING CHEMISTRY AND INNOVATION
CERM 2014

The 45th Central Regional Meeting

Oct. 29 – Nov. 1, 2014

Doubletree by Hilton
Pittsburgh - Green Tree

WCC Luncheon

Thursday, October 30, 2014

11:40 AM - 12:50 PM

Duqesne Room

Featuring Dr. Kathleen M. Schulz

ACS BOARD OF DIRECTORS

Kathleen Schulz is president of Business Results, Inc., a consulting company that provides coaching, consulting and facilitation to help leaders get results. She is an ACS Fellow who currently serves on the ACS Board of Directors, where she chairs the ACS Board Committee on Public Affairs and Public Relations. Kathleen is a Co-Founder of the ACS Leadership Development System, and is certified to facilitate six ACS leadership courses and the Strategic Planning Retreat.

Kathleen earned her B.S. summa cum laude from Eastern New Mexico University, and holds a Ph.D. in analytical chemistry from the University of Missouri-Columbia. She has worked in all sectors of the chemical enterprise: academe, industry/government contracting, not-for-profit and small business. She has worked for companies including Hewlett-Packard, Lockheed-Martin and Midwest Research Institute. In fifty years as an ACS member, Kathleen has been active at all levels in ACS: local sections, technical divisions, national committees and task forces. She has been an ACS Tour and Webinar Speaker, and served on recent ACS Presidential task forces and working groups on Innovation and Climate Science.

For more information contact:

Michelle Ward

Pittsburgh WCC Chair

muscat@pitt.edu

2014 ACS Central Regional Meeting

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BRIDGING CHEMISTRY AND INNOVATION
CERM 2014

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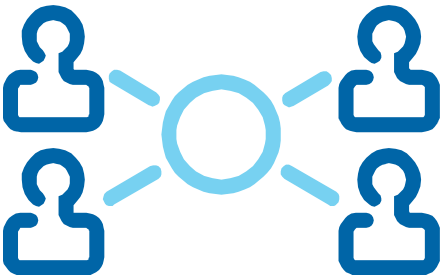
Undergraduate Student Networking Luncheon



October 31 - Duquesne Room

11:30 AM - 1:00 PM

Featuring Dr. Joseph Jolson

Since 2004, when he became chair of the ACS-Pittsburgh Section employment committee, Dr. Joseph Jolson made changes to the Job Searching for Chemical Professionals workshop that quadrupled annual attendance. He has been an ACS National career counselor since 2008, has chaired the SACP employment committee since 2010, and is employment committee chair for the 2014 CERM meeting.

Dr Jolson founded Custom Client Solutions in 2004 to provide battery, gas detection, and respiratory protection services to clients. From 2000 – 2004, he oversaw the development of emergency-breathing devices and air quality monitors for the CSE Corporation. From 1979 – 2000, he analyzed detection technologies for potential use in emerging markets; facilitated qualification testing and applications support for gas detectors; led teams that developed gas sensors, gas detectors, and lithium batteries; and set up a specialty battery facility for the Mine Safety Appliances Company, Inc. Dr. Jolson has 11 U.S. Patents, 13 publications, and has given 27 presentations. He has a Ph.D. in analytical chemistry from SUNY at Buffalo.

For more information contact:

Evonne Baldauff

EBALDAUF@WAYNESBURG.EDU

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Project SEED Luncheon

Saturday, November 1, 2014 - Salons 3, 4

11:30 AM to 1:30 PM

An informal lunch to promote the great work of Project SEED within the central region.

The luncheon will include informal presentations on the programming of Project SEED from program coordinators and advisors. Students who have participated in Project SEED will be present their work in a poster session. Some former participants will also be discussing the impact that Project SEED has had on their scientific career path as well as their personal successes.

Project SEED was established in 1968 to help economically disadvantaged high school students expand their education and career outlook. The program provides opportunities for students who historically lack exposure to scientific careers to spend a summer conducting hands-on research with a scientist in academic, industry, and government research laboratories. Students receive a fellowship award for their efforts and a chance to receive a SEED college scholarship.

For more information contact:
Mackenzie Speer
Pittsburgh ACS Chair-elect
mackenzie.speer@reaxis.com

Program Events

DoubleTree by Hilton, Pittsburgh—Green Tree

9:00 am — 5:00 pm **Graduate School and Recruitment Fair**
Junior Ballroom

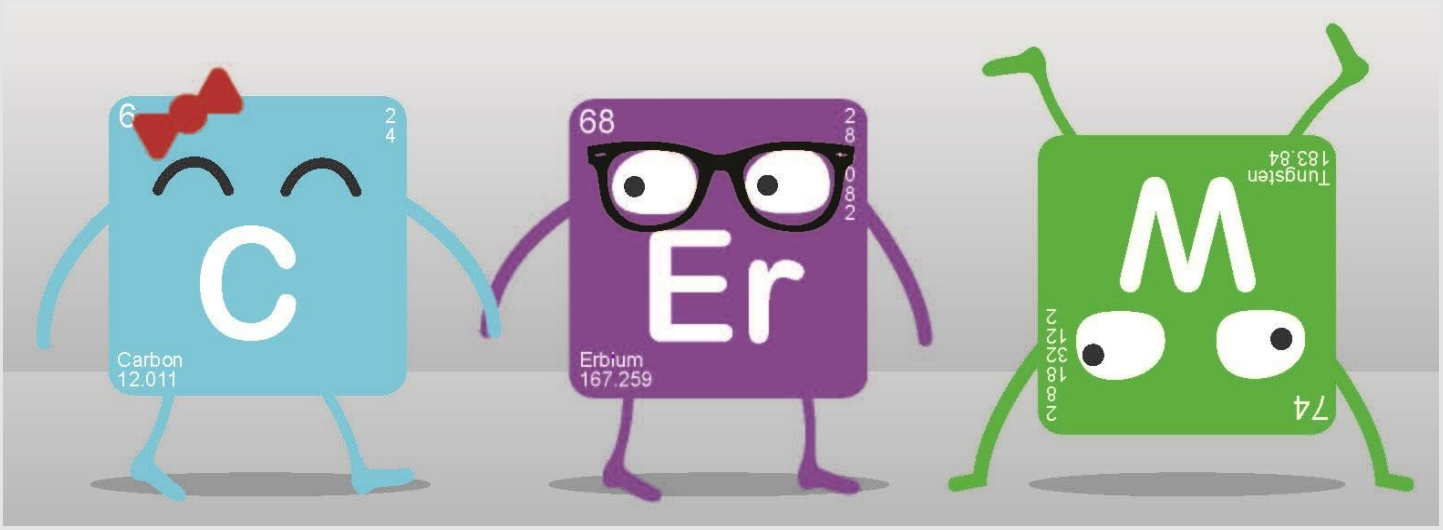
10:00 am — 11:30 am **Undergraduate Poster Session**
Salons D, E

11:30 am — 12:45 pm **Undergraduate Network and Resume Luncheon**
Duquesne Room
Pittsburgh ACS member, Dr. Joseph Jolson, Ph.D., will lead a discussion on current trends in resumes, networking and hiring. Participants will have the opportunity to network with area professionals.

1:00 pm — 2:00 pm **Keynote Speaker**
Salons D, E
Dr. Sara E. Skrabalak, Assistant Professor of Chemistry at IU Bloomington, will discuss her research in nanomaterial design and synthesis.

2:00 pm — 3:30 pm **Workshop: How to be an Award-Winning Student Chapter**
Duquesne Room
Local chapters will lead a forum to share ideas to increase the effectiveness of chemistry outreach in the region.

5:30 pm — 7:30 pm **Undergraduate Member Social Hour and Tailgate**
Patio (Duquesne Room if Inclement Weather)



@cermundergrad14 facebook.com/CERMUndergrad14

Teacher Programming at CERM 2014

SATURDAY, NOVEMBER 1, 2014 • 8:30 AM – 5:10 PM • SALON A • DOUBLE TREE BY HILTON GREEN TREE

Listen to engaging talks by past Excellence Award winners

8:30 am – 8:50 am

Introduction/Award Ceremony/2014 Excellence Presentation

8:50 am – 9:20 am

Leslie McSparrin, Indiana Academy for Science, Mathematics, and Humanities, Muncie, IN, Penn Ohio Border, 2005. *"Using the Synthesis and Characterization of potassium trisoralatoferrate(III) as a Culminating Authentic Assessment in AP Chemistry"*

9:20 am – 9:50 am

Jack Randall, Director of Chemistry, Vernier Software & Technology. *" Vernier Mini GC Plus Demonstration"*

9:50 am – 10:00

Coffee Break

10:00 am – 10:30 am

Laura E. Slocum, Heathwood Hall Episcopal School, Columbia, SC, Indiana, 2012. *"Designing and Teaching Outside the 'Traditional' Box"*

10:30 am – 11:00 am

Elizabeth (Betty) Dabrowski, retired Magnificat High School, Rocky River, OH, Cleveland, 2013. *"Chemistry Outside the Textbook Covers"*

11:00 am – 11:30 am

Linda Ford, Seven Hills High School, Cincinnati, OH, Cincinnati, 2000 (2003 James Conant Award Winner). *"Evolution of a Chemistry Teacher"*

11:30 am – 1:30 pm

A Celebration of Project SEED Luncheon

SEED Poster Session

SEED Alumni Presentations

1:30 pm – 2:00 pm

Kathy Kitzmann, Mercy High School, Farmington Hills, MI, Detroit, 1997 (2014 James Conant Award Winner). *"Kathy's Favorite (Chemistry) Things"*

2:00 pm – 2:30 pm

Judith M. Lachvayder, retired St. Ignatius High School, Cleveland, OH, Cleveland, 2011. *"Sherlock Holmes and Chemistry"*

2:30 pm – 3:00 pm

Jack Randall, Director of Chemistry, Vernier Software & Technology. *"Wireless Data Collection with Vernier Sensors"*

3:00 pm – 3:10 pm

Coffee Break

3:10 pm – 3:40 pm

William E. Snyder, Mentor for 'College in the High School' Chemistry Teachers, Youngstown State University, retired, Poland Seminary High School, Poland, OH, Penn Ohio Border, 2009. *"How Do You Know What You Know?"*

3:40 pm – 4:10 pm

Rachel Badanowski, Wayne State University & Michigan State University, retired Southfield High School, Southfield, MI, Detroit, 2007. *"Time of Useful Consciousness in Chemistry"*

4:10 pm – 4:40 pm

Bonnie Buddendeck, Centerville High School, Centerville, Dayton, OH 1996. *"Chemistry is Just Too Hard"*

4:40 pm – 5:10 pm

Kelly Weston, Seneca Valley Senior High School, Harmony, PA, *"A STARs (Siemens Teachers as Research Fellows) Experience – Combining Research and Professional Development in STEM"*

2014 ACS Central Regional Meeting

CERM Social Events & Activities

Wednesday, October 29

Rum Science - Pittsburgh Style - 7:30-9:15 pm

Tickets are $45.00 and include transportation, tour, & delicious rum samplings. Learn a little rum science the old-fashioned way—through a tasty sampling of rum and a tour of Pittsburgh's only rum distillery in the city's Historic Strip District! Learn the story behind Maggie's Farm Rum Distillery—the first manufacturer of craft rum since Colonial Times! Afterwards, grab dinner on your own in the historic neighborhood!

Wii, Wine, and 'Wiches - 7:00-9:00 pm

This kickoff reception is the place to be with raffle prizes and light hors d'oeuvres. Show our vendors your competitive side by challenging them in the Wii tournament. There will be a cash bar and raffle prizes provided by our vendors. A grand prize of a free overnight stay at the DoubleTree will be raffled away. Tickets are $12.00 and include 10 raffle tickets.

Friday, October 31

Rum Science & a View - 5:30-10:20 pm

Take a taste and a ride as tonight's science lesson includes Maggie's Farm Rum Tour & tasting and then a ride up the historic Duquesne Incline where visitors will get a behind-the-scenes tour of the incline. Afterward, explore Station Square, the former Pittsburgh & Lake Erie railroad complex! Enjoy dinner and nightlife on your own with choices that include Pittsburgh's Hard Rock Café, Bar Louie, Buca di Beppo, Melting Pot, Joe's Crab Shack and many more! Tickets are $55.00 and include transportation, tours, and rum samplings!

Saturday, November 1

'Burgh, Bits & Bites Food Tour - 10:30 am OR 1:30 pm

The Strip District Market tour is a late morning/early afternoon tour featuring a behind-the-counter look at a variety of eateries in Pittsburgh's historic market district. This tour links local history with the eating establishments peppered along Penn Avenue with taste samples from around the world including Italian pastries, Mediterranean and Polish specialties, European meats and French bread. CERM attendees receive 20% off ticket prices. See the CERM website for more details about the discount!

Carrie Blast Furnace Tour - 10:00 am

Learn about Pittsburgh history as the former steel-making capital of the world. The Carrie Blast Furnace tour is a 2-hour retired steelworker guided tour of the only blast furnace left in Pittsburgh. People from all over the world come to visit this historic location! CERM 2014 members and guests will receive a 20% discount on the Carrie Blast Furnace Tour. See the CERM website for more information about the discount! Transportation is not included.

More information and how to register can be found at www.acscerm2014.org.

Featuring presentations of

Section Awards

Greater Pittsburgh WCC Award for Encouraging Women into the Chemical Sciences
Greater Pittsburgh WCC Award for Career Excellence in the Chemical Sciences
Distinguished Service Award
Pittsburgh Award

Regional Awards

Current and Former Section Chairs
60 Year Members
50 Year Members
Regional Award for Excellence in High School Teaching
E. Ann Nalley Award for Volunteer Service to the American Chemical Society
Stanley C. Israel Regional Award for Advancing Diversity in the Chemical Sciences

CERM 2014 *Awards Banquet*

Thursday, October 30
Salons D, E

Cash Bar 5:00 pm
Dinner: 6:00 pm
Awards 7:00 pm

MEET-U wants to MEET YOU in the parking lot

As part of our energy programming and in honor of one of our National Historic Chemical Landmarks, we welcome the MEET-U Truck to CERM

The Friends of Drake Well, Inc.'s Mobile Energy Education Training Unit (MEET-U) spreads awareness of energy creation, development and utilization through a partnership with the Friends of Drake Well and Drake Well Museum by educating school children and the public on the historic and modern uses of energy in the hope they will improve the future of energy consumption.

Since opening in the summer of 2009, over 100,000 people have visited the educational exhibits in MEET-U in a number of cities, towns, fairs and other events in Pennsylvania, New York, and Ohio. In 2013 over 30,000 people saw MEET-U. Many of those who have seen the trailer are students.

WHEN: Thursday, October 30, 2014
10:00 am – 3:00 pm
WHAT: Mobile Energy Museum
WHERE: East Parking Lot of the Double Tree

We challenge the students to come up with new and creative ideas for energy independence. We stress the value of education in being able to compete in an energy driven workforce. It is this generation that will discover new ways of harnessing energy. While those who visit the trailer learn about their oil and gas heritage, they are also encouraged to think about ways to change the future of energy consumption to minimize the adverse impacts on the environment.

"We challenge students to come up with new and creative ideas for energy independence."

During the winter of 2011-2012 MEET-U developed and implemented the MEET-U in the Classroom. This program travels into local classrooms targeting 4th graders and meets state and national standards in social studies, economics, and science. We currently have a menu of options for the teachers to choose from, so they are able to pick a lesson that best fits their needs. They are able to choose from programs based on Social Studies, Science, and Energy.

BRIDGING CHEMISTRY AND INNOVATION
CERM 2014

SPEAKER INSTRUCTIONS

GENERAL INFORMATION

All speakers and poster presenters must register and pay the appropriate registration fee to attend the meeting. Invited speakers should contact their symposium organizer to clarify the terms of their invitation. All presenters should prepare for their presentation by verifying the following details: the status of your abstract at abstracts.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. If you need to withdraw your presentation, please send a withdrawal notice to pacs@acs.org and contact your symposium organizer immediately.

ORAL SESSIONS

Speakers should arrive in their presentation rooms at least 15 minutes before their scheduled session. Each technical session meeting room will be equipped with the following: LCD projector, screen, podium, laser pointer, and timer. Speakers need to provide their own laptops and necessary connection adapters or arrange for specialty equipment directly with their symposium organizer. Speakers are asked to bring their presentation on a jump drive as well.

GENERAL AND SCI-MIX POSTER SESSIONS

Posters should be 3'x4.' Posters will be mounted to a foam board resting on an easel. Presenters must mount their poster 30 minutes 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 immediately following the poster session.

UNDERGRADUATE POSTER SESSION

Undergraduate presenters are strongly encouraged to place their posters by 9:00 am on Friday. Posters must be placed by 9:45 am. Posters should be 3'x4.' Posters will be mounted to a foam board resting on an easel. 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. All posters must remain up until the session ends and then immediately removed.

PROJECT SEED ORAL AND POSTER PRESENTATIONS

Project SEED Presenters are strongly encouraged to arrive at the 10:00 am break on Saturday to place their poster. Posters must be placed by 11:00 am and done so quietly so as not to disrupt the teacher programming that will be in progress. Posters should be 3'x4.' Posters will be mounted to a foam board resting on an easel. 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. A laptop with Microsoft Windows® will be provided for oral presenters.

2014 ACS Central Regional Meeting

October 29 - November 1, 2014

Pittsburgh, Pennsylvania

Doubletree by Hilton Green Tree Hotel

A. Michael and M. Ward, *Program Chairs*

T E C H N I C A L P R O G R A M

WEDNESDAY MORNING

Plenary I
Salons D, E

M. Ward, A. Michael, *Organizers, Presiding*

9:00 1. Smart molecules for imaging, therapy, and health. **B. D. Smith**

Kickoff Poster Session
Junior Ballroom Hallway

M. Ward, A. Michael, *Organizers*

10:20 - 12:00

2. Synthesizing cyanine binding ligands with high fidelity to g-quadruplex DNA in pursuit of novel chemotherapeutics. **E. A. Owens**, R. Nanjunda, E. M. Stroeva, H. T. Huynh, M. W. Germann, W. Wilson, M. M. Henary

3. Human waste markers in an agricultural watershed: How much do septic systems contribute to nutrient loading? **C. E. Spiese**, J. M. Berry, M. N. Bowling, A. G. Thayer, L. M. Streacker, B. O. Boulanger

4. Structure-activity relationship of ruthenium complexes to inhibit breast cancer growth and metastasis. **E. T. Bell-Loncella**, M. L. Purazo, Y. Lu, J. Iida, C. D. Shriver

5. Using fluorine NMR to study HIV-1 reverse transcriptase. **N. G. Sharaf**, R. Ishima, A. Gronenborn

6. Electronic notebooks in the teaching and research laboratory. **D. Miller**

7. N-Hydroxysulfonamides RSO_2NHOH as nitroxyl (HNO) donors: Improved preparation and kinetics of nitroxyl generation. **S. K. Adas**, N. E. Brasch, P. Sampson

~~**8.** Exploring reductions of the pyranopterin dithiolene moiety of the Molybdenum Cofactor (Moco). **R. Kleiner**, S. Burgmayer~~ withdrawn

~~**9.** Development of new CO_2 responsive macromolecular nanomaterials. **B. Barkakaty**, B. S. Lokitz, J. Browning, J. Ankner, B. Sumpter, D. Uhrig, I. Ivanov, J. M. Messman, S. Kilbey II~~ withdrawn

10. In situ measurements of pH during barley mashing. **R. Barth**

11. Transport and conformational change of the dopamine transporter. **E. Benner**, M. Acevedo, J. D. Madura

12. Synthesis and characterization of substituted pyrazole ligands capable of hydrogen bonding for copper-catalyzed atom transfer radical cyclization. **G. J. Pros**, T. Pintauer

13. Infrared-detected admittance spectroscopic investigation of hybrid organic/inorganic photovoltaic materials. **R. J. Stewart**, J. B. Asbury

14. Improving the tensile properties of bulk carbon nanotube materials through covalent modification. **J. S. Baker**, S. Miller, T. Williams, M. A. Meador

~~**15.** Stereoselective catalyst design principles for the Diels–Alder reaction of alpha, beta-unsaturated aldehydes with 1,3-dienes. B. Vernier, A. Ahmed, A. Kelly, J. J. Rohde, **J. D. Evanseck**~~ withdrawn

16. Transition state stabilization of substituted enals in Diels-Alder reactions by Group 13 chiral Lewis acids. **B. T. Vernier**, A. N. Ahmed, A. Kelly, J. J. Rohde, J. D. Evanseck

17. Interactions of phosphazene superbases with phosphonitrilic chloride. **N. A. Johnson**, M. J. Panzner, W. J. Youngs, C. A. Tessier

18. Understanding the interplay between morphology and charge recombination in block copolymer photovoltaics. **C. Grieco**, A. Rimshaw, Y. Lee, E. D. Gomez, J. B. Asbury

19. Unraveling the potential of sulfur-substituted DNA and RNA bases as photosensitizers. **M. Pollum**, C. E. Crespo-Hernández

20. Ultrafast structure and dynamics in ionic liquids. **Z. Ren**, T. Brinzer, S. Garrett-Roe

21. Comparison of time-resolved fluorescence spectroscopy techniques of DNA standards using confocal microscopy. **M. J. Kaliszewski**, A. W. Smith

22. Synthesis of planar polycationic metal complexes for G4-DNA quadruplex stabilization. **D. H. Robinson**, **G. M. Marqus**, C. H. Leung

23. Sensitivity to membrane-bound peptidase rates using electroosmotic push-pull perfusion. **Y. Ou**, S. G. Weber

24. Cyclophosphazene based drug delivery systems. **J. A. McQuilkin**, N. A. Johnson, M. J. Panzner, W. J. Youngs, C. A. Tessier

25. Gas permeation properties of polyoxanorbornenes bearing lateral cyclic pendant groups: The development of CO_2 selective membranes . **J. C. Worch**, K. J. Noonan, H. Nulwala

26. Synthesis and characterization of a praseodymium coordination polymer with 4,4'-bipyridine N,N'-dioxide. M. L. Stromyer, M. Zeller, **J. M. Knaust**

27. Temperature-assisted on-column solute focusing: Enhancing preconcentration and separation performance in fast capillary liquid chromatography. **S. R. Groskreutz**, S. G. Weber

WEDNESDAY AFTERNOON

At the Forefront of Proteomics
Salk

Sponsored by AB SCIEX
R. Robinson, *Organizer, Presiding*

1:30 28. Robust liquid chromatography-tandem mass spectrometry approaches to understand protein changes that occur in cancer. **M. A. Freitas**

2:00 29. Re-thinking and re-creating the modern scientific data analysis paradigm: Mass spectrometry moves big data out of the lab and on to the Cloud. **N. Yates**

2:20 30. Phosphoproteomics reveals new mechanistic insight into Fibroblast growth factor 2-mediated cardioprotection. **K. D. Greis**, A. B. Wijeratne, J. R. Manning, J. J. Schultz

2:40 31. Combined Precursor Isotopic Labeling with Isobaric Tagging (cPILOT) to increase sample multiplexing. **R. A. Robinson**

3:00 Break

3:30 32. Applying data-independent acquisition to interrogate signaling networks. **J. M. Held**

4:00 33. Development of a general proteomic strategy for global characterization of protein complexes. **M. C. Hall**, U. K. Aryal, Y. Xiong, Z. McBride, D. Kihara, J. Xie, D. B. Szymanski

4:20 34. IMS-MS instrumentation for high-throughput comparative and structural proteomics analyses. **S. J. Valentine**, J. Arndt, M. Khakinejad, S. Ghassabi-Kondalaji, G. Donohoe, M. Maurer, H. Maleki

4:40 35. Proteomic analyses of saliva from individuals undergoing cold pressor test. **D. Isailovic**, R. Marvin, B. Saepo, J. Tomko, K. Hensley, D. Giovannucci

Electricity: Generation, Storage, and Transmission

Monongahela

J. Jolson, *Organizer*
M. Treblow, *Organizer, Presiding*

1:30 Introductory Remarks

1:35 36. Thinking beyond energy technology and energy resources. **D. Keairns**

2:00 37. The new 21st century war of the currents: AC vs. DC electricity. **G. Reed**

2:40 38. Pumped Storage hydro plants: Their history & operation. **R. M. Kovach**

3:00 Break

~~**3:30 39.** Nuclear power, safety, and new plant construction. **B. R. Beebe**~~ withdrawn

4:00 40. Electric vehicles: Future innovation. **I. R. Nourbakhsh**

4:20 41. A survey of regulatory, technical, and economic drivers affecting the future of coal- and gas-fired electricity generation in the United States. **D. P. Connell**

4:40 42. Sustainable geothermal heating and cooling solutions using the natural refrigerant, recycled carbon dioxide. **M. A. Portnoff**

Electronic Materials for Device Applications: Energy Transfer, Charge Separation, and Morphology

Interstate

L. Peteanu, *Organizer, Presiding*

1:30 43. Reversible photoluminescence quenching in conjugated polymers. **L. Rothberg**, B. W. Martin

2:00 44. Novel intensity fluctuations in annealed single conjugated polymer chains. **B. W. Martin**, L. Rothberg

2:20 45. Modeling electric field-induced quenching in conjugated polymers and oligomers. **C. M. Legaspi**, L. A. Peteanu, D. J. Yaron

2:40 46. Surface potential heterogeneity in organic semiconductors. **P. B. Hoffmann**, A. G. Gagorik, G. R. Hutchison

3:00 Break

3:30 47. Ultrafast infrared spectroscopy of charge generation in organic photovoltaic materials. **J. B. Asbury**

4:00 48. Simulating charge transport and morphology in organic photovoltaics: Finding an ideal morphology through inverse design. **G. R. Hutchison**, P. B. Hoffmann, A. G. Gagorik, J. W. Mohin, T. Kowalewski

4:20 49. Phosphorus and sulfur building blocks for electronic materials. **K. J. Noonan**

4:40 50. The effects of water on charge carrier dynamics in organo halide perovskite materials. **A. V. Larsen**, J. B. Asbury

Fresh Faces in (Bio)Inorganic Chemistry
Carnegie

P. Basu, *Organizer, Presiding*

1:30 51. pH dependent ligands: Electronic properties of ruthenium complexes containing hydoxyl-substituted-polypyridyl ligands. D. J. Charboneau, M. H. Roeder, I. Nieto, T. J. Dudley, E. T. Papish, **J. J. Paul**

2:00 52. Spectroscopic studies of a novel paramagnetic iron(III)-superoxo complex. **H. D. Stout**, S. R. Kleespies, C. Chiang, M. K. Katlyn, P. Li, W. Lee, E. L. Bominaar, Q. Lawrence, E. Munck

2:20 53. Electron spin resonance analysis of metal histidine coordination in amyloid-β. **K. Silva**, B. C. Michael, S. J. Geib, S. Saxena

2:40 54. New highly fluorescent and symmetric pyrrole−BF2 chromophore: BOPHY. **I. Tamgho**, S. A. Hasheminasab, J. T. Engle, C. J. Ziegler, V. Nemykin, J. J. Rack

3:00 Break

3:30 55. Stereoinversion reaction mechanism and beyond in the biosynthesis of carbapenem antibiotics. **W. Chang**, J. M. Bollinger, C. Krebs, A. Boal, Y. Guo, A. Rosenzweig

4:00 56. Kinetics study of recombinant NapA and C176S mutant NapA from *Campylobacter jejuni*. **B. Mintmier**, J. Thomas, C. Sparacino-Watkins, P. Basu

4:20 57. Controlling pyran cyclization in molybdenum pyranopterin dithiolene complexes: It's… dielectric. **D. Gisewhite**, B. Williams, S. Burgmayer

4:40 58. 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

General Session (Part I)
Starlz

M. Ward, M. Speer, *Organizers*
L. Miller, *Organizer, Presiding*

1:30 59. Prototype IMS-MS instrumentation for high-throuhput comparative and structural proteomics analyses. **S. J. Valentine**, J. Arndt, G. Donohoe, M. Khakinejad, H. Maleki, S. Kondalaji

~~**2:00 60.** Preparation of functional DNA block copolymers for biological applications. S. R. Das, K. Matyjaszewski, **S. Averick**~~ withdrawn

2:20 61. Noncovalent binding of RNA monomers to RNA and DNA oligonucleotide duplexes. **E. C. Izgu**, A. C. Fahrenbach, N. Zhang, L. Li, W. Zhang, J. C. Blain, J. W. Szostak

2:40 62. *In vitro* binding study of iron-regulatory protein onto iron-responsive element mRNA. **M. Rahman**, B. S. Day, W. L. Patterson, C. Warner, E. T. Mendenhall, B. Wang, M. L. Norton

3:00 Break

3:30 63. Hierarchical approach of frequent assessment in chemistry. G. A. Buckholtz, M. N. Srnec, E. S. Gawalt, **J. D. Evanseck**

4:00 64. Success of an interdisciplinary approach to introducing electrostatic potential energy for introductory chemistry. **M. Nagel**, B. Lindsey

4:20 65. Size-controlled nanoMOFs for near-infrared biological imaging. **K. Gogick**, N. L. Rosi, S. Petoud

4:40 66. Analysis of detergent in diesel fuel by gas chromatography-mass spectrometry (GCMS). **J. R. Parish**, H. L. Juzwa

Solid-State Materials (Part I)
Allegheny

J. Aitken, *Organizer*
P. Maggard, P. A. Salvador, *Presiding*

1:30 67. Photocatalytic applications of delafossite materials: Organic dye degradation and CO_2 reduction. **J. W. Lekse**, J. P. Lewis, C. Matranga, B. J. Haycock

2:00 68. Analysis of novel polymorphic Li_2-II-IV-S_4 diamond-like semiconductors using synchrotron x-ray powder diffraction. **K. P. Devlin**, K. R. Daley, M. A. Moreau, J. A. Brant, J. A. Aitken

2:20 69. Synthesis, structure and transport properties of $Cu_2Mg_{3-2x}Ti_xSe_4$ ($0 \le x \le 1.5$). **E. Chen**, A. Olvera, P. P. Poudeu

~~**2:40 70.** New diamond-like semiconductors that violate Pauling's second rule of local electroneutrality: Crystal structures and physicochemical characterization. **C. W. Sinagra**, J. Zhang, J. A. Brant, K. A. Rosmus, J. A. Aitken~~ withdrawn

3:00 Break

3:30 71. Controlling polymorphism and morphology: Low temperature routes to metal sulfides. **C. Lind-Kovacs**, R. Kaur

4:00 72. Surface modification of ZrW_2O_8 and $ZrW_2O_7(OH)\bullet 2H_2O$ by in-situ polymerization: Enhanced filler particles for use in composites. **X. Gao**, C. Lind, M. R. Coleman

4:20 73. Isolation of columbite SnO_2 with combinatorial substrate epitaxy. **J. Wittkamper**, P. Salvador, G. Rohrer, M. DeGraef

4:40 74. Shape actuation of dual-cured networks. **J. Jiang**, Y. Meng, M. L. Anthamatten

Surface Chemistry: Polymer Science and Biointerfaces

PPG

R. Quiñones, *Organizer, Presiding*

1:30 75. Bioinspired adhesives and coatings: Lessons learnt from spiders and geckos. **A. Dhinojwala**

2:00 76. Solid-state NMR and computational chemistry studies of reactive surface area. **K. Mueller**, N. Washton, P. O'Day, J. Kubicki, H. Watts, S. Estok, E. Poweleit

2:20 77. Multi-functionalized ceramic biomaterials. **E. S. Gawalt**

2:40 78. Understanding the underlying mechanisms of simultaneously oleophobic/hydrophilic polymer coatings. **Y. Wang**, L. Li

3:00 Break

3:30 79. Low cost and effective solid sorbents for carbon dioxide capture. E. A. Roth, S. Agarwal, **R. K. Gupta**

4:00 80. Developments in finite, nanoscale DNA scaffold arrays for sensing applications. M. Rahman, T. Wu, T. Bakhshi, D. Neff, **M. L. Norton**

~~**4:20 81.** Second Harmonic Generation study of the structure and molecular adsorption on Hexadecane/water interface. **W. Gan**, H. Fang, Y. Sang, W. Wu, S. Chen~~ withdrawn

~~**4:40 82.** Synthesis and biomedical applications of boronic acid-installed polycarbonates. **M. Herrera-Alonso**~~ withdrawn

Synthetic Organic Methods and Total Synthesis
Ohio

R. Lettan, *Organizer, Presiding*

1:30 83. Copper-mediated oxidative decarboxylative cross-coupling reactions. **J. Hoover**

2:00 84. Anionic conjugate additions of arylsulfonylalkeneisonitriles. **S. V. Chepyshev**, F. F. Fleming

2:20 85. Development and application of novel glycosylating agent in complex oligosaccharide assembly. **A. Sasmal**, Y. Li, X. Liu

2:40 86. Synthesis and anti-tumor activity of N, N'-bisnaphthylated imidazole salts with lipophilic or hydrophilic substituents in the 4 and 5 positions of the imidazole rings. **K. L. Shelton**, P. O. Wagers, M. A. DeBord, M. J. Panzner, N. K. Robishaw, C. A. Tessier, W. J. Youngs

3:00 Break

3:30 87. Bronsted acid-catalyzed acetalizations and reactions of acetals. **P. Nagorny**

4:00 88. Total synthesis of an anti-fouling sesquiterpene furan natural product. **C. N. Ungarean**, S. S. Murphree

4:20 89. A scaffold with rich biological activity but no commercial availability. **A. S. Bayden**

4:40 90. Design, synthesis, and evaluation of peptidyl emetine prodrugs as cancer therapy. **E. S. Akinboye**, W. Brennen, M. D. Rosen, O. Bakare, S. R. Denmeade

Sci-Mix Poster Session I
Salons D, E

M. Ward, A. Michael, *Organizers*

5:00 - 7:00

91. ACS International and you. **H. Cheng**

92. Hollow spherical gold nanoparticle superstructures with visible to near infrared extinction and size-dependent drug release properties. **C. Zhang**, Y. Zhou, T. Brinzer, A. Merg, C. Song, C. Liu, G. C. Schatz, S. Garrett-Roe, N. L. Rosi

93. Ligand exchange for mesoporous metal-organic framework functionalization. **C. Liu**, T. Luo, E. S. Feura, C. Zhang, N. L. Rosi

~~**94.** Core-shell metal-organic frameworks: Design, construction, and gas adsorption properties. **T. Luo**, C. Liu, A. B. Spore, N. L. Rosi~~ withdrawn

~~**95.** Novel antibacterial nanocomposites based on PLLA/Triclosan/Nanohydroxyappatite. S. Davachi, B. Kaffashi, **M. Bahrami**~~ withdrawn

~~**96.** Multivalent peptide conjugates for rationally controlling the metrics and assembly of nanoparticle superstructures. **A. Merg**, N. Rosi~~ withdrawn

97. Copper detection and analysis in marine systems: Toward the development of an *in situ* sensor. **W. M. Cunning**, W. R. LaCourse

98. Design and synthesis of small-molecule inhibitors of the hypoxia inducible factor-1 as anticancer therapeutics. **Z. A. De los Santos**

99. Surface modification of polymer nanoparticles for nitric oxide delivery . **N. A. Reger**, W. S. Meng, E. S. Gawalt

100. Design, synthesis, and characterization of asymmetric monooxo molybdenum complexes containing dithiolene units. **S. Dille**, B. Mogesa, P. Basu

~~**101.** Reaction of aqueous organomercury compounds with aluminum. **J. S. Thayer**, N. Kaval~~ withdrawn

102. One pot in-situ synthesis of poly(3-hexylthiophene) vanadium oxide composites. **J. N. Gadient**, C. Lind-Kovacs, M. N. Coleman

103. Drug discovery in undergraduate research: Defining an appropriate target in the struggle with LPS. **R. Woodward**, A. Greenwell, E. Loosli, L. Gosser

104. Novel quaternary diamond-like selenides and their nonlinear optical properties. **J. Zhang**, D. Clark, J. Brant, K. Rosmus, Y. Kim, J. Jang, J. Aitken

105. Photophysical and electrochemical properties of novel Mn carbonyl complexes containing substituted phenanthroline ligands. **R. J. Hulme**, D. A. Kurtz, B. Dhakal, G. S. Nichol, G. A. Felton

106. Synthesis and biological activity of 4-substituted pyrrolo[2,3-d]pyrimidines as inhibitors of mitotic kinases. **S. Kurup**, B. McAllister, T. Mistry

107. Scalable stereodivergent synthesis of biologically active clopidogrel metabolites and UV active analytes. **B. P. Vokits**, B. Balasubramanian, J. Caceres-Cortes, J. Dai, P. Y. Lam, F. Qui, R. R. Wexler, Y. Zhang, S. A. Shaw

108. Ionically cross-linked poly(ethers)-based membranes for CO_2/N_2 separation. **X. Zhou**, S. R. Venna, E. A. Roth, D. R. Luebke, E. J. Albenze, H. B. Nulwala

109. Single molecule magnet $Mn_{12}O_{12}(C_xH_{2x-1}O_2)_{16}\cdot 4H_2O$: Characterization and surface organization. **N. M. Khatri**, K. R. Lincoln, K. D. Pires, T. M. Hughes, K. E. Plass, J. A. Borchers, S. E. Lofland, K. Jorabchi, M. Pileni, S. L. Stoll

110. Exploring the importance of zinc binding and steric factors in novel HCV replication inhibitors. **D. C. Talley**, P. J. Smith

111. Synthetic approaches to iron selenide nanostructures. **S. E. Ingram**, S. L. Stoll

112. Hybrid metal-oxo polymer nanobeads as potential MRI contrast agents. **V. A. Dahanayake**, W. J. Hickling, S. L. Stoll

113. Using ssNMR spectroscopy to study the binding and disruption of mitochondrial lipid bilayers by a peripheral membrane protein. **A. Mandal**, M. L. DeLucia, C. L. Hoop, R. B. Kodali, J. Ahn, P. C. van der Wel

114. New Research Experience for Summer Scholars (RESS) program at Indiana University of Pennsylvania. A. E. Kondo, **J. D. Fair**

115. Atomically precise Au_{25} clusters for electrocatalytic CO_2 conversion. **J. A. Thakkar**, D. R. Kauffman

116. Effect of doping on the magnetostructural transition in MnAs nanoparticles: Optimizing properties for magnetic refrigeration. **S. R. Pimmachcharige**, S. L. Brock

117. Determining K_D's of Ricin aptamers in DNA origami compatible buffer. **J. N. Botkin**, M. L. Norton, H. Zhong

118. Laser ionization methodology for the quantitative analysis of a biomedically relevant analyte. **L. T. Miller**, S. Shuttleworth, S. Sheffield, M. Pamukcu, H. Kingston

119. Observation of the human FTH1 IRE/IRP complex under various conditions using three different techniques. **E. T. Mendenhall**, B. Wang, M. L. Norton, W. L. Patterson III, M. Rahman, B. S. Day

120. Assessing polyglutamine conformation and aggregation with molecular dynamics techniques. **R. J. Workman**, J. D. Madura

121. 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

122. IRMPD spectroscopy reveals a novel rearrangement reaction for modified peptides that involves elimination of the N-terminal amino acid. **K. L. Patterson**, M. J. Van Stipdonk, J. K. Gibson, G. Berden, J. Oomens

123. Graphene nanostructured metalloporphyrin interfaces: Improved selectivity and sensitivity of peroxynitrite sensors. **H. Kalil**, M. Bayachou

124. Novel, low-energy, pseudo-chair conformation of carboxyphosphate with implications for ATP-dependent carboxylase enzymes through charge-assisted proton shuttling. **T. M. Clymer**, V. S. Pakkala, S. P. Hebert, S. E. Kochanek, S. M. Firestine, J. D. Evanseck

125. Workshop for high school chemistry teachers: Enhanced chemistry learning through instrument access and personalized secondary educator training. **C. Spiese**, C. P. Bowers

126. Regulation of the 3' UTR in BDNF mRNA at the DNA level. **B. DeMarco**, R. Mihailescu

127. Investigation of the role played by the RNA G-quadruplex structure in ALS/FTD pathology. **D. S. McAninch**, M. Mihailescu

128. G quadruplex RNA structures in PSD-95 mRNA: Potential regulators of miR-125a seed binding site accessibility. **S. Stefanovic**, R. Mihailescu

~~**129.** Photosensitive polymers for controlled release of a PEGylated singlet oxygen photosensitizer. **M. Minnis**, G. Ghosh, I. Abramova, A. Greer~~ withdrawn

130. 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

131. Effects of domain size and composition on physical properties of MoS_xSe_{2-x} and WS_xSe_{2-x} solid solutions. **M. T. Nguyen**, Z. Lin, J. Shevrin, A. L. Elías, S. Feng, J. Zhu, M. Terrones, T. E. Mallouk

132. Magnetic mesoporous silica nanoparticles as potential MRI contrast agents. **W. J. Hickling**, V. Dahanayake, S. L. Stoll

133. Phase transfer of gold-silver alloy nanoparticles. **T. R. Brewer**, B. T. Comstock-Reid, R. Fiedler, V. Marcu

134. Role of lipid membranes in modulating the activity of endothelial nitric oxide synthase. **G. Altawallbeh**, M. Bayachou, C. Verdi, M. Haque, D. Stuehr

135. Improving rational drug design of a selective serotonin reuptake inhibitor using FEP. **B. Jean**, J. D. Madura

136. Density functional characterization of the iron-sulfur cluster in human mitoNEET. **A. M. Koval**, B. R. Jagger, R. A. Wheeler

137. Synthesis, characterization, and efficacy study of alkyl substituted hydrophobic imidazolium salts. **M. A. DeBord**, P. O. Wagers, M. J. Panzner, C. A. Tessier, W. J. Youngs

~~**138.** Selective hydroperoxidation of an olefin sulfonate detergent by airborne singlet oxygen. **A. A. Ghogare**, B. Malek, R. Choudhury, A. Greer~~ withdrawn

139. Physical effects of extending the conjugation of rhodamine dyes in straight or bent configurations. **M. F. Mark**, M. W. Kryman, R. P. Sabatini, D. J. Mark, M. R. Detty, R. Eisenberg, D. W. McCamant

140. Combining the advantages of siloxane and ethylene oxide moieties in cross-linked polymers for gas separation membranes. **V. A. Kusuma**, S. R. Venna, E. A. Roth, E. Albenze, D. R. Luebke, D. Hopkinson, H. B. Nulwala

~~**141.** Influence of molecular structure on charge separation dynamics in perylene diimides. **A. Rimshaw**, C. Grieco, J. Asbury~~ withdrawn

142. Lewis acid strength of cyclic chlorophosphazenes. **B. S. Thome**, B. D. Wright, P. O. Wagers, W. J. Youngs, C. A. Tessier

143. Investigation of acidity for group 13 & 15 superacids. **J. A. Stiel**, Z. Tun, C. Tessier

144. Pulse radiolysis studies of the reaction of nitrogen dioxide with the vitamin B_{12} complexes cob(II)alamin and nitrocobalamin. **R. S. Dassanayake**, D. E. Cabelli, N. E. Brasch

145. Excited state torsional processes in an asymmetric chalcogenopyrylium monomethine dye: Toward applications for photodynamic therapy and solar hydrogen generation. **D. J. Mark**, R. P. Sabitini, M. Bedics, M. Mark, M. Detty, D. W. McCamant

~~**146.** Temperature-resolved kinetics of pyrene excimer formation in cyclohexane. **J. R. Weaver**, B. H. Milosavljevic~~ withdrawn

147. Characterization of self-aggregation of different chalcogenorhodamine dyes on nanocrystalline films using Doubly Resonance Sum Frequency Generation. **S. Sengupta**, S. K. Das, L. Bromley, L. Velarde

148. Preventing corrosion by controlling cathodic reaction kinetics. **V. B. Oyeyemi**, J. A. Keith

149. Computational and spectroscopic studies of heterogeneities in room temperature ionic liquids. **E. C. Wu**, H. J. Kim, L. A. Peteanu

150. Synthesis of 2-carboxylate-1,3-thiazole esters. **S. M. Carney**, A. Seed, P. Sampson

151. CD44+ tumor targeting pentium complex for more efficient drug delivery. **N. Beals**, E. Soehnlen, A. Das, S. Basu

152. Engineering transaminases for dynamic kinetic resolution of α-substituted β-keto esters. **A. L. Snyder**, J. Rogers, J. Johnson, E. M. Brustad

153. ~~Designer plasmid enabled identification of a prenylated cyclopentenedione containing bis-indole alkaloid from in vivo biosynthesis of fungal natural product terrequinone in escherichia coli: Insights into the origin of divergent regioselectivity of prenyltransferase TdiB. **Q. Zhu**, X. Liu~~ withdrawn

154. ~~Ring strain energy in ether- and lactone-containing spiro compounds. **J. D. Augspurger**, M. K. Stedjan~~ withdrawn

155. Ligand-bound cation-anion pairs in the gas-phase. **T. Souza**, D. Martin, C. O'Malley, M. Van Stipdonk

156. Sub-picosecond intersystem crossing dynamics of 2-thiocytosine in aqueous buffer solution. **N. J. Dunn**, M. Pollum, S. Mai, L. Martínez-Fernández, P. Marquetand, I. Corral Pérez, L. González, C. E. Crespo-Hernández

157. Examining the interface of pyrimidine pathway enzymes using synthetic peptides. **N. Alyami**, **D. Ganti**, D. Evans, F. Hachem, D. Heyl, H. Evans

158. ~~Computer simulation study of ionic liquid/water mixtures. **F. Yan**, H. J. Kim~~ withdrawn

159. Copper mediated oxidative decarboxylative trifluoromethylation of C-H bonds with trifluoroacetic acid as the CF_3 source. **L. Ju**, J. Hoover

160. ~~Guided Compassion and Relaxation App: Changing the way people react to daily personal conflicts. **A. V. DelGiorno**, A. Prabhu, J. Brefczynski-Lewis~~ withdrawn

161. ~~Novel $p18^{INK4C}$ small molecule inhibitors for hematopoietic stem cell expansion. **P. Yang**, P. Zhang, Y. Zhang, L. Wang, Q. Ji, Q. Tong, H. Cheng, M. Yang, p. Huang, Y. Ding, T. Cheng, Y. Gao, X. Xie~~ withdrawn

162. Catalytic drugs targeting stem loop IV of the IRES HCV RNA. **M. J. Ross**, S. S. Bradford, J. A. Cowan

163. Screening antibodies with labeled gold nanoparticle DLS assays. **Y. H. Lai**, J. D. Driskell

164. Structure-activity relationships of linear derivatives of tachyplesin containing fluorophenylalanine. **N. Kanneganti**, S. Wood, D. Heyl-Clegg

165. Enhanced osteoblast response on a composite calcium-based ceramic. **G. A. Buckholtz**, M. C. Miller, E. S. Gawalt

166. Oxygen/chlorine transfer reactions of cyclic chlorophosphazenes using methane sulfonic acid. **S. R. Snyder**, B. S. Thome, C. A. Tessier

THURSDAY MORNING

Computational Modeling in Energy Research

Ohio

D. Lambrecht, *Organizer, Presiding*
J. Keith, S. Garrett-Roe, *Presiding*

8:30 167. Accurate and efficient density functional theory approaches for modeling catalysis. **H. J. Kulik**

9:00 168. Electro-chemical trends in organic molecular crystals: A high-throughput DFT investigation. **B. Schatschneider**

9:20 169. Rapid computational screening for new energy materials: Organic piezoelectrics and photovoltaics. **G. R. Hutchison**

9:40 Break

10:00 170. How to achieve quantitative accuracy in calculations for strongly correlated solids. **D. Zgid**

10:30 171. Quantitative analysis of Pt nanoparticles on amorphous silica supports using density functional theory. **C. S. Ewing**, M. J. Hartmann, D. S. Lambrecht, G. Veser, J. J. McCarthy, J. Johnson

10:50 172. Ultrafast vibrational spectroscopy (2D-IR) probes structure and dynamics in ionic liquids. **S. Garrett-Roe**, Z. Ren, T. Brinzer, S. Dutta

11:10 173. Unraveling mechanistic aspects of heterocycle-promoted CO_2 electroreduction with quantum chemistry. **J. A. Keith**

Diversity in the Chemical Sciences (Part I)

Foster

M. Ward, K. Brummond, *Organizers*
R. Robinson, *Organizer, Presiding*

8:30 174. Adventures with the dehydro-Diels–Alder reaction: Cracking a mechanistic mystery. **K. M. Brummond**

9:00 175. Nanoscale science and the environment. **S. O. Obare**

9:20 176. Stimuli sensitive hydrogels: Metal oxidation-state control of crosslink density. **T. Y. Meyer**, J. T. Auletta, G. J. LeDonne, K. C. Gronborg, C. D. Ladd, H. Liu, W. C. Clark

9:40 Break

10:00 177. DNA under attack: Electronic and structural elements that regulate nucleic acids photostability. **C. E. Crespo-Hernández**

10:30 178. Optical properties of conjugated materials and their aggregates: Toward imaging of films and devices. **L. A. Peteanu**, S. Jeon, J. Hong, J. Kim, D. Devi, J. Wildeman, J. H. Werner, A. P. Shreve

10:50 179. Gas-phase radical ion chemistry: A new avenue to bio-analysis. **Y. Xia**

11:10 180. Distinct allosteric inhibitors may share common mechanisms of action in the Hepatitis C virus polymerase. **I. F. Thorpe**

General Session (Part II)

Interstate

M. Ward, *Organizer*
M. Speer, *Organizer, Presiding*

8:30 181. Double-acceptor as a superior organic dye design for p-type DSSCs: High photocurrents and observed light soaking effect. **K. A. Click**, B. R. Garrett, Z. Huang, D. R. Beauchamp, Y. Wu

9:00 182. Synthesis of acetate-type ionic liquids: Applications in carbon capture. **M. K. Macala**, H. Nulwala, W. Shi

9:20 183. Investigations of nitrogen doping density in graphene and hydrogen adsorption by DFT. **E. Gottlieb**, J. A. Keith, D. J. Yaron

9:40 Break

10:00 184. Exploring vibrational dynamics and catalytic functions of heme proteins: The case of cytochrome c and myoglobin. **M. I. Galinato**, N. Lehnert, K. L. Bren, J. G. Kleingardner, S. E. Bowman, E. Alp, J. Zhao, W. Sturhahn, A. Stetz, R. S. Fogle

10:30 185. Computational exploration of spring-like single molecule piezoelectrics. **C. W. Marvin**

10:50 186. Atomically precise gold nanoclusters as model catalysts for solution and gas phase reactions. **Y. Chen**, G. Li, C. Zeng, R. Jin

11:10 187. Measuring noncovalent interactions in fluorous solvent using isothermal titration calorimetry. **A. R. Horner**, T. Brinzer, S. Garrett-Roe, S. G. Weber

Green Chemistry Success Stories
Frick

G. Ruger, *Organizer, Presiding*

8:30 188. Progress report on a roadmap for green chemistry education. **J. MacKellar**, D. Constable

9:00 189. Spreading green chemistry education in New York and beyond. **G. W. Ruger, Jr**

9:20 190. Green chemistry and engineering at the University of Toledo. **M. Mason**, A. Jorgensen

9:40 Break

10:00 191. Chemical Hygiene Officer: A curriculum long overdue. **M. F. Charlton-Smith**, J. Webb

10:30 192. Interrogating the microenvironment of ionic liquids by two-dimensional infrared spectroscopy. **S. Dutta**, S. Garrett-Roe

10:50 193. New water soluble organometallic catalysts for waterborne coatings. **L. D. Venham**, B. Parks

11:10 194. Synthesis, characterization and immobilization on NiO of FeFe-hydrogenase mimics bearing carboxylic acids and investigation of their electrochemical degradation pathway. **B. R. Garrett**, C. Hadad, Y. Wu

Nucleic Acid Based Materials (Part I)
PPG

C. Achim, D. Waldeck, H. Liu, *Organizers, Presiding*

8:30 195. Degradable lipid nanoparticles with predictable in vivo siRNA delivery activity. **K. Whitehead**

9:00 196. DNA computation in mammalian cells: microRNA logic operations. **J. Hemphill**, A. Deiters

9:20 197. ~~Discrete and cooperative DNA triplex formation with bifacial polymer nucleic acid. **D. Bong**~~ withdrawn

9:40 Break

10:00 198. DNA: Not merely the secret of life. **N. C. Seeman**

10:30 199. Stability of DNA origami nanostructure under diverse chemical environments. **H. Kim**, S. P. Surwade, A. Powell, C. O'Donnell, H. Liu

10:50 200. Attached to DNA . **S. R. Das**

11:10 201. Directed self-assembly of DNA tiles into complex nanocages. **C. Tian**, X. Li, Z. Liu, W. Jiang, G. Wang, C. Mao

Oil, Gas, and Chemicals from Shale Formations (Part I)
Monongahela

J. Miller, *Organizer, Presiding*

8:30 202. The history of gas and oil in Western Pennsylvania. **A. N. Mann**

9:00 203. Shale gas and the chemical industry: Impacts on process chemistry needs. **J. J. Siirola**

9:40 Break

10:00 204. Shale Gas in the US: Potential opportunities and challenges to address. **K. Mertins**

10:30 205. Evolving microbial communities in produced water from hydraulic fracturing: Implications for water management. **K. B. Gregory**

11:10 206. Chemicals required for chemical extractions from shale: Learning opportunities for our students. **M. A. Benvenuto**

Organic Process Research and Development: Utilization and Recovery of Precious Metal Catalysts
Salk

J. Fisk, M. Grandbois, *Organizers, Presiding*

8:30 207. Ion exchange processes for precious metal catalyst recovery. **B. Kern**, J. Hwang

9:00 208. Photosensitization and beyond: Leveraging an uncommon iridium architecture for applications in solar fuel production. **D. N. Chirdon**, W. J. Transue, H. N. Kagalwala, A. Kaur, A. B. Maurer, T. Pintauer, S. Bernhard

9:20 209. [FeFe]-and [FeNi]-Hydrogenase-inspired proton reduction electrocatalysts. **R. J. Day**, R. J. Hulme, G. S. Nichol, G. A. Felton

9:40 Break

10:00 210. Ligand design in palladium-catalyzed cross-coupling reactions to optimize catalyst performance, selectivity, and recovery. **K. H. Shaughnessy**

10:30 211. The synthesis, characterization and biochemical studies of ru-arene complexes bearing electroneutral phosphane ligands. N. G. Petrochko, T. Wignot, R. G. Baughman, **R. Peters**

~~**10:50 212.** Divergent chemoselectivity preferences of *N*-Lithiated and *C*-Magnesiated nitriles. **X. Yang**, D. Nath, F. Fleming~~ withdrawn

11:10 Concluding Remarks

Solid-State Materials (Part II)
Allegheny

J. Aitken, *Organizer*
C. Oertel, C. Lind, *Presiding*

8:30 213. Looking for order-disorder or displacive nature of the BaTiO3 ferro-to para-electric phase transition with high-resolution single crystal neutron diffraction. **C. Hoffmann**

9:00 214. Domain-specific photochemical surface reactivity on ferroelastic $BiVO_4$. **R. Munprom**, P. A. Saldavor, G. S. Rohrer

9:20 215. Density-functional study of the $La_2Zr_2O_7$ low-index faces. **Y. Mantz**, Y. Duan

9:40 Break

10:00 216. Competing magnetic interactions in the osmate double perovskites. **P. Woodward**, R. M. Morrow

10:30 217. Mixed-metal oxides and the impact of structure and composition on their optical, electronic, and photocatalytic properties. **J. Boltersdorf**, T. Wong, P. A. Maggard

10:50 218. Fast lithium-ion conductivity in thiogermanate and thiostannate compounds. J. A. Brant, J. H. MacNeil, D. M. Massi, K. P. Devlin, A. P. Douvalis, T. Bakas, C. Bischoff, S. M. Martin, **J. A. Aitken**

11:10 219. Complex magnetism in the Sr2-xCaxCoOsO6 system. **R. Morrow**, P. M. Woodward

THURSDAY AFTERNOON

Plenary II
Salons D, E

M. Ward, A. Michael, *Organizers, Presiding*

1:00 220. Native MS of protein complexes: Surface-induced dissociation coupled to ion mobility. **V. Wysocki**, S. Harvey, R. Quintyn, Y. Song, Y. Ju, J. Yan, A. Sahasrabuddhe

Careers Related to Chemical Education
Frick

J. Grabowski, D. Hoover, *Organizers, Presiding*

2:20 221. Teaching and research in a MS and BS granting chemistry program. **J. J. Paul**

2:50 222. Nelson Diversity Surveys: Significance, utility, and impact of their data. **D. J. Nelson**

3:10 223. Teaching, scholarship, and service: Early career experiences at a liberal arts university. **D. Hoover**

3:30 Break

3:50 224. Sharing one's passion for chemistry at a two-year college: Producing high yields of professional and personal fulfillment. **D. R. Brown**

4:20 225. Transforming Walsh University's first forensic science course into an online learning experience: A course for both science and non-science majors. **A. J. Heston**

4:40 226. Breaking Bad: Science behind the show. **D. Nelson**

Cope Symposium in Honor of Jeff Johnston
Ohio

Sponsored by ACS Division of Organic Chemistry
R. Lettan, *Organizer*
J. Hoover, *Presiding*

2:20 227. Legacy of Cope: On what a plant, a fungus, and a bacterium have been speaking to us through organic chemical mechanisms. **R. Viswanathan**, K. Thandavamurthy, D. Sharma, S. K. Porwal, D. Ray

2:50 228. MK-7655: Surprising synthetic complexity for seemingly straightforward steps. **R. T. Ruck**

3:20 Break

3:50 229. Progress toward the total synthesis of Haouamine A. **P. Wipf**, L. Cao

4:20 230. Reagent and reaction development in the service of complex target synthesis and therapeutic development. **J. N. Johnston**

Diversity in the Chemical Sciences (Part II)
Foster

K. Brummond, R. Robinson, *Organizers*
M. Ward, *Organizer, Presiding*

2:20 231. Understanding interests: Exploring patterns and predictors in the career decision-making of science PhDs by race and gender. **K. Griffin**, K. Gibbs, Jr.

2:50 232. Who is minding the gaps? **C. M. Rankins**

3:30 Break

3:50 233. Recruitment and retention efforts for underrepresented and first generation STEM graduate and undergraduates students. **S. V. Olesik**, C. Turro, D. Tomasko, J. S. Ridgway

4:20 234. Inclusive excellence in research-active chemistry departments. **R. Hernandez**, S. Watt

General Session (Part III)
Interstate

M. Ward, *Organizer*
M. Speer, *Organizer, Presiding*

2:20 235. Pointsource photodynamic therapy of glioma cells in vitro: Development of polymer probe tips for use as a singlet oxygen scalpel to localize the delivery of PDT. **A. A. Ghogare**, I. Rizvi, T. Hasan, A. Greer

2:50 236. CMDdescriptor - 1D and 3D descriptors for addressing ADME/Tox challenges in peptide-based drug discovery. **A. S. Bayden**, D. J. Diller, J. Audie

3:10 237. A proteomics-driven elucidation of the disparate determinants of osteosarcoma cells that differ in metastatic potential. **I. Motorykin**, S. Bracha, M. Milovancev, C. S. Maier

3:30 Break

3:50 238. ~~Bifacial PNA as an allosteric switch for aptamer and ribozyme function. **D. Bong**~~ withdrawn

4:20 239. Relative free energies of binding for enantiomers of nerve agents bound to Paraxonase-1 enzyme: A TIMD study. **S. Oottikkal**, C. M. Hadad

4:40 240. Increased throughput and purity of combinatorial libraries utilizing a targeted gradient profile based on preliminary analytical screening. **T. M. Anderson**, H. L. Juzwa

Nucleic Acid Based Materials (Part II)
PPG

C. Achim, D. Waldeck, H. Liu, *Organizers, Presiding*

2:20 241. Developments in finite, nanoscale 1D DNA scaffold arrays for opto-electronic applications. M. Rahman, T. Wu, T. Bakhshi, D. Neff, **M. Norton**

2:50 242. Incorporation of metal complexes in nucleic acid triplexes. **D. R. Jayarathna**, C. Achim

3:10 243. Designing mechanical dynamics of DNA origami nanostructures. A. Marras, L. Zhou, M. Hudoba, J. Johnson, M. Poirier, H. Su, **C. Castro**

3:30 Break

3:50 244. Engineering molecular assembly for 3D electronics. **T. LaBean**

4:20 245. Dexter energy transfer pathways in donor-bridge-acceptor systems. **D. N. Beratan**

4:40 246. Photophysical studies of oligopeptide linked Ru-Cu, Ru-Pd and Ru-Zn complexes. **S. Sun**, C. P. Myers, M. E. Williams

Oil, Gas, and Chemicals from Shale Formations (Part II)
Monongahela

J. Miller, *Organizer, Presiding*

2:20 247. Synthesis gas from methane-rich shale and natural gas by dry reforming. **D. B. Dadyburjor**, E. L. Kugler

2:50 248. Risk management for unconventional oil and gas development: Might better scientific information be helpful? **M. J. Small**

3:30 Break

3:50 249. Thermal maturity in the marcellus and utica formations. **J. C. Corbett**

4:20 250. Understanding rates of methane leakage and the GHG footprint of gas production. J. Littlefield, **J. Marriott**, G. Cooney, T. J. Skone

Solid-State Materials (Part III)
Allegheny

J. Aitken, *Organizer*
J. Lekse, R. Schaak, *Presiding*

2:20 251. Hydrothermal synthesis and post-synthetic processing of lead oxide carboxylates. **C. M. Oertel**, V. S. Mandala, E. E. Liu, I. Yamakawa, M. Zeller

2:50 252. Manganese vanadate/organic hybrids: Structures, bandgap sizes, and photocatalytic activities. **L. Luo**, Y. Zeng, P. A. Maggard

3:10 253. Functionalizable porous organic crystals of triphenylarenes. **J. Rowsell**

3:30 Break

3:50 254. Peptide-directed synthesis and assembly of hollow spherical nanoparticle superstructures: Syntheses, structures, and emergent properties. **N. L. Rosi**

4:20 255. Light-responsive MOFs: Functionalization of metal-organic frameworks with diarylethene based organic linkers. **I. M. Walton**, J. B. Benedict, D. G. Patel

4:40 256. Gradient-index networks based on thiol-ene reactions. Y. Meng, **M. Tsai**, M. Anthamatten

Sci-Mix Poster Session II
Junior Ballroom Hallway

M. Ward, A. Michael, *Organizers*

4:00 - 6:00

257. Effects of initial COD and conductivity on MFC performance. A. Casasús, L. Bava, **J. Lee**

258. Dinuclear ruthenium(I) complexes with N-heterocyclic carbene ligands. T. N. Rohrabaugh, E. D. Sawyer, J. C. Doverspike, **T. J. Malosh**

259. Visible light driven alcohol dehydrogenation using a rhodium catalyst. **H. N. Kagalwala**, A. B. Maurer, I. N. Mills, S. Bernhard

260. First quantitative *in vitro* assay to characterize the *Saccharomyces cerevisiae* GPI-Transamidase. **S. Amarasingha Ekanayaka**, D. N. Gamage, T. L. Hendrickson

261. Abiotic degradation of chlorinated hydrocarbons by copper amended nanoscale zero-valent iron stabilized with carboxymethylcellulose. **A. Franze**, A. Agrawal

262. Development, validation and application of various biophysical modules in CMDInventus to enable structure-based peptide drug design and discovery. **A. S. Bayden**, D. J. Diller, M. Jarosinski, D. G. Sprous, J. T. Swanson, J. Audie

263. Incorporation of a design your own experiment into an undergraduate instrumental analysis course. **A. M. Reinsel**

264. Chemistry is fun! A quantitative analysis laboratory adventure. **S. Yochum**

265. Two-dimensional infrared spectroscopy probes carbon dioxide solvation dynamics in imidazolium ionic liquids. **T. Brinzer**, Z. Ren, A. S. Ivanova, J. D. Watkins, N. R. Washburn, H. B. Nulwala, S. Garrett-Roe

266. Overexpression and purification of human aconitase 1 for the study of its iron-responsive element-binding properties. **W. Patterson**, E. Mendenhall, M. Rahman, A. Belalcazar, B. Wang, M. Norton

267. Who ordered that? Exciting new behavior of gas-phase uranyl complexes. **M. J. Van Stipdonk**, A. Plaviak, C. O'Malley, S. M. Osburn

268. Electrostatic interactions between anionic phospholipids and polycationic macromolecules: PIE-FCCS study of effect of polycationic macromolecule on the mobility. **X. Shi**, X. Li, X. Zhuang, A. W. Smith

269. Complex kinetics of TAML activators with tert-butyl hydroperoxide. **M. R. Mills**, A. E. Burton, A. D. Ryabov, T. J. Collins

270. Synthesis and characterization of chromium-based ternary chalcogenides. **H. A. Dalafu**, K. R. Lincoln, H. Nguyen, S. L. Stoll

271. High-throughput screening of erratic cell volume regulation using hydrogel-based single cell microwell array. **J. Heo**, C. Brown, V. Fleischauer

272. Molecular docking study of organophosphorus pesticides with G3C9 and its variants. **K. J. Cahill**, K. Doddapaneni, S. Oottikkal, T. J. Magliery, C. Hadad

273. Structure-dependent fluorescence properties of Au_{25} nanoclusters. L. Peteanu, **W. So**

274. Multi-functional reagent ions for CI-MS. **M. Barth**

275. Computer simulation study of the ionic liquid, chloline acetate, and its mixtures with water. **J. Willcox**, H. Kim, H. Kim

276. Exploring the interaction of humanin and its analogs with IGFBP-3 and regulation of apoptosis in Alzheimer's disease. **S. P. Herath Gedara**, D. Heyl, H. Evans

277. Effect of metal films on photoluminescence and electroluminescence properties of conjugated polymers: Photostability effect. L. Peteanu, **S. Abbas**

278. Structure-function relationship of NFU1 in iron-sulfur cluster biosynthesis. **C. Wachnowsky**, J. A. Cowan

279. 5-substituted 2(3H)-Thienones as building blocks for the synthesis of o-thienyl carboxylate-based liquid crystals. **J. Zhang**, P. Sampson, A. Seed

~~**280.** Morbidity and mortality due to severe malarial anemia in Kasungu District, Central Malawi. **A. S. Jung**, **C. B. Lee**, S. B. Baek, S. B. Chung~~ withdrawn

281. Single molecule fluorescence studies on conformation of backbone branched RNA. **S. Dey**, D. Grahacharya, L. A. Peteanu, S. R. Das

~~**282.** Adjusting metal-organic framework pore environment via cation exchange to tune kinetic stability in the presence of water. **A. B. Spore**, N. L. Rosi~~ withdrawn

FRIDAY MORNING

Analytical Chemistry in the Central Region (Part I)

Ohio

A. Michael, *Organizer, Presiding*

8:30 283. Identifying ovarian cancer aptamers with multiple selection modes and bioinformatics. **R. Whelan**, J. Shallcross, R. Eaton, T. Uhm, M. Felder, A. Kapur, M. Patankar

9:00 284. Influx of aqueous cholesterol to the cell plasma membrane. **J. Burgess**

9:20 285. Understanding and improving ferriprotoporphyrin electropolymerization for selective detection of physiological H_2S. **J. A. Bennett**

9:40 Break

10:00 286. Simple approaches for achieving quantitative point-of-care assays. **S. T. Phillips**

10:30 287. Multidimensional NMR characterization of pentafluorophenyl-terminated hyperbranchedpolyfluorinated poly(benzyl ether) samples. **F. J. Wyzgoski**, M. J. Quast, A. Mueller, C. Gao, P. L. Rinaldi

10:50 288. Investigating the structural modifications of the iron-responsive element in the human FTH1 IRE/IRP complex under various conditions. **E. T. Mendenhall**, B. Wang, M. L. Norton, W. L. Patterson III, M. Rahman

11:10 289. Ruthenium-modified sensitive no sensors: Quantifying nitric oxide in the pathobiology of cystic fibrosis. **T. Bose**

Entrepreneurs' Tool Kit: Resources and True Stories (Part I)

Foster

Sponsored by ACS Division of Small Chemical Businesses
J. Sabol, X. Ling, *Organizers*
R. Taylor, *Organizer, Presiding*

8:30 290. IP basics, securing intellectual property (IP) and avoiding common IP pitfalls. **P. C. Lauro**

9:00 291. Grow your business with recipes for marketing success. **S. Cohen**

9:20 292. Creating and sustaining a viable service-based business in the chemical sector. **J. Sabol**

9:40 Break

10:00 293. Top 10 steps to business success... and missteps to avoid. **J. Allen**, G. Arnold

10:30 294. Helping your company grow: Your free, confidential SCORE Advisory Board. **S. Cohen**

10:50 295. The story of Cohera Medical, Inc. **E. Beckman**

General Session (Part IV)

Salk

M. Ward, M. Speer, *Organizers*
K. Ricardo, *Organizer, Presiding*

~~**8:30 296.** Anti-reflection glass with characterization of anti-degradation and developed by Grafting Silane. **L. Liang**~~ withdrawn

9:00 297. Transition metal PARACEST and PARASHIFT molecular imaging probes responsive to temperature, pH and redox. **P. B. Tsitovich**, J. R. Morrow

9:20 298. Interaction between proteins and quinone methide precursors: Toward realkylation of aged acetylcholinesterase. **Q. Zhuang**, C. S. Callam, &. Dogan-Ekici, T. Secor, A. Smith, B. Sauner, C. M. Hadad

9:40 Break

10:00 299. B-Site substituted perovskites for oxygen storage applications. **J. W. Lekse**, S. Natesakhawat, D. Alfonso, C. Matranga

10:30 300. Sequence matters: Determining the sequence effect of conjugated trimers, tetramers and hexamers on electronic structure properties. **I. Y. Kanal**, G. Hutchison, J. Bechtel, T. Meyer, S. Zhang

~~**10:50 301.** Enhanced room-temperature corrosion of copper in the presence of graphene. **F. Zhou**, Z. Li, G. Shenoy, L. Li, H. Liu~~ withdrawn

11:10 302. Gas phase formation and reactivity of mixed metal cluster cations containing silver and calcium. **S. Osburn**, A. Plaviak, M. Van Stipdonk

Innovations in Undergraduate Chemistry Education

Interstate

J. Grabowski, D. Hoover, *Organizers, Presiding*

8:30 303. Use of online homework in general chemistry: Sex-differentiated attitudes and success rates. **M. Richards-Babb**, J. Jackson

9:00 304. Critical thinking inspired by reflective journals in chemistry. M. N. Srnec, G. A. Buckholtz, E. S. Gawalt, **J. D. Evanseck**

9:20 305. "Everything old is new again": Teaching general chemistry using the flipped classroom and with the iPad. **J. R. Zubricky**

9:40 Break

10:00 306. Support for innovation in undergraduate chemistry education from the National Science Foundation. **D. R. Brown**, D. Rickey, N. Bennett

10:30 307. Diverse techniques used to teach green chemistry. **S. Kennedy**

10:50 308. Recitation hour or guided inquiry learning: How do students fare in an organic chemistry course under these two approaches? **F. Yepez Castillo**

11:10 309. Using team-based learning strategies to promote student engagement in a thermodynamics course. **D. Miller**

Molecular Recognition of and by Nucleic Acids
PPG

Sponsored by Waters Corporation
B. Armitage, *Organizer, Presiding*

8:30 310. Challenges and progress in DNA recognition. **D. H. Ly**

9:00 311. Label-free molecular beacons for biomolecular detection. **X. Tan**, Y. Wang, B. Armitage, M. Bruchez

9:20 312. Building bright fluorescent dye labeled peptide nucleic acid probes. **E. E. Rastede**, B. A. Armitage

9:40 Break

10:00 313. Capture and quantitation of cell-free telomeric DNA from cancer cells. K. W. Harris, K. L. Hayden, K. S. Selander, B. A. Armitage, **D. E. Graves**

10:30 314. Hybridization of G-quadruplex-forming peptide nucleic acids to guanine-rich DNA templates inhibits DNA polymerase η extension. **C. T. Murphy**, A. Gupta, B. A. Armitage, P. L. Opresko

10:50 315. Optical control of oligonucleotide function in cells and animals. **A. Deiters**

11:10 316. Sequence-directed labeling and manipulation of ribonucleoprotein machines. **M. Bruchez**

Solid-State Materials (Part IV)
Allegheny

J. Aitken, *Organizer, Presiding*
P. Woodward, *Presiding*

8:30 317. Nanostructured solids as a platform for materials discovery. **R. Schaak**

9:00 318. Observing polytypism in multi-shell giant quantum dots. **S. Majumder**, M. M. Maye

9:20 319. Synthesis and magnetism of electron- and hole-doped europium chalcogenides. **N. Rosa**, W. L. Boncher, L. Figueroa, S. Pineda, S. L. Stoll

9:40 Break

10:00 320. Towards predictive synthesis of metastable solid state materials. **P. A. Salvador**, G. S. Rohrer, J. R. Kitchin, W. Prellier

10:30 321. Molecular silver nanoparticles and their assemblies. **T. P. Bigioni**

10:50 322. Probing gas-solid reactions at the atomic level using environmental TEM. **R. Wang**

11:10 323. Au_{23}, Au_{24} and Au_{25} protected by thiolates: A trio of nanoclusters. **A. Das**, R. Jin

Surface and Microscopic Characterization of Manufactured Nanomaterials (Part I)
Westinghouse

B. R. Strohmeier, *Organizer, Presiding*

8:30 324. Surface characterization of S-tolerant PdCuAu H_2 separation alloys. **J. B. Miller**, C. Yin, G. Gumuslu, A. J. Gellman

9:00 325. Surface characterization of nanoparticle-incorporated thin film oxides in support of gas sensor development. **J. P. Baltrus**, P. R. Ohodinicki, T. R. Brown

9:20 326. Effects of solvent environment on electron injection into TiO_2: Differences between DSSCs and H_2 generating systems. **R. P. Sabatini**, W. T. Eckenhoff, A. Orchard, K. R. Liwosz, M. R. Detty, D. F. Watson, D. W. McCamant, R. Eisenberg

9:40 Break

10:00 327. On the intrinsic wettability of graphitic surfaces. **L. Li**, Z. Li, A. Kozbial, Y. Wang, H. Liu

10:30 328. Effective method to protect graphitic surface from airborne hydrocarbon contamination. **Z. Li**, A. Kozbial, L. Li, H. Liu

10:50 329. Two color sum frequency generation spectroscopy on size selective enriched single walled carbon nanotubes. **S. K. Das**, S. Sengupta, L. Velarde

11:10 330. Advanced surface characterization of thin film nanostructures using x-ray photoelectron spectroscopy (XPS) and argon cluster ion depth profiling. **B. R. Strohmeier**, R. G. White, T. S. Nunney, P. Mack, A. E. Wright

The Science of CO_2 Capture in Energy Production (Part I)
Monongahela

J. Steckel, K. Johnson, *Organizers*
H. Nulwala, *Organizer, Presiding*

8:30 331. CO2-reactive ionic liquids: Alkyl-substituted triazolides and amine-substituted cholines. **R. L. Thompson**, H. Nulwala, K. Damodaran, W. Shi, E. Albenze, D. R. Luebke

9:00 332. Overview of carbon capture research and development at the National Energy Technology Laboratory. **M. Matuszewski**

9:20 333. Ultrafast 2D-IR spectroscopy probes CO_2 uptake in ionic liquids. **S. Garrett-Roe**, T. Brinzer, Z. Ren, S. Dutta

9:40 Break

10:00 334. Core-shell MOFs designed for selective CO_2 capture. **N. L. Rosi**

10:30 335. Design of Lewis Pairs-Functionalized metal organic frameworks for CO_2 hydrogenation. **J. Ye**, K. Johnson

10:50 336. Evaluation of kinetic models to describe sigmoidal adsorption rates in gate-opening metal organic frameworks for kinetic separations. **A. D. Lueking**, S. Sircar, C. Wang, C. Malencia

11:10 337. FE-NI Bi-metallic carriers for chemical looping dry reforming of methane. **A. More**, G. Veser

Undergraduate Poster Session
Salons D, E

E. Baldauff, *Organizer*

10:00 - 11:30

338. Investigation of the role of chlorine and fluorine on CH/pi binding. **K. Wolfe**, M. R. Ams

339. Influence of angle strain on the CH/pi interaction: A systematic study using the Wilcox molecular torsion balance. **J. Patterson**, M. R. Ams

340. Systematic study of the influence of fluorine on the CH-pi interaction: Implications for drug design. **R. Sheridan**, M. R. Ams, M. Fields, T. Grabnic

341. Changes to membrane permeability by perfluorinated compounds. **E. A. Tatarkov**, C. E. Spiese

342. Effects of targeted combinations of kinase inhibitors and low dose radiation on erbB2+ cancer cells. **A. E. Walter**, **C. J. Kuhnheim**, D. L. Jones, **C. E. Taylor**

343. Progress towards the development of an organocatalytic method for generating imine nucleophiles. **Z. W. Taylor**, **C. E. Taylor**

344. Treatment of hydraulic fracturing contaminated water using *Closterium moniliferum*: Protein expression and Ba and Sr elemental analysis. **L. Jubic**, H. Boylan, K. Resendes, L. Miller

345. Chemical signaling between algae species in a Wisconsin river. **A. Baert**, D. Poister, A. Schaefer, J. Tracey, K. Richards

346. Chemical loss of *agr* quorum sensing and virulence pathway function leads to early growth advantage in *staphylococcus aureus* infection. **A. Winnett**, J. K. Femling

347. Analysis of the open limestone channel at the Swank 13 abandoned coal mine: Reade Township, PA. **J. P. Krug**, R. C. Krupa, **C. J. Weyant**, D. R. Mosier, B. Kebede, W. H. Strosnider, E. P. Zovinka

348. Characterization of the photocleavage mechanisms of ruthenium(II) polypyridyl complexes. **S. Yang**, **K. Wang**, S. J. Burgmayer

349. Potential allosteric modulators of focal adhesion kinase activity determined by virtual screening techniques. **B. C. Neeley**, B. Mertz

350. Nicotine-triggered dopamine response in pheochromocytoma rat cell lines: Bringing metabolomics into the sophomore organic chemistry laboratory. **J. Osko**, F. Yepez Castillo

351. Metal-dependent stability change of DJ-1 protein carrying a Parkinson's Disease mutation. **A. A. Geraets**, E. Shuman, N. Smith, M. Wilson, J. Lee

352. Electronic properties of halide perovskites with organic cations. **J. F. Khoury**, P. M. Woodward

353. Evaluation of a redox-active NHC pincer ligand nickel(II) complex as a catalyst for oxidative C-C coupling reactions. **J. E. Hertzog**, C. F. Harris, J. D. Soper

~~**354.** Computational modeling of temporary anion states in the field of a dipole or quadrupole moment. **E. Tharnish**, M. F. Falcetta~~ withdrawn

355. Computational modeling of resonant vibrational excitation of CO by electron impact. **L. Williams**, M. F. Falcetta

356. Comparing effects of added acid verses added base on a buffer's pH. **M. A. Hawranick**, K. Alzouhayli, E. Echi, **M. Han**

357. Determining the amount of caffeine and theobromine in dark chocolates from unique sources in Africa. **B. Ho**, K. S. Wendling

358. Therapeutic potential of cerium oxide nanoparticles for the treatment of sepsis induced kidney dysfunction. **R. Goydel**, K. Rice, E. Fankhanel, N. D. Manne, E. Blough

359. Application of a new DFT method to a small peptide. **M. A. Shebel**, J. A. Thomas

360. Electro-chemical genome of homo-halogenated benzenes: A DFT investigation. B. X. Schatschneider, **R. P. Baer**

361. Electrochemical reduction of graphene oxide on platinum electrodes from aqueous and non-aqueous solutions. **I. Agbere**, J. A. Bennett

362. Engineering self-assembling peptide amphiphiles for cancer imaging. **M. J. Nicholl**, A. Ghosh, C. Buettner, M. F. Tweedle, J. E. Goldberger

363. Evaluating Pt black as an electrocatalyst support for H_2S detection. **R. Custer**, J. A. Bennett

364. Synthesis and characterization of $(pip_2NNN)Co(Cl)_2$. **B. Hakey**, M. Sabat, J. R. Webb

365. Synthesis, characterization, and electrochemical studies of water soluble ruthenium complexes. **A. Jain**, A. Kishlock, E. A. Stimmell

366. Pyrolysis products from the thermal decomposition of pivaldehyde and isovaleraldehyde. **B. J. Warner**, E. M. Wright, E. R. Sias, C. D. Hatten, L. R. McCunn

367. Identifying products of the thermal decomposition of 3-oxetanone. **E. M. Wright**, B. J. Warner, H. E. Foreman, E. R. Sias, L. R. McCunn

368. Reactivity of rhodium peroxido complexes. **L. Moneypenny**, J. R. Webb

369. Molecular modeling of iron porphyrins and platinum surfaces. **S. N. Simkovitch**, S. Simpson, J. Bennett, E. Zurek

370. Isolation of cyanobacterial secondary metabolites with activity at the 5-HT_7 receptor. **C. R. Work**, K. J. Tidgewell, T. Ahmed

371. Modified surface of zinc oxide nanoparticles using pPerfluorophosphonic acid self assembled monolayers. **C. Peck**, R. Quiñones

372. Polymorphism: Screening active pharmaceuticals using SAMs and metal plates. R. Quiñones, **N. Searls**

373. Synthesis of biodiesel using nanoparticles in the inorganic chemistry laboratory. **R. C. Krupa**, D. D'Andrea, B. D. Smith, E. P. Zovinka

374. Mild and direct amination of tertiary alkyl halides with imido-iodinanes. **A. C. Brueckner**, **E. J. Anders**, A. A. Lamar

375. Mild, iodine-promoted synthesis of *N*-sulfonyl imines using imido-iodinanes. **J. A. MacGruder**, A. A. Lamar

376. Utilizing electrochemical impedance spectroscopy for detection of 2,2',4,4'-tetrabromodiphenyl ether. **N. Balfe**, L. Zheng, I. I. Suni

377. Crystal stabilization energy in organic molecular crystals: A case study of Rubrene Polymorphs. B. Schatschneider, **T. Garcia**

378. Synthesis of a rhodium complex bearing a C_1-symmetric bis(imino)pyridine ligand for asymmetric hydrogenation. **N. N. Baughman**, J. R. Webb

379. Developing a cost-effective Raman spectroscopy instrument for use in the college classroom. **J. Wierszewski**, D. Miller

380. Computational analysis of hydrogen and chlorine adsorption to graphene. **K. G. Mulugeta**, R. C. Brown

381. Picolinicamides derivatives as ligands in Ullmann type O-Arylation. **J. Malone**, **C. Ludwig**, **E. Vik**, F. Damkaci

382. Synthesis of novel cyclic amino acids with basic side-chain. **W. A. Shee**, M. J. Jones, B. Hargittai

383. Synthesis of lactam analogues of α-conotoxin SI. **C. M. Fry**, J. R. Teachout, M. R. Hargittai, B. Hargittai

384. Synthesis of chiral cation selective crown ethers. S. M. Ciraula, **C. R. Evans**, B. Hargittai

385. Application of copper catalyzed Atom Transfer Radical Addition (ATRA) for the synthesis of highly functional nitrogen containing monoadducts. **J. P. Martin**, G. J. Pros, T. Pintauer

386. Thermal decomposition of 4-nitrosooxy-2-butanone. **E. R. Sias**, B. J. Warner, E. M. Wright, L. R. McCunn

387. Zinc dehalogenation of organohalides. **D. P. Mallory**, M. F. Charlton-Smith

388. Ab initio dynamics of the unfolding and decarboxylation of pseudo-chair carboxyphosphate in aqueous solution using QM/MM and QM/QM models. **E. Jesikiewicz**, S. Boesch, S. M. Firestine, J. D. Evanseck

389. Biochemical and biophysical analyses of *CDK5R2* mRNA G-quadruplex secondary structures and their influence on the pathogenesis of fragile x syndrome. **C. M. Gaetano**, M. Mihailescu

390. Kinetics and mechanism of pyrene fluorescence quenching by iodide in water-ethanol mixture. **T. S. Breidenbaugh**, K. M. Kufta, B. H. Milosavljevic

391. Effect of linker length and structure on DNA probe binding capacity. **D. D. Carte**, C. Warner, T. Skidmore, Z. Hunter, B. S. Day

392. Laser ablation inductively coupled plasma for the quantitative analysis of inorganic elements in dried blood spots. **S. Sheffield**, L. Miller, H. Kingston

393. Quantum models of methylphosphonate adsorption onto the rutile (110) surface. **S. W. Clifford**, M. N. Srnec, E. S. Gawalt, J. D. Evanseck

394. Atom transfer radical addition of copper complexes with TPEN and TPEN* ligands in polar aprotic solvent system. **E. E. Gorse**, T. Pintauer, A. Kaur, G. Pros

395. Expression, transfection optimization, and production of major hominoid semen coagulation proteins. **M. Hockman**, M. Jensen-Seaman

396. Ferrocene as a bio-fuel additive: Ferrocene's effects on the thermodynamic properties of corn oil. **H. Landis**, **M. Allen**, K. Brock, P. Cristofari, L. Zook-Gerdau, R. Rataiczak

397. Water quality study of the Salt Creek Watershed. **K. Brock**, L. Zook-Gerdau

398. Elevated temperature investigation of copper catalyzed atom transfer radical addition (ATRA) utilizing monohalogenated alkyl halides. **A. Jansto**, T. Pintauer

399. Quantitation of the DNA binding specificity of human mitochondrial transcription factor A to the light strand promoter. **S. A. Mitarnowski**, J. N. Scott, M. R. Hargittai

400. 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. Ahmed, J. Rohde, J. D. Evanseck

401. High-throughput computational analysis of electro-structural properties for polycyclic aromatic hydrocarbons. **S. Monaco**

402. Interaction of phenanthridine fused quinazoliniminiums with double stranded DNA. **O. M. Pishnak**, T. Liyange, S. Rayat

403. Methods for grafting short polymeric units onto Kraft lignin. **C. Godfrey**, **N. Carroll**, E. Schurter, K. Zheng

404. Competitive uptake of 23 metals on five functionalized solid supports. **B. J. Foley**, B. Torre, J. M. Fitzsimmons

405. Design, synthesis, and characterization of zinc (II) complexes of dithiolene and dithione ligands. **S. C. Ratvasky**, B. Mogesa, M. van Stipdonk, P. Basu

406. Soil lead content in urban community gardens. **C. Hemmingsen**, J. Hemmingsen

407. Computational assessment of electron density in metallo-organic catalytic species for formation of C-P bonds. **J. Eller**, K. E. Downey

408. Computational SSNMR chemical shift peak matching of geometry optimized organic crystals. **S. Upadhyay**, M. Srnec, J. Madura, R. Iuliucci

409. Analysis of organic capture capabilities of advanced functionalized sorbents. **V. Smith**, B. White, K. Nell, D. Johnson

410. Orientation and conformation of surfactants with amino acid head groups at aqueous interfaces investigated with VSFG spectroscopy. **S. Wilson**, M. Silva, M. Williams, L. Clark, M. R. Watry

411. Effects of the inhalation anesthetic halothane on the conformation and orientation of lipids in lipid monolayers at water interfaces examined by VSFG spectroscopy. **M. Williams**, M. R. Watry

412. Sythesis and catalytic testing of Au dendrimer encapsulated nanoparticles. **M. McCoy**, B. S. Day

413. Organic synthesis of novel SSRI analogues. **E. Kantor**, B. Jean, R. B. Lettan, J. D. Madura

414. Characterization of substrate specificity of β-Glucosidase BglX from Esherichia coli. **J. W. Weimer**, **M. S. Welsh**, L. Sui, N. V. Stourman

~~**415.** Synthesis of [4]ferrocenophane toward a general route to [4]metallocenophanes. **B. D. Coleman**, M. Castellani~~ withdrawn

416. Amine synthesis and their effects on dithiocarbamates. **N. B. King**

417. Presentation of the peptide sequence, RGD, (arginine, glycine, aspartic acid) tethered to polyethylene glycol hydrogels as examined by VSFG spectroscopy. **D. Schmitt**, R. Asawa, J. McGee, H. Baca, D. Doroski, M. R. Watry

418. Synthesis of cobalt dithiocarbamate complexes. **G. Azzarello**, E. Sylvester

419. Influence of competitive, attractive, ground state, complex interactions on the stereochemical outcome of Diels-Alder reactions of enals catalyzed by Group 13 chiral Lewis acids. **A. Ahmed**, A. Kelly, B. Vernier, J. J. Rohde, J. D. Evanseck

420. Utilization of novel binuclear copper complexes in atom transfer radical addition (ATRA). **E. Perez**, A. Kaur, T. Pintauer

421. Structural analysis of a proposed intrinsically unstructured protein region using fluorescence spectroscopic techniques. **M. R. Limbacher**, **J. L. Villemain**

422. Synthesis and solid state structures of a library of substituted N,N-diaryl ureas. **M. Hakimian**, O. Pishnak, K. Epa, B. Sandhu, J. Desper, C. B. Aakeroy, S. Rayat

423. Peptide sequencing using gas-phase peptide carbocations. **A. Plaviak**, M. J. Van Stipdonk

424. Quantum modeling of molecular orientation of alkylcarboxylic acids adsorbed to α-Al_2O_3(0001) surface. **S. O. Neel**

425. Isolation of cyanobacterial secondary metabolites with activity at the 5-HT_7 receptor. R. A. Clark, **B. Jones**, D. Reckner

426. Toward synthesis of a P-stereogenic frustrated Lewis pair. **A. S. Porter**, T. W. Chapp

427. Electrochemical dissolution of pyrite. R. A. Clark, **K. Kozak**, B. Jones, **B. Herman**

428. Additions to the chemistry curriculum and optimization of an existing lab. **J. E. Jurczyk**, T. W. Chapp

429. Reduction of a racemic P-stereogenic phosphine oxide and a new one-step approach for preparation of its reduced form. **J. Hong**, T. W. Chapp

430. Molecular dynamics simulations of human γD-crystallin aggregates found in cataracts. **S. A. Richards**, R. A. Wheeler

431. Synthesis and characterization of metal complexes from Schiff base ligands derived from amino acids. **E. Bain**, S. Caddies

432. Experimental optimization of DNA aptamer usage conditions. **K. Humphreys**, K. M. Hickey, P. M. Gannett, K. L. Pisane

433. Exchange between Fe(III) and In(III)/Ga(III) dithiocarbamates in solution. **N. M. Barker**, N. V. Duffy, M. Logan, J. Coffield

434. Investigation of macromolecular crowding in ferredoxin and ferredoxin NADP+ reductase kinetics. **D. Bautista**, S. Owen, D. Seybert

435. Mixed carboxylic and phosphonic acid monolayers on titanium and Ti-6Al-4V surface. **A. A. Dalal**, N. A. Reger, E. S. Gawalt

436. Free radical production and inhibition demonstrated by luminometry. **A. M. Predmore**, C. Saladino

437. Investigations of solvent and steric effects on aldimine synthesis. **R. Neldon**, K. Blaha, B. W. Knettle

438. Mixed mitigation by antioxidants and green tea extract of the mutagenicity of 3-nitrobenzanthrone in the Ames *Salmonella*/microsome mutagenicity assay. **W. Wang**

439. Photophysical studies of pyrenyl attached polymers. **J. C. Becca**, M. J. Bertocchi, R. G. Weiss

440. Infinitely large kinetic isotope effect in parallel dissociation reactions of acetone+ and acetone-d6 cations. **N. K. Wells**

441. Microwave-assisted organic synthesis of 4′-substituted 2,2′:6′,2″-terpyridines. **D. Waugh**, **I. Williams**, C. Shreiner

442. Substrate transport and conformational change of the monoamine transporters. **M. J. Acevedo**, E. M. Benner, J. D. Madura

443. Coordination cyclopolymerization of bis(allyl)organosilanes for the formation of polycarbosilanes: Investigation of the Thorpe-Ingold Effect. **K. F. Augustine**, K. E. Crawford, L. R. Sita

444. Conformational analysis of cyclic disulfides and selenenyl sulfides in peptide redox motifs. **D. B. Pollard**, C. A. Bayse

445. Substituent effects on the properties of short oligothiophenes: A combined physical and theoretical approach. **A. P. Hu**, C. M. Legaspi, R. C. Jemison, K. A. Penrod, L. A. Peteanu, D. J. Yaron, R. D. McCullough

446. Investigation of genetic material transfer during the laundering process. **D. Matt**, C. Pickard, S. Wiechman

447. Effectiveness of various spectroscopic methods in the analysis of drug mixtures. **A. Heinle**, M. Cipoletti

448. Quantification of met-enkephalin and leu-enkephalin using microdialysis sampling coupled on-line with micro-extraction by packed sorbent (MEPS). **C. D. Rugh**, H. Fletcher

449. Using SRB assays to explore the growth inhibition of canine TCC cells: A study involving Tl^{+} and Cu^{2+}. **A. M. Zimmer**, A. J. Heston

450. Development of a safe and efficient near-infrared diagnostic method for Alzheimer's Disease. **J. G. Tawney**, E. A. Owens, M. Henary

451. Synthesis of novel rare-earth substituted pyrochlores. **J. D. Aldridge**, D. P. Sunderland

452. Impact of lanthanum doping on Fe/ceria oxygen carriers for chemical looping combustion. **N. Isenberg**, S. Bhavsar, G. Veser

453. Dynamic reactor simulations of chemical looping combustion in a fixed-bed reactor. **J. D. Hughes**, G. Veser

454. Progress toward the synthesis of the Choi framework. **J. Tropp**, M. S. Leonard

455. Real-world applications in the organic laboratory: Sunscreen production. **B. C. Dominguez**, J. D. Fair

456. The use of weak base to restore catalytic activity of [Cu(Me_6TREN)Cl]Cl in ATRA in the presence of ascorbic acid as a reducing agent. **M. C. Wasson**, G. J. Pros, A. Kaur, T. Pintauer

457. ^{15}N vibrational frequency shifts of the Rieske iron-sulfur cluster distinguish the protonation states of histidine ligands from cytochromes bc1 and b6f. **B. R. Jagger**, A. M. Koval, R. A. Wheeler

458. Short-strong hydrogen bond strength in pseudo-chair carboxyphosphate. **S. E. Kochanek**, T. M. Clymer, V. S. Pakkala, S. P. Hebert, S. M. Firestine, J. D. Evanseck

459. An electrochemical approach to control ring size of cyclic polyesters. **E. J. Helenbrook**, G. Faughnan, M. Cross, C. Porterfield, K. Arumugam

460. Synthesis of varying ferrocenylated *N*-heterocyclic carbene supported gold complexes. **K. J. Sidoran**, J. Arambula, K. Arumugam

461. Effects of viscosity and macromolecular crowding on the diffusion-controlled rate constant of Ferredoxin $NADP^{+}$ reductase. **S. R. Sweger**, J. D. Madura

462. Biophysical analysis of CDK5R2 DNA secondary structures. **K. J. Bandi**, B. A. DeMarco, R. Mihailescu

463. Determination of the activation energy and rate constants of the isomerization of 4-anilino-4'-nitroazobenzene using flash photolysis. **C. J. Park**

FRIDAY AFTERNOON

Plenary III

Salons D, E

M. Ward, A. Michael, *Organizers, Presiding*

1:00 464. From synthesis to materials design: New nanostructures and new catalysts. **S. E. Skrabalak**

Analytical Chemistry in the Central Region (Part II)
Ohio

A. Michael, *Organizer, Presiding*

2:20 465. Multifunctional nanogels for integrated biomolecule processing and separation. **L. A. Holland**, B. C. Durney, T. A. Davis, S. A. Gattu

2:50 466. Ultrafast infrared and computational study of the formation of alkynylcarbenes from cyclopropanated phenanthrene derivatives. **J. Joseph**, M. Chakraborty, J. M. Suzuki, D. M. Thamattoor, C. M. Hadad

3:10 467. Nanoparticle formation for colorimetric glucose detection. **S. A. Unser**, I. Campbell, D. Jana, L. B. Sagle

3:30 Break

3:50 468. Examining brain tissue during microdialysis probe insertion in real time using 2-photon microscopy. **A. Jaquins-Gerstl**, T. D. Kozai, X. T. Cui, A. C. Michael

4:20 469. Insights into iron storage in the metalloprotein, ferritin as analyzed by MALDI TOF mass spectrometry with superconducting tunnel junction cryodetection. **L. D. Plath**, A. A. Aksenov, M. E. Bier

4:40 470. Strategies for designing Fe(II) selective optical sensors. **T. Y. Tittiris**, J. R. Morrow

Beyond the Cookbook: Moving Undergraduate Laboratory Courses Forward
Interstate

J. Grabowski, D. Hoover, *Organizers, Presiding*

~~**2:20 471.** Employing practices from industry and academia in undergraduate analytical laboratory courses. **M. M. Ward**~~ withdrawn

2:50 472. Merger of the scientific method and communication skills with laboratory research experiences. M. N. Srnec, G. A. Buckholtz, E. S. Gawalt, **J. D. Evanseck**

3:10 473. Qualitative assessment and the hidden value of general chemistry lab. **G. R. Long**

3:30 Break

3:50 474. Active learning strategies in introductory organic laboratory courses. **J. A. Cramer**

4:20 475. Independent student research projects on crystal growth in the undergraduate inorganic chemistry laboratory. **D. A. Czegan**

4:40 476. Using solid phase microextraction in undergraduate organic chemistry laboratories: It doesn't get any greener! **J. D. Williams**, M. F. Antunez, D. C. Green

Entrepreneurs' Tool Kit: Resources and True Stories (Part II)

Foster

Sponsored by ACS Division of Small Chemical Businesses
R. Taylor, X. Ling, *Organizers*
J. Sabol, *Organizer, Presiding*

2:20 477. The Institute for Entrepreneurial Excellence: Helping your business start, grow, and prosper. **J. Ciotti**

2:50 478. True story: A wandering career path based on instinct and intuition. **P. E. Yeske**

3:10 479. Traveling from academia to entrepreneurship. **C. P. Horwitz**

3:30 Break

3:50 480. Bootstrapping a chemical company in the Steel City. **B. Bosley**, B. Bosley

4:20 481. The story of Liquid X Printed Metals. **B. Vasy**

4:40 482. Member benefits, programming, and entrepreneurial activities from the ACS Division of Small Chemical Businesses SCHB. **J. Sabol**

Spectroscopic Studies of Protein Structure and (Mal)Function

PPG

P. Van Der Wel, *Organizer, Presiding*

2:20 483. Paramagnetic metal based ESR distance rulers and their application in understanding protein-DNA interactions. **S. K. Saxena**

2:50 484. Structural dynamics of the NMDA recepter as determined by single molecule FRET. **D. Cooper**, D. Dolino, H. Jaurich, J. Chen, V. Jayaraman, C. F. Landes

3:10 485. Using 31P-NMR and 15N-NMR to understand the structural basis of substrate specificity for PI-PLC and GDPD Enzymes. **T. L. Selby**

3:30 Break

3:50 486. Structural mechanisms of HIV-1 capsid assembly and maturation. **P. Zhang**, G. Zhao, J. R. Perilla, E. l. Yufenyuy, X. Meng, J. Ning, J. Ahn, A. M. Gronenborn, K. Schulten, C. Aiken

4:20 487. Fragile X Mental Retardation Protein interactions with G quadruplex structures formed by dendritic mRNA targets. **R. Mihailescu**

4:40 488. Proteomics to understand immunity in Alzheimer's Disease. **R. A. Robinson**

Surface and Microscopic Characterization of Manufactured Nanomaterials (Part II)

Westinghouse

B. R. Strohmeier, *Organizer, Presiding*

2:20 489. Solution phase strategies for metal nanoparticle growth on colloidal plasmonic substrates. **J. Millstone**

2:50 490. Gold-thiolate ring as protecting motif in the $Au_{20}(SR)_{16}$ nanocluster and implications. **C. Zeng**, R. Jin

3:10 491. Surfactant-free exfoliation of graphite in aqueous solutions. **K. B. Ricardo**, H. Liu

3:30 Break

3:50 492. Probing micro and nanoscale behavior across the life cycle of materials used in life science applications. **M. Sparrow**, C. Morrison, K. Bunker, J. Mastovich

4:20 493. Single molecule protein patterning by hole mask colloidal lithography. **W. Lum**, M. Vieweger, H. Zhao, P. Guo, L. B. Sagle

4:40 494. Epitaxial electrodeposition of single crystal germanium nanowire arrays at room temperature in water. **E. Fahrenkrug**, J. Gu, S. Maldonado

The Science of CO_2 Capture in Energy Production (Part II)
Monongahela

J. Steckel, H. Nulwala, *Organizers*
K. Johnson, *Organizer, Presiding*

2:20 495. Structured membranes for CO_2 separations. **M. Mauter**, B. Adzima, S. Venna, S. Klara, H. He, M. Zhong, D. Leubke, K. Matyjaszewski, H. Nulwala

2:50 496. Nanostructured porous organic polymers for CO_2 capture and separation. **A. K. Sekizkardes**, S. Altarawneh, Z. Kahveci, T. Islamoglu, H. M. El-Kaderi

3:10 497. Thermodynamic descriptors to identify molecular co-catalysts for efficient electroreductions. **J. A. Keith**

3:30 Break

3:50 498. Computational study of transport behaviors of choline-based ionic liquids. **H. Kim**, F. Yan, H. Nulwala

4:20 499. Molecular models of carbon dioxide retention in hydrated smectite minerals using molecular dynamics and Monte Carlo simulations. **M. Makaremi**, K. D. Jordan, G. D. Guthrie, E. M. Myshakin

~~**4:40 500.** Structure-function relationship of NFU1 in iron-sulfur cluster biosynthesis. **J. Mao**, K. Damodaran~~ withdrawn

Culinary Chemistry: Bridging Innovations in Food and Science
Allegheny

S. Das, *Organizer, Presiding*

2:30 501. Teaching an "atoms first" food chemistry course using an integrated lecture/lab format. **J. K. Vohs**

3:00 502. Chemistry of fermented beverages as a component of an undergraduate curriculum. **C. D. Emal**

3:30 Break

3:50 503. Taste of chemistry. **S. R. Das**

4:20 Demonstrations

SATURDAY MORNING

CERM Award for Excellence in High School Teaching (Part I)
Salon A

D. Zimmerman, *Organizer, Presiding*

8:30 504. Preparation and analysis of potassium tris(oxalato)ferrate(III)trihydrate as a review for the AP Chemistry Examination. **L. McSparrin**

9:00 505. Vernier Mini GC Plus demonstration. **J. Randall**

9:30 Break

9:40 506. Designing and teaching outside the traditional box. **L. E. Slocum**

10:10 507. Chemistry outside the textbook covers. **E. Dabrowski**

10:40 508. Evolution of a chemistry teacher. **L. Ford**

Project SEED Poster Session
Salon A

J. Aitken, *Organizer*

11:30 - 12:30

509. Absolute binding free energy calculations bovine pancreas beta-trypsin in complex with benzamidine. **S. Lau**, B. Jean, J. Madura

510. Probing Serotonin transporter (SERT) structure by mutagenesis. **C. Perez**, E. Perez, R. Veeramachaneni, M. Cascio

511. Synthesis and characterization of quaternary diamond-like semiconductors. **C. Simmons**, J. Aitken, J. A. Brant

512. Synthesis and characterization of dithione ligands for metal chelation. **K. O'Kelley**, S. A. Dille, P. Basu

513. The investigation of the presence of organic GSR on SEM stubs. **K. Pesta**, L. Ali, S. Wetzel

514. Negative thermal expansion materials. **T. K. Reditt**, L. Young, C. Lind-Kovacs

~~**515.** Synthesis and characterization of blue pigments: An undergraduate laboratory module. **A. Latona**, C. W. Sinagra III, J. A. Aitken~~ withdrawn

516. Stability of self-assembled monolayers of organic acids on cobalt. **N. Kodjo**, N. Reger, E. Gawalt

~~**517.** Investigating substituent effects on the fragmentation spectra of protonated peptides modified to create N-terminal imines. **R. Nelson**, M. VanStipdonk, K. Patterson~~ withdrawn

518. Gecko adhesion on various substrates. **L. Edding**, M. Klittich, G. Amarpuri, A. Dhinojwala

~~**519.** R-value temperature dependence and LTTR of rigid polyurethane foams. **Z. Thompson**, G. Combs~~ withdrawn

520. The functional and structural studies on the COS domain of MID1. **M. Dagnachew**

521. Alcoa SEED-Alcoa Internship Experience: High School Teacher Perspective. N. Dando, **K. Stack**, **P. Kolek**

SATURDAY AFTERNOON

Project SEED Symposium

Salon A

J. Aitken, *Organizer*
M. Speer, *Presiding*

12:00 522. Ten ways in which Project SEED can benefit students. **J. A. Aitken**

12:15 523. How participation in two summers of Project SEED helped me to succeed. **C. M. Sidun**

CERM Award for Excellence in High School Teaching (Part II)
Salon A

D. Zimmerman, *Organizer, Presiding*

1:30 524. Kathy's favorite (chemistry) things. **K. Kitzmann**

2:00 525. Using Sherlock Holmes and reverse engineering strategies to hone problem solving skills in chemistry and beyond. **J. Lachvayder**

2:30 526. Wireless data collection with vernier sensors. **J. Randall**

3:00 Break

~~**3:10 527.** How do you know what you know? **W. Snyder**~~ withdrawn

~~**3:40 528.** Time of useful consciousness in chemistry. **R. Badanowski**~~ withdrawn

4:10 529. Chemistry is just too hard! **B. Buddendeck**

4:40 530. A STARs experience – combining research and professional development in STEM. **K. Weston**

CERM2014

The 45th Central Regional Meeting of the American Chemical Society

Oct. 29th - Nov. 1st, 2014

Exhibitor Directory

Wednesday, Oct. 29th & Thursday, Oct. 30th

9:00 am – 5:00 pm

Junior Ballroom

Advion

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www.advion.com

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CERM ACS 2015

www.jglcrm2015.com

Donna Nelson for ACS President

www.drdonnajnelson.com

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www.gatewayanalytical.com

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The 45th Central Regional Meeting of the American Chemical Society

Oct. 29th - Nov. 1st, 2014

Graduate School and Recruitment Fair Directory

Friday, Oct. 31st

9:00 am – 5:00 pm Junior Ballroom

Bryn Mawr College

www.brynmawr.edu

Carnegie Mellon University

www.cmu.edu

CERM ACS 2015

www.jglcrm2015.com

Chatham University

www.chatham.edu

Duquesne University

www.duq.edu

Indiana University of Pennsylvania

www.iup.edu

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SOUTH CAROLINA

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www.utoledo.edu

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West Virginia University

WestVirginiaUniversity.

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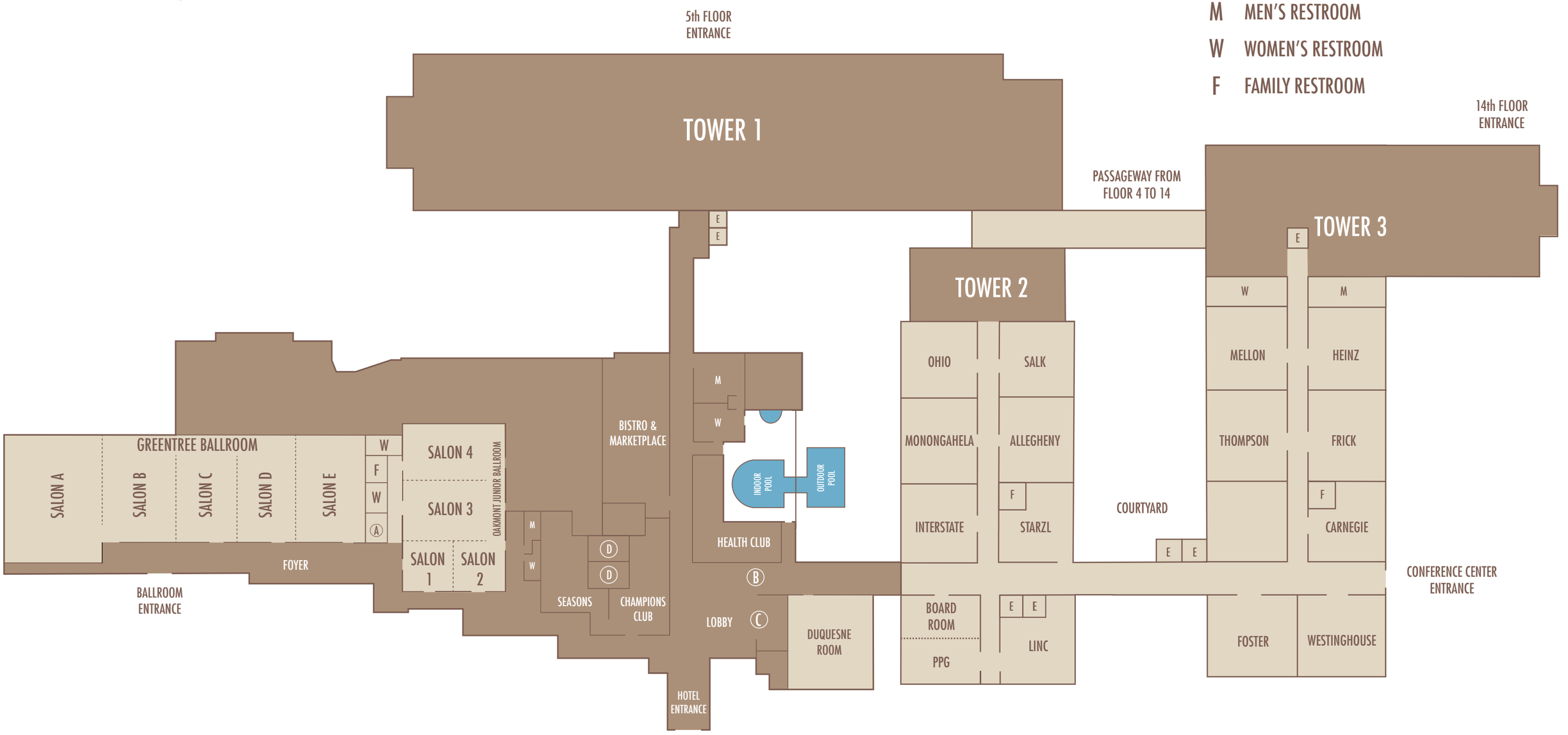
- E ELEVATORS
- A MEETING PLANNER'S OFFICE
- B BUSINESS CENTER
- C FRONT DESK
- D PRIVATE DINING ROOM
- M MEN'S RESTROOM
- W WOMEN'S RESTROOM
- F FAMILY RESTROOM



TRANSPORTATION

COURTESY SHUTTLE

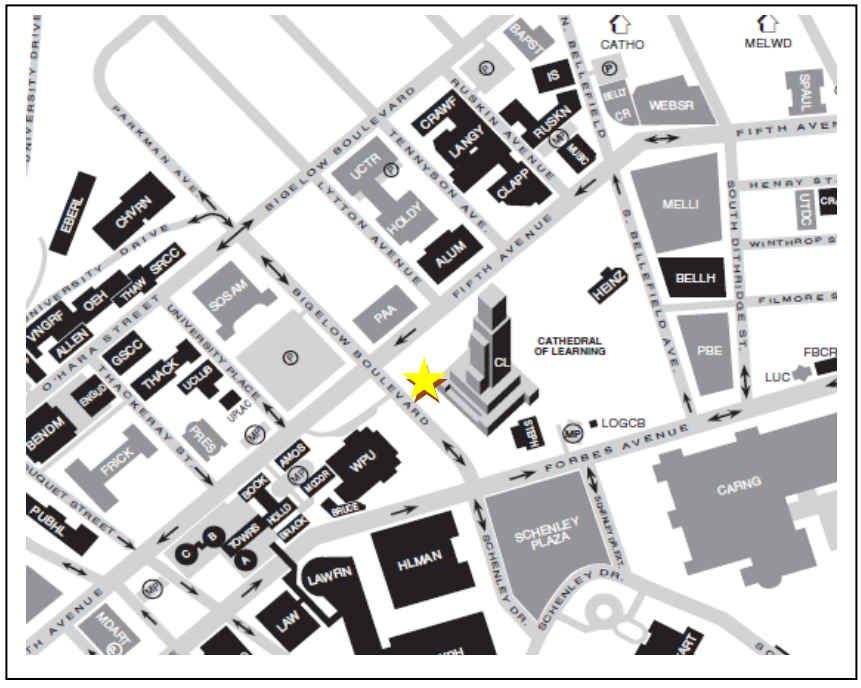
All service can be expected every 30-45 minutes, depending on traffic.

Oakland Shuttle Pickup: Fifth & Bigelow
Hotel Shuttle Pickup: Main Lobby Door

WEDNESDAY, October 29
7:00 AM - 12:00 PM
3:30 PM - 7:30 PM
9:30 PM - 11:00 PM

THURSDAY, October 30
7:00 AM - 12:00 PM
4:00 PM - 6:30 PM
9:30 PM - 11:00 PM

FRIDAY, October 31
7:00 AM - 12:00 PM
5:00 PM - 8:00 PM



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PUBLIC TRANSPORTATION FREQUENTLY ASKED QUESTIONS

Where does the Green Tree bus leave people off?

The Route 38 stop that is nearest to the hotel drops off at the corner of Green Tree and Mansfield Roads. Pedestrians will walk 0.6 miles down Mansfield before reaching the hotel on the right.

How long will my trip from Oakland take using PAT?

The Port Authority indicates a commute of one hour to one hour and fifteen minutes. Attendees are encouraged to use the Advanced Route Planner.

Can Duquesne University registrants pick up a PAT bus and ride it straight to the DoubleTree Green Tree?

The main PAT bus route that services Green Tree is Route 38 and runs on weekdays. Walk about 3 blocks to the corner of 5th Avenue and Washington Place (southwest corner of the Consol Energy Center). There, pick up one of the buses on Routes 65, 67, or 69 and take one of them inbound to Stanwix Street (Opposite 4th Avenue). Catch Route 38 at Stanwix Street (at Forbes Ave). Board the Outbound (Green Tree to Mt. Lebanon Station). The trip should take about 11 minutes.

Where can I find all PAT bus schedules?

The Port Authority website (www.portauthority.org) has complete schedules. The Route Planner is recommended for CERM 2014. *travelers.*

2014 ACS Central Regional Meeting

October 29 - November 1, 2014

Pittsburgh, Pennsylvania

AUTHOR INDEX

NOTES PAGE

BRIDGING CHEMISTRY AND INNOVATION

CERM 2014

NOTES PAGE

BRIDGING CHEMISTRY AND INNOVATION

CERM 2014

NOTES PAGE

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*The co-hosting Sections are the **Kalamazoo Section** in the **Great Lakes Region** and the **Western Michigan Section** in the **Central Region**.*

Program co-chairs

James J. Kiddle
Kalamazoo Section
James.Kiddle@wmich.edu

and

Mark Thomson
Western Michigan Section
MarkThomson@ferris.edu

General co-chairs

Lydia E. M. Hines
Kalamazoo Section
lemhwgh@gmail.com

and

Neal Fox
Western Michigan Section
NealFox@comcast.net

THEME:

Chemistry
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Plenary Speaker:

Scott Denmark
11 a.m., May 27 (Wed)

Keynote Speakers:

Joan Brennecke (ENVN)
4:30 p.m., May 27 (Wed)

Dustin Mergot (HEALTH)
4:30 p.m., May 28 (Thu)

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Food, Health, Environment

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