



## GORDON RESEARCH CONFERENCES

### FINAL PROGRESS REPORT

Department of Energy

Metals in Biology GRC & Bioinorganic Chemistry GRS

Grant Number DE-SC0019145

January 27, 2019 – February 3, 2019

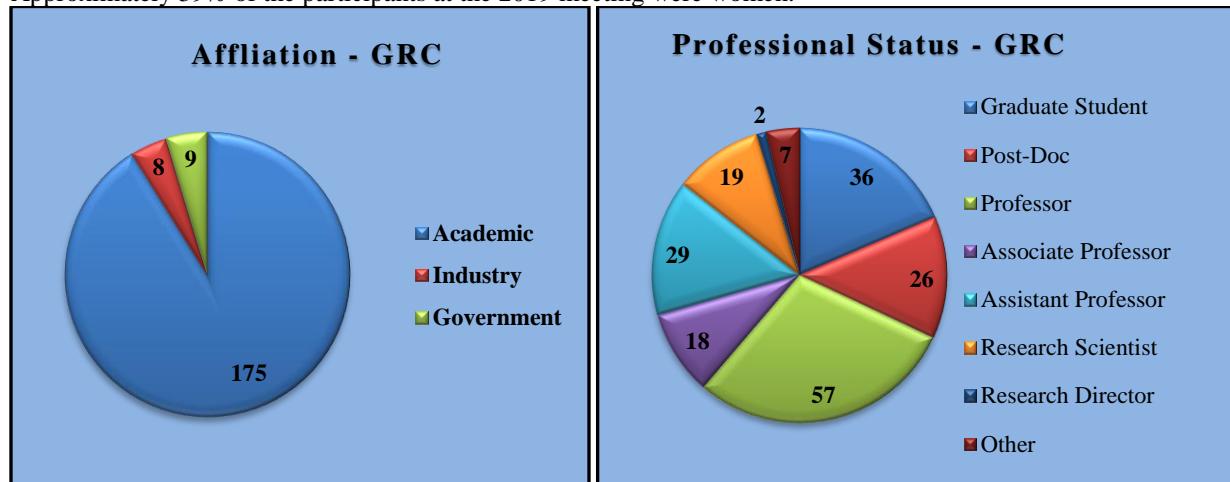
#### **Operational Summary**

The Gordon Research Conference (GRC) on Metals in Biology was held at the Four Points Sheraton/Holiday Inn Express in Ventura, California, on January 27 – February 1, 2019 and the accompany Gordon Research Seminar (GRS) on Bioinorganic Chemistry was held at the same location on January 31 - February 3, 2019. The meetings covered a variety of scientific topics and the content presented was highly rated by participants.



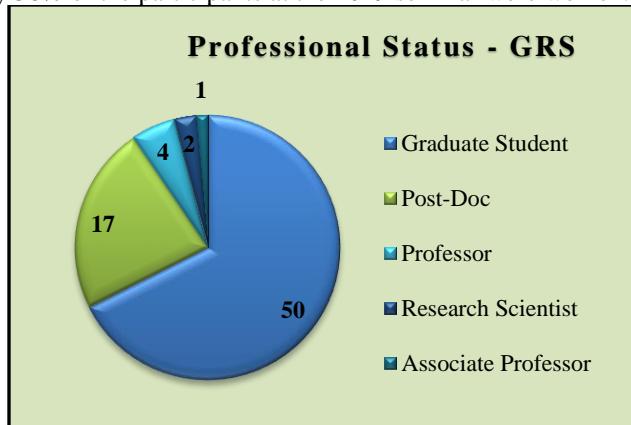
#### Conference Participants

The Conference was well-attended with 194 participants. Scientists from academia represented 90% of the participants while attendees from government accounted for 5% and those from industry totaled 4%. The meeting also attracted a strong mix of young investigators and senior scientists. Students and post-docs accounted for 32% of all attendees. Approximately 39% of the participants at the 2019 meeting were women.



#### Seminar Participants

The Conference was well attended with 74 participants. Scientists from academia represented 99% of the participants while there were no attendees from government or industry. Students and post docs combined accounted for 99% of all attendees. Approximately 38% of the participants at the 2019 seminar were women.



## **Conference Program**

The Metals in Biology Gordon Research Conference (MIB GRC) addresses long-standing, central challenges and emerging trends in the field of bioinorganic chemistry. The 2019 MIB GRC focused on novel, complex transformations in natural product biosynthesis, complex metallocofactor assembly and function, metal trafficking relevant to infectious disease, deployment of metalloenzymes for energy and commercial applications, and elucidation of modern metallobiogeochemistry and how it evolved. A primary goal of the 2019 meeting was to increase participation by scientists from underrepresented groups and ensure equitable gender representation among speakers and discussion leaders.

Metalloenzymes catalyze the most challenging and consequential chemical reactions on earth, including ATP-driven dinitrogen reduction and photochemical water oxidation. The complex clusters of redox-active transition metal ions and exogenous (in)organic ligands that support these reactions must be assembled/inserted into proteins by elegant biosynthetic machinery. Delineating the pathways for construction and the mechanisms of function of these elaborate multi-electron redox catalysts is a central challenge to the field of bioinorganic chemistry; analysis of how they arose on earth is fundamental to our understanding of our origins.

In addition to these central players in earth's element and energy economy, organisms have evolved an astounding array of metalloenzymes, powered by simple and complex metal cofactors, that promote reactions meeting specialized needs of diverse organisms in varied ecological niches. Some of these enzymes support basic metabolism and regulation, while others assemble Nature's astounding inventory of complex secondary metabolites, installing unusual functional groups that confer potent bioactivities. The direct deployment, engineering, and mimicry of these enzymes for research and commercial applications, another primary goal of bioinorganic chemists, holds great promise for society.

Most metalloproteins function only with a specific metal ion or cluster. This stringent metal specificity is one reason why cells must maintain concentrations within a relatively narrow range: too little of a trace metal can deprive essential metalloenzymes of their cofactors; too much can cause mismetallation of other biomolecules, blocking their functions. Cells and organisms balance uptake and efflux of each trace metal and control its distribution. Homeostasis is often antagonized by host or competing organisms that actively sequester (or, less commonly, induce overload of) essential metals. Mapping this complex metal-trafficking network, and exploiting it for disease therapy, are important goals of the field.

As sophisticated as Nature's catalysts are, they deploy only a small fraction of the periodic table. Abiological metals have surprising and useful bioactivities that have been leveraged for treatment of cancer, arthritis, and infectious diseases. In other cases, such metals are the basis for imaging diagnostics. When incorporated into proteins, these metals can enable reactions not represented among natural enzymes. Bioinorganic chemists continue to extract general principals underlying catalysis by metalloenzymes and marry them with the known chemistry of abiological metals to develop novel catalysts. Biomimetic and bioinspired chemistry is a vibrant focus of the field and provides underpinnings for innovation of new processes and deeper insight into Nature's elegant inorganic chemistry.

Bioinorganic chemistry is at the crossroads of biology and chemistry. From the primordial soup to present day diagnostic imaging agents, metals have occupied a central role in both biological processes and chemical reactions. Their critical roles in electron transport, cellular homeostasis, the regulation of global gas cycles, biomedical applications, and chemical catalysis are the reason why bioinorganic chemists continue to be inspired by metals in biology and seek to study, model, and replicate the chemistry these metals accomplish in nature. This Gordon Research Seminar focused on research at the frontier of metallobiochemistry, aimed not only at elucidating the myriad of roles metals play in biological processes and chemical transformations, but also understanding the roles of metals in emerging biological materials and the novel computational and modelling tools being employed to better understand their roles.

Celebrating its 23rd year, the Bioinorganic Chemistry GRS was established in 1996 due to the routinely oversubscribed Metals in Biology Gordon Research Conference (GRC) to provide a platform for young scientists to participate in a forum that focuses on novel research among a collaborative environment for scientists from a variety of fields. A joint session with the Metals in Biology GRC provided a unique opportunity for younger scientists to network with senior researchers in the field of bioinorganic chemistry.

## **Conference Budget**

Funding provided by the Department of Energy supported partial registration for 4 assistant professors and 1 postdoc at the GRC and partial registration for 8 graduate students and 2 postdocs at the GRS.

### **Conference Feedback**

Participants had an opportunity to provide feedback at the end of the Conference. The feedback collected from the meeting was extremely positive. Evaluations included numerous positive remarks regarding poster sessions, variety of talks, and the format of the conference. Evaluations from the GRS included positive comments, including “Poster sessions are very informative,” and “non-intimidating opportunity to ask questions.” Other positive comments included interactions and networking with peers, and “discussions and the explanations of the experimental data.”

GRC would like to thank the Department of Energy for its continued support of the meetings. The contributions received have been critical to the success of the conferences and are having a measurable impact in advancing the frontiers of science worldwide.

J. Martin Bollinger, GRC Chair  
The Pennsylvania State University

Dr. Victoria DeRose, GRC Vice Chair  
University of Oregon

Anastasia Manesis, GRS Chair  
Ohio State University

Kyle Rodriguez, GRS Chair  
University of Fribourg

Dr. Nancy Ryan Gray  
President and Chief Executive Officer  
Gordon Research Conferences

**Metals in Biology**  
**Gordon Research Conference**  
**Conference Program**

Sunday

4:00 pm - 8:00 pm Arrival and Check-in  
6:00 pm - 7:00 pm Dinner  
7:30 pm - 7:40 pm Introductory Comments by GRC Site Staff / Welcome from the GRC Chair  
7:40 pm - 9:30 pm Oxidative Rearrangements to Unusual Functional Groups in Bioactive Natural Products  
Discussion Leader: Amie Boal (Pennsylvania State University, USA)  
7:40 pm - 8:20 pm Michelle Chang (University of California, Berkeley, USA)  
"Discovery and Engineering of a Terminal Alkyne Pathway"  
8:20 pm - 8:35 pm Discussion  
8:35 pm - 9:15 pm Emily Balskus (Harvard University, USA)  
"Metalloenzyme Discovery in the Microbial World"  
9:15 pm - 9:30 pm Discussion

Monday

7:30 am - 8:30 am Breakfast  
8:30 am - 9:00 am Group Photo  
9:00 am - 12:30 pm Metal Acquisition, Restriction and Deployment at Host Disease Interfaces  
Discussion Leader: Elizabeth Nolan (Massachusetts Institute of Technology, USA)  
9:00 am - 9:30 am Paul Donnelly (University of Melbourne, Australia)  
"The Use of Radioactive Metal Ions for Diagnosis and Targeted Therapy of Cancer"  
9:30 am - 9:40 am Discussion  
9:40 am - 10:10 am Eric Skaar (Vanderbilt University Medical Center, USA)  
"The Intersection of Nutrition and Infection at the Host-Pathogen Interface"  
10:10 am - 10:20 am Discussion  
10:20 am - 10:45 am Coffee Break  
10:45 am - 11:10 am Ellen Heber-Katz (Lankenau Institute for Medical Research, USA)  
"Potent Regenerative Effects of Iron-Containing Prolyl Hydroxylases and Their Inhibitors"  
11:10 am - 11:20 am Discussion  
11:20 am - 11:45 am Bo Li (University of North Carolina at Chapel Hill, USA)  
"Metals and Mechanism of Dithiolopyrrolones"  
11:45 am - 11:55 am Discussion  
11:55 am - 12:20 pm Martin Hogbom (Stockholm University, Sweden)  
"Doing Without Metals: Metal-Free Class Ie Ribonucleotide Reductase"  
12:20 pm - 12:30 pm Discussion  
12:30 pm - 1:30 pm Lunch  
1:30 pm - 4:00 pm Free Time  
3:00 pm - 4:00 pm Power Hour  
The GRC Power Hour is an optional informal gathering open to all meeting participants. It is designed to help address the challenges women face in science and support the professional growth of women in our communities by providing an open forum for discussion and mentoring.

	Organizers: Zarath Summers (ExxonMobil Research and Engineering, USA), Anne-Frances Miller (University of Kentucky, USA) and Anastasia Manesis (Ohio State University, USA)
4:00 pm - 6:00 pm	Poster Session
6:00 pm - 7:00 pm	Dinner
7:30 pm - 9:30 pm	Iron-Sulfur Cluster Assembly and Disassembly in Catalysis and Regulation Discussion Leader: Patricia Dos Santos (Wake Forest University, USA)
7:30 pm - 7:40 pm	Introduction by Discussion Leader: Iron-Sulfur Cluster Dynamics: Past, Present and Future
7:40 pm - 8:10 pm	Tracey Rouault (National Institute of Child Health and Human Development, NIH, USA) "Biogenesis and Functions of Mammalian Iron-Sulfur Proteins in Multiple Pivotal Mammalian Metabolic Pathways"
8:10 pm - 8:20 pm	Discussion
8:20 pm - 8:50 pm	Carsten Krebs (Pennsylvania State University, USA) "New Roles for an Old Cofactor"
8:50 pm - 9:00 pm	Discussion
9:00 pm - 9:20 pm	Deborah Perlstein (Boston University, USA) "Dre2 and Nar1 Collaborate with the Nbp35-Cfd1 Iron-Sulfur Cluster Scaffold During the Early Steps in Cytosolic Iron-Sulfur Cluster Assembly"
9:20 pm - 9:30 pm	Discussion
Tuesday	
7:30 am - 8:30 am	Breakfast
9:00 am - 12:30 pm	Assembly and Function of Multielectron Redox Cofactors Discussion Leader: Joan Broderick (Montana State University, USA)
9:00 am - 9:30 am	R. David Britt (University of California, Davis, USA) "Spectroscopic Studies of Fe-S Enzyme Assembly"
9:30 am - 9:40 am	Discussion
9:40 am - 10:10 am	Oliver Einsle (University of Freiburg, Germany) "What Happened to Nitrogenase Cofactor ... During Catalysis"
10:10 am - 10:20 am	Discussion
10:20 am - 10:50 am	Coffee Break
10:50 am - 11:10 am	Steven Mansoorabadi (Auburn University, USA) "Biosynthesis of Coenzyme F430 and Assembly of Methyl-Coenzyme M Reductase"
11:10 am - 11:20 am	Discussion
11:20 am - 11:40 am	Jenny Yang (University of California, Irvine, USA) "Thermodynamic Considerations for Selective CO <sub>2</sub> Reduction to Formate"
11:40 am - 11:50 am	Discussion
11:50 am - 12:20 pm	Hannah Shafaat (The Ohio State University, USA) "If I Had a Nickel... Model Metalloenzymes for Energy Conversion"
12:20 pm - 12:30 pm	Discussion
12:30 pm - 1:30 pm	Lunch
1:30 pm - 4:00 pm	Free Time
4:00 pm - 6:00 pm	Poster Session
6:00 pm - 7:00 pm	Dinner
7:30 pm - 9:30 pm	Metalloenzymes for Commerce Discussion Leader: Victoria DeRose (University of Oregon, USA)

7:30 pm - 8:00 pm	Lana Saleh (New England Biolabs, USA) "Mechanism of TET Enzyme and Its Utility in Methylome Sequencing"
8:00 pm - 8:10 pm	Discussion
8:10 pm - 8:40 pm	Zarath Summers (ExxonMobil Research and Engineering, USA) "Heme Oxygenase: A Small Enzyme Tackling a Big Problem for Crude Oil Refining"
8:40 pm - 8:50 pm	Discussion
8:50 pm - 9:20 pm	Anna Fryszkowska (Merck & Co, Inc., USA) "Metalloenzymes in the Synthesis of Active Pharmaceutical Ingredients"
9:20 pm - 9:30 pm	Discussion
Wednesday	
7:30 am - 8:30 am	Breakfast
9:00 am - 12:30 pm	Toxicity, Signaling and Catalysis in the Biochemistry of Reactive O/N/S Species Discussion Leader: Anne-Frances Miller (University of Kentucky, USA)
9:00 am - 9:30 am	James Imlay (University of Illinois at Urbana-Champaign, USA) "Molecular Explanations for the Toxicity of Oxygen"
9:30 am - 9:40 am	Discussion
9:40 am - 10:10 am	Valeria Culotta (Johns Hopkins University, USA) "A New Family of Cu-Only Superoxide Dismutases for Fungal Pathogens"
10:10 am - 10:20 am	Discussion
10:20 am - 10:35 am	Julia Diaz (University of California, San Diego, USA) "A Role for NADPH-Dependent Extracellular Superoxide Production in Phytoplankton Photophysiology: Insights from the Marine Diatom <i>Thalassiosira oceanica</i> "
10:35 am - 10:40 am	Discussion
10:40 am - 11:10 am	Coffee Break
11:10 am - 11:40 am	Vincent Eijsink (Norwegian University of Life Sciences, Norway) "Hydrogen Peroxide-Driven Oxidative Cleavage of Polysaccharides by Monocopper Enzymes"
11:40 am - 11:50 am	Discussion
11:50 am - 12:20 pm	David Giedroc (Indiana University, USA) "Sensing Persulfides: Hydrogen Sulfide Homeostasis and Signaling in Bacterial Pathogens"
12:20 pm - 12:30 pm	Discussion
12:30 pm - 1:30 pm	Lunch
1:30 pm - 4:00 pm	Free Time
4:00 pm - 6:00 pm	Poster Session
6:00 pm - 7:00 pm	Dinner
7:00 pm - 7:30 pm	Business Meeting Nominations for the Next Vice Chair; Fill in Conference Evaluation Forms; Discuss Future Site and Scheduling Preferences; Election of the Next Vice Chair
7:30 pm - 9:30 pm	Microbes and Enzymes for a Sustainable Future Discussion Leader: Harry Gray (California Institute of Technology, USA)
7:30 pm - 7:40 pm	Introduction by Discussion Leader: The Role of Biology in Renewable Energy Science
7:40 pm - 8:10 pm	Shelley Minteer (University of Utah, USA) "Enzymatic Bioelectrocatalysis for Green Synthesis and Energy Harvesting"
8:10 pm - 8:20 pm	Discussion

8:20 pm - 8:50 pm	Syed Shams Yazdani (International Centre for Genetic Engineering and Biotechnology, India) "Engineering Aldehyde Deformylating Oxygenase (ADO) for Production of Hydrocarbon Fuels in Bacteria"
8:50 pm - 9:00 pm	Discussion
9:00 pm - 9:20 pm	Denis Proshlyakov (Michigan State University, USA) "Transient Intermediates in Aldehyde Deformylation Reaction by the Diiron Cluster of ADO"
9:20 pm - 9:30 pm	Discussion
Thursday	
7:30 am - 8:30 am	Breakfast
9:00 am - 12:30 pm	Modern and Ancient Metallobiogeochemistry Discussion Leader: John Peters (Washington State University, USA)
9:00 am - 9:30 am	Amy Rosenzweig (Northwestern University, USA) "Biological Methane Oxidation"
9:30 am - 9:40 am	Discussion
9:40 am - 10:10 am	Mak Saito (Woods Hole Oceanographic Institution, USA) "The Influence of Trace Elements and Vitamins on Productivity in Ocean Environments"
10:10 am - 10:20 am	Discussion
10:20 am - 10:35 am	Megen Culpepper (Appalachian State University, USA) "Deciphering the Metal Binding of Dimethylsulfide Degradation"
10:35 am - 10:40 am	Discussion
10:40 am - 11:10 am	Coffee Break
11:10 am - 11:40 am	Gerrit Schut (University of Georgia, USA) "Evolutionary Path of Modern Day Respiratory Complexes from a Proton-Reducing [NiFe]-Hydrogenase Ancestor"
11:40 am - 11:50 am	Discussion
11:50 am - 12:20 pm	Victoria Orphan (California Institute of Technology, USA) "Genomic Distinctions and Evolutionary Transitions from Methanogenic to Methanotrophic Archaea"
12:20 pm - 12:30 pm	Discussion
12:30 pm - 1:30 pm	Lunch
1:30 pm - 4:00 pm	Free Time
4:00 pm - 6:00 pm	Poster Session
6:00 pm - 7:00 pm	Dinner
7:30 pm - 9:30 pm	New Free Radical and Organometallic Enzyme Chemistry Discussion Leader: Vahe Bandarian (University of Utah, USA)
7:30 pm - 7:50 pm	Daniel Suess (Massachusetts Institute of Technology, USA) "Fe4S4 Clusters Featuring a Reactive Fe Site: Preparation of Alkyl Complexes Relevant to Radical-SAM Enzymes"
7:50 pm - 8:00 pm	Discussion
8:00 pm - 8:20 pm	Tyler Grove (Albert Einstein College of Medicine, USA) "From Interferon-Stimulated to a New Antiviral: The Story of Viperin"
8:20 pm - 8:30 pm	Discussion
8:30 pm - 9:15 pm	Squire Booker (Pennsylvania State University, USA) "New Insight into Cobalamin-Dependent Methylation"

9:15 pm - 9:30 pm Discussion

Friday

7:30 am - 8:30 am Breakfast

9:00 am Departure

Contributors



Gordon Research  
Conferences  
*Frontiers of Science*



Carl Storm  
Underrepresented  
Minority Fellowship  
Program



Carl Storm  
International  
Diversity  
Fellowship Program



Predominantly  
Undergraduate  
Institution Fund

**STREAM**  
CHEMICALS, INC.

**ExxonMobil**

**AMERICAN ELEMENTS**  
THE ADVANCED MATERIALS MANUFACTURER®

**JBC** JOURNAL OF  
BIOLOGICAL  
CHEMISTRY

AGOURON  
INSTITUTE



**PennState**



**magnetech**  
by Freiberg Instruments



 NEW ENGLAND  
**BioLabs** Inc.

**Chemical  
Science**  
Editor-in-chief  
Andrew Cooper  
OPEN ACCESS  
IMPACT FACTOR  
9.063\*

**Inorganic Chemistry**

**SENSORS**  
ACS

**ACCOUNTS**  
of chemical research

**analytical  
chemistry**

**SBIC**  
Bringing Inorganic Chemistry To Life

**CORTEVA**  
agriculture

Agriculture Division of DowDuPont™

  
ELSEVIER

**nature  
chemical biology**

**BRUKER**

The Saltman Lecturer Fund

The Stiefel Young Investigator Fund

Sessler Family Charitable Trust

This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Science Financial Assistance Program under Award Number DE-SC0019145. The report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any

agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation or favoring by the U.S. Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

Support provided by Argonne National Laboratory.

**Bioinorganic Chemistry (GRS)**  
**Gordon Research Seminar**

**Conference Program**

**Thursday**

4:00 pm - 8:00 pm Arrival and Check-in

6:00 pm - 7:00 pm Dinner

7:30 pm - 9:30 pm New Free Radical and Organometallic Enzyme Chemistry  
Discussion Leader: Vahe Bandarian (University of Utah, USA)

7:30 pm - 7:50 pm Daniel Suess (Massachusetts Institute of Technology, USA)  
"Fe4S4 Clusters Featuring a Reactive Fe Site: Preparation of Alkyl Complexes Relevant to Radical-SAM Enzymes"

7:50 pm - 8:00 pm Discussion

8:00 pm - 8:20 pm Tyler Grove (Albert Einstein College of Medicine, USA)  
"From Interferon-Stimulated to a New Antiviral: The Story of Viperin"

8:20 pm - 8:30 pm Discussion

8:30 pm - 9:15 pm Squire Booker (Pennsylvania State University, USA)  
"New Insight into Cobalamin-Dependent Methylation"

9:15 pm - 9:30 pm Discussion

9:30 pm - 11:00 pm Poster Session  
Joint Poster Session with the Metals in Biology GRC

**Friday**

7:30 am - 8:30 am Breakfast

8:30 am - 9:00 am Group Photo

9:00 am - 12:30 pm Using the Bioinorganic Toolbox: New Methods and Techniques to Understand the Role of Metals in Nature  
Discussion Leader: R. David Britt (University of California, Davis, USA)

9:00 am - 9:20 am Jose Alvarez-Hernandez (University of Rochester, USA)  
"Electrochemical Hydrogen Evolution Catalyzed by CoMP11-Ac: Who Is the Substrate?"

9:20 am - 9:30 am Discussion

9:30 am - 9:50 am Hannah Rose (Pennsylvania State University, USA)

"Structural Basis for Superoxide Activation of Class IId Ribonucleotide Reductases"

9:50 am - 10:00 am Discussion

10:00 am - 10:20 am Shannon Rivera (Emory University, USA)

"Determining the Effects of Heme Pocket Residues on the Signal Transduction Within Globin Coupled Sensors"

10:20 am - 10:30 am Discussion

10:30 am - 11:00 am Coffee Break

11:00 am - 11:20 am Matthew Ross (Northwestern University, USA)

"Biological Methane Oxidation Is Catalyzed by a Mononuclear Copper Center"

11:20 am - 11:30 am Discussion

11:30 am - 11:50 am Anindita Sarkar (University of Michigan, USA)

"The Curious Case of Reverb $\beta$ : Chemical Reaction Coupling of Electron Transfer Makes Ferric Heme a Gas Sensor"

11:50 am - 12:00 pm Discussion

12:00 pm - 12:20 pm Richard Sayler (University of California, Davis, USA)

"Substrate Analogue Reactivity in HydG: Radical Counterparts of Relevant Intermediates"

12:20 pm - 12:30 pm Discussion

12:30 pm - 1:30 pm Lunch

1:30 pm - 4:00 pm Free Time

4:00 pm - 6:00 pm Poster Session

6:00 pm - 7:00 pm Dinner

7:30 pm - 9:30 pm Applications of Metals in Biology: Biological Materials, Biomineralization, Therapeutics and Imaging

Discussion Leader: Akif Tezcan (University of California, San Diego, USA)

7:30 pm - 7:45 pm Zahra Bahrami-Dizicheh (Arizona State University, USA)

"Repeat Proteins as Versatile Scaffolds for Arrays of Redox-Active Fe-S Clusters"

7:45 pm - 7:50 pm Discussion

7:50 pm - 8:05 pm Kelsey Miller (University of California, Irvine, USA)

"Designed Artificial Iron Proteins"

8:05 pm - 8:10 pm Discussion

8:10 pm - 8:25 pm Ryan Riskowski (Colorado State University, USA)  
"Enzyme-Catalyzed CdSe Quantum Dot Growth and Functionalization"

8:25 pm - 8:30 pm Discussion

8:30 pm - 8:45 pm Viktoria Steck (University of Rochester, USA)  
"Chemoselective Cyclopropanation over Carbene Y-H Insertion Catalyzed by an Engineered Carbene Transferase"

8:45 pm - 8:50 pm Discussion

8:50 pm - 9:05 pm Chung-Jui Yu (Northwestern University, USA)  
"Spin Dynamics of Coordination Complexes and Materials as Model Systems for Biology"

9:05 pm - 9:10 pm Discussion

9:10 pm - 9:25 pm Juner Zhang (California Institute of Technology, USA)  
"Repurposing Cytochrome P450s for Selective C(sp<sub>3</sub>)-H Perfluoroalkylation Using Directed Evolution"

9:25 pm - 9:30 pm Discussion

Saturday

7:30 am - 8:30 am Breakfast

9:00 am - 12:30 pm Inspired by Nature: Understanding the Role of Metals and Structure-Function Relationships in Catalysis  
Discussion Leader: Kyle Lancaster (Cornell University, USA)

9:00 am - 9:20 am Jamey Bower (The Ohio State University, USA)  
"A Four-Coordinate {CuNO}10 by Nitrite Reduction and Implications for Oxidative Stress"

9:20 am - 9:30 am Discussion

9:30 am - 9:50 am Zachary Butz (Colorado State University, USA)  
"Utilizing Metal Reducing Enzymes as Tags in Optical and Electron Microscopy"

9:50 am - 10:00 am Discussion

10:00 am - 10:20 am Jesse Gordon (Johns Hopkins University, USA)  
"Structures, Spectroscopic Properties and Dioxygen Reactivity of 5- and 6-Coordinate Nonheme Iron(II) Complexes: A Combined Enzyme/Model Study of Thiol Dioxygenases"

10:20 am - 10:30 am Discussion

10:30 am - 11:00 am Coffee Break

11:00 am - 11:20 am Eric Koehn (University of California, Berkeley, USA)

"PQQ Biosynthesis Is Resolved by the Discovery of Unprecedented Functions for the Enzyme PqqB"

11:20 am - 11:30 am Discussion

11:30 am - 11:50 am Casey Van Stappen (Max-Planck Institute for Chemical Energy Conversion, Germany)

"Insight into the E1 State of Mo Nitrogenase"

11:50 am - 12:00 pm Discussion

12:00 pm - 12:20 pm Aaron Ledray (University of California, Irvine, USA)

"Understanding Ferryl Basicity in a Histidine-Ligated Peroxidase"

12:20 pm - 12:30 pm Discussion

12:30 pm - 1:30 pm Lunch

1:30 pm - 4:00 pm Free Time

4:00 pm - 6:00 pm Poster Session

6:00 pm - 7:00 pm Dinner

7:00 pm - 7:30 pm Evaluation Period  
Fill in GRS Evaluation Forms

7:30 pm - 9:30 pm Metals on the Move: Sequestration, Affinity and Transport of Metals in and out of the Cell  
Discussion Leader: Kelly Chacon (Reed College, USA)

7:30 pm - 7:45 pm Rahul Purohit (California Institute of Technology, USA)

"Cu+-Specific CopB Transporter: Revisiting CopA and CopB Classification"

7:45 pm - 7:50 pm Discussion

7:50 pm - 8:05 pm Sambuddha Sen (The Ohio State University, USA)

"Molecular Basis of Multiple Mitochondrial Dysfunctions Syndrome 2 (MMDS2): Impact of a Disease Causing Ile67Asn Mutation on BOLA3"

8:05 pm - 8:10 pm Discussion

8:10 pm - 8:25 pm Maria-Eugenia Llases (Instituto de Biología Molecular y Celular de Rosario, Argentina)

"Towards the Mechanisms of Copper Insertion in Plant Cytochrome c Oxidase"

8:25 pm - 8:30 pm Discussion

8:30 pm - 8:45 pm Michael Stevenson (University of California, Davis, USA)

"Investigating the Dependence of Proinsulin C-Peptide on Metal Micronutrients"

8:45 pm - 8:50 pm Discussion

8:50 pm - 9:05 pm Jasmine Tutol (University of Texas at Dallas, USA)  
"Genetically Encoded Fluorescent Biosensors for Probing Cellular Chloride"

9:05 pm - 9:10 pm Discussion

9:10 pm - 9:25 pm Clifford Hardy (University of California, Santa Barbara, USA)  
"Coordination Chemistry and Photoreactivity of Pacifibactin, a Marine Siderophore Identified Through Genome Mining"

9:25 pm - 9:30 pm Discussion

Sunday

7:30 am - 8:30 am Breakfast

9:00 am - 12:30 pm The Origins of Life: The Role of Metals in Evolution, Early Metabolism and Biogeochemical Cycles  
Discussion Leader: Stephen Ragsdale (University of Michigan Medical School, USA)

9:00 am - 9:20 am Steven Cohen (Massachusetts Institute of Technology, USA)  
"Conformational Flexibility of Carbon Monoxide Dehydrogenase/Acetyl-CoA Synthase Revealed by Electron Microscopy"

9:20 am - 9:30 am Discussion

9:30 am - 9:50 am Natasha Pence (Washington State University, USA)  
"Unraveling the Interactions of the Physiological Reductant Flavodoxin with the Different Conformations of the Fe Protein in the Nitrogenase Cycle"

9:50 am - 10:00 am Discussion

10:00 am - 10:20 am Michael Mazzotta (Woods Hole Oceanographic Institution, USA)  
"Characterization of the Metalloproteome of the Marine Bacteria, Alteromonas"

10:20 am - 10:30 am Discussion

10:30 am - 11:00 am Coffee Break

11:00 am - 11:20 am Patricia Rodriguez Macia (Max Planck Institute for Chemical Energy Conversion, Germany)  
"Functional and Spectroscopic Investigations of CODH-I from Carboxydothermus hydrogenoformans"

11:20 am - 11:30 am Discussion

11:30 am - 11:50 am Chi Nguyen (Massachusetts Institute of Technology, USA)

"Flipping the Anaerobic Switch: [4Fe-4S] Cluster Mediated Oxygen Sensing and Global Transcription Regulation by FNR"

11:50 am - 12:00 pm Discussion

12:00 pm - 12:20 pm Melissa Marquez (Boston University, USA)

"Conservation of Leu1's C-Terminus Is Essential for Its Recognition by the Cytosolic Iron-Sulfur Cluster Assembly Targeting Complex"

12:20 pm - 12:30 pm Discussion

12:30 pm - 1:30 pm Lunch

1:30 pm Departure

### Contributors



Carl Storm  
International  
Diversity  
Fellowship Program



This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Science Financial Assistance Program under Award Number DE-SC0019145. The report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation or favoring by the U.S. Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

## Metals in Biology GRC Registration List

Name	Organization	Participation
Abhyankar, Nandita	University of Maryland	Poster Presenter
Alvarez-Hernandez, Jose	University of Rochester	Poster Presenter
Anderson, Vernon E	NIH/NIGMS	Attendee
Angerhofer, Alexander	University of Florida	Poster Presenter
Baldwin, Michael J	University of Cincinnati	Poster Presenter
Balskus, Emily P	Harvard University	Speaker
Bandarian, Vahe	University of Utah	Discussion Leader
Basu, Partha	Indiana University-Purdue University Indianapolis	Poster Presenter
Berggren, Gustav O	Uppsala University	Poster Presenter
Birrell, James A	Max Planck Institute for Chemical Energy Conversion	Poster Presenter
Blakely, Maike N	University of Washington	Poster Presenter
Boal, Amie K	Pennsylvania State University	Discussion Leader
Bohle, Scott	McGill University	Poster Presenter
Bollinger, J. Martin	The Pennsylvania State University	Chair
Bollinger, Samuel S	Lankenau Institute for Medical Research	Attendee
Booker, Squire	Pennsylvania State University	Speaker
Bren, Kara L	University of Rochester	Poster Presenter
Bridwell-Rabb, Jennifer	University of Michigan	Poster Presenter
Britt, R. David	University of California, Davis	Speaker
Broderick, Joan B	Montana State University	Discussion Leader
Burger, Richard M	Brooklyn College of CUNY	Attendee
Butler, Alison	University of California, Santa Barbara	Poster Presenter
Butz, Zachary	Colorado State University	Poster Presenter
Caruso, Alessio	Princeton University	Poster Presenter
Chang, Michelle	University of California, Berkeley	Speaker
Chica, Bryant	National Renewable Energy Laboratory	Poster Presenter
Cho, Jaeheung	DGIST	Poster Presenter
Confer, Alex M	Johns Hopkins University	Poster Presenter
Corrigan, Patrick S	Penn State	Poster Presenter
Cotruvo, Jr., Joseph A	Penn State University	Poster Presenter
Culotta, Valeria	Johns Hopkins University	Speaker
Culpepper, Megen A	Appalachian State University	Speaker
Cutsail, George E	MPI for Chemical Energy Conversion	Poster Presenter
Dassama, Laura MK	Stanford University	Attendee
Davidson, Victor L	University of Central Florida	Attendee
Dawson, John H	Univ of South Carolina	Attendee
Deane, Caitlin D	Nature Chemical Biology	Attendee
DeRose, Victoria J	University of Oregon	Vice Chair
Diaz, Julia	University of California, San Diego	Speaker
Dodani, Sheel C	The University of Texas at Dallas	Poster Presenter
Donnelly, Paul S	University of Melbourne	Speaker

Dos Santos, Patricia C	Wake Forest University	Discussion Leader
DuBois, Jennifer L	Montana State University	Poster Presenter
Dwaraknath, Sudharsan	University of Illinois at Urbana-Champaign	Poster Presenter
Eijsink, Vincent G.H.	Norwegian University of Life Sciences	Speaker
Einsle, Oliver	University of Freiburg	Speaker
Fernandez, Rebeca L	University of Wisconsin Madison	Poster Presenter
Fryszkowska, Anna	Merck & Co, Inc.	Speaker
Gale, Eric M	MGH/ Harvard Medical School	Poster Presenter
Giedroc, David P	Indiana University	Speaker
Goldberg, David P	Johns Hopkins University	Attendee
Goldsmith, Christian R	Auburn University	Poster Presenter
Gomez Castillo, Rebeca	Max Planck Institute for Chemical Energy Conversion	Poster Presenter
Gordon, Jesse	Johns Hopkins University	Attendee
Gray, Harry B	California Institute of Technology	Discussion Leader
Green, Anthony	University of Manchester	Attendee
Green, Michael T	University of California, Irvine	Poster Presenter
Greenhalgh, Elizabeth	University of Wisconsin-Madison	Poster Presenter
Grove, Tyler L	Albert Einstein College of Medicine	Speaker
Groves, John T	Princeton University	Poster Presenter
Guo, Yisong	Carnegie Mellon University	Poster Presenter
Hakkinen, Hannu	University of Jyvaskyla	Attendee
Heber-Katz, Ellen	Lankenau Institute for Medical Research	Speaker
Heffern, Marie	University of California, Davis	Poster Presenter
Hegg, Eric L	Michigan State University	Poster Presenter
Heinrichs, David E	University of Western Ontario	Poster Presenter
Hoffman, Brian M	Northwestern University	Attendee
Hogbom, Martin	Stockholm University	Speaker
Holland, Patrick	Yale University	Poster Presenter
Hu, Jian	Michigan state university	Poster Presenter
Imlay, James A	University of Illinois at Urbana-Champaign	Speaker
Jameson, Guy NL	The University of Melbourne	Poster Presenter
Johnson, Russell	Nature Chemistry	Attendee
Jollie, David R	National Institutes of Health	Attendee
Kern, Jan	Lawrence Berkeley National Laboratory	Poster Presenter
Kieber-Emmons, Matthew	University of Utah	Poster Presenter
Kielb, Patrycja	California Institute of Technology	Poster Presenter
Kiernicki, John J.	University of Michigan	Poster Presenter
Kirk, Martin L	The University of New Mexico	Poster Presenter
Knox, Hayley L	The Pennsylvania State University	Poster Presenter
Kovacs, Julie A	University of Washington	Poster Presenter
Krebs, Carsten	Pennsylvania State University	Speaker
Lancaster, Kyle M	Cornell University	Poster Presenter
Ledray, Aaron P	University of California, Irvine	Poster Presenter

Lehnert, Nicolai A	University of Michigan	Poster Presenter
Li, Bo	University of North Carolina at Chapel Hill	Speaker
Lippard, Stephen J.	Massachusetts Institute of Technology	Attendee
Lipscomb, John D	University of Minnesota	Poster Presenter
Liptak, Matthew D	University of Vermont	Poster Presenter
Liu, Gang	National Institute of Child Health and Human Development/NIH	Poster Presenter
Liu, Aimin	University of Texas at San Antonio	Poster Presenter
Llases, Maria-Eugenia	Instituto de Biología Molecular y Celular de Rosario	Poster Presenter
Lu, Yi	University of Illinois	Poster Presenter
Lubner, Carolyn E	National Renewable Energy Laboratory	Poster Presenter
MacArdle, Siobhan G	California Institute of Technology	Poster Presenter
Machonkin, Timothy E	Whitman College	Poster Presenter
Magyar, John S	California Institute of Technology	Poster Presenter
Manesis, Anastasia C	Ohio State University	Attendee
Mann, Samuel I	UCSF	Poster Presenter
Mansoorabadi, Steven	Auburn University	Speaker
Marquez, Melissa D	Boston University	Poster Presenter
Martins, Maria C.	ITQB NOVA - Instituto de Tecnologia Química e Biológica António Xavier, Universidade Nova de Lisboa	Poster Presenter
Mazzotta, Michael G	Woods Hole Oceanographic Institution	Poster Presenter
Miller, Anne-Frances	University of Kentucky	Discussion Leader
Minter, Shelley	University of Utah	Speaker
Mukherjee, Anusree	University of Alabama in Huntsville	Poster Presenter
Murray, Leslie J	University of Florida	Poster Presenter
Nawrat, Chris C	Process Chemistry, Merck & Co., Inc.	Poster Presenter
Neugebauer, Monica E	UC Berkeley	Poster Presenter
Ng, Tai L	Harvard University	Poster Presenter
Nguyen, Chi H	Massachusetts Institute of Technology	Poster Presenter
Niemand, Nandi	Stellenbosch University	Poster Presenter
Niklas, Jens	Argonne National Laboratory	Poster Presenter
Nolan, Elizabeth M	Massachusetts Institute of Technology	Discussion Leader
Nouairia, Ghada	Stockholm University	Attendee
Ok, Kiwon	University of Maryland School of Pharmacy	Poster Presenter
Olszansky, Lisa	University of Illinois at Urbana-Champaign	Attendee
Orphan, Victoria J	California Institute of Technology	Speaker
Ortmayer, Mary	University of Manchester	Poster Presenter
Oyala, Paul H	California Institute of Technology	Poster Presenter
Palowitch, Gavin	The Pennsylvania State University	Poster Presenter
Parker, Mackenzie J	New England Biolabs	Poster Presenter
Pence, Natasha	Washington State University	Poster Presenter
Perlstein, Deborah L	Boston University	Speaker
Peters, John W	Washington State University	Discussion Leader
Pham, Cindy	Lawrence Berkeley National Laboratory	Poster Presenter

Pierce, Brad S	The University of Texas at Arlington	Poster Presenter
Pletneva, Ekaterina V	Dartmouth College	Poster Presenter
Pollock, Chris	Cornell High Energy Synchrotron Source	Poster Presenter
Prier, Christopher	Merck & Co.	Poster Presenter
Proshlyakov, Denis A	Michigan State University	Speaker
Que, Emily L	University of Texas at Austin	Poster Presenter
Ragsdale, Stephen W.	University of Michigan Medical School	Poster Presenter
Rao, Guodong	University of California, Davis	Poster Presenter
Richards, Nigel G	Cardiff University	Attendee
Riskowski, Ryan A	Colorado State University	Poster Presenter
Rodriguez, Kyle J	Adolphe Merkle Institute, University of Fribourg	Poster Presenter
Rodriguez Macia, P	Max Planck Institute for Chemical Energy Conversion	Poster Presenter
Romao, Celia V.	Instituto de Tecnologia Química e Biológica António Xavier, Universidade Nova de Lisboa	
Rose, Hannah R	Pennsylvania State University	Poster Presenter
Rose, Michael J	University of Texas at Austin	Poster Presenter
Rosenzweig, Amy C	Northwestern University	Speaker
Ross, Matthew O	Northwestern University	Poster Presenter
Rouault, Tracey	National Institute of Child Health and Human Development, NIH	Speaker
Rozman Grinberg, Inna	Stockholm University	Poster Presenter
Saito, Mak	Woods Hole Oceanographic Institution	Speaker
Saleh, Lana	New England Biolabs	Speaker
Sarfatti, David E.	Lankenau Inst. of Medical Research	Attendee
Sarkar, Anindita	University of Michigan	Poster Presenter
Sayler, Richard I	University of California, Davis	Poster Presenter
Schut, Gerrit Jan	University of Georgia	Speaker
Sen, Sajal	University of Texas at Austin	Poster Presenter
Shafaat, Hannah S	The Ohio State University	Speaker
Shearer, Jason M	Trinity University	Attendee
Shin, Jieun	California Institute of Technology (Caltech)	Poster Presenter
Silakov, Alexey	Pennsylvania State University	Poster Presenter
Sjöberg, Britt-Marie	Stockholm University	Attendee
Skaar, Eric P	Vanderbilt University Medical Center	Speaker
Speina, Kevin J	Princeton University	Poster Presenter
Spiro, Thomas G	U of Washington	Poster Presenter
Stack, Robert J	Basic Energy Sciences, U.S. Department of Energy	Attendee
Steck, Viktoria C	University of Rochester	Poster Presenter
Stevenson, Michael J	University of California, Davis	Poster Presenter
Stich, Troy A	Wake Forest University	Attendee
Streit, Bennett R	Montana State University	Poster Presenter
Suess, Daniel	Massachusetts Institute of Technology	Speaker
Summers, Zarath M	ExxonMobil Research and Engineering	Speaker
Sutherlin, Kyle D	Lawrence Berkeley National Laboratory	Poster Presenter

Tao, Lizhi	University of California, Davis	Poster Presenter
Thompson, Emily J	University of California, Berkeley	Poster Presenter
Tomat, Elisa	University of Arizona	Poster Presenter
Tommos, Cecilia	University of Pennsylvania	Poster Presenter
Tutol, Jasmine N	University of Texas at Dallas	Poster Presenter
Valentine, Joan S	University of California, Los Angeles	Attendee
Van Stappen, Casey M	Max-Planck Institute for Chemical Energy Conversion	Poster Presenter
Villa, Alejandro j	IBR - University of Rosario	Poster Presenter
Walsh, Brenna J.C.	Indiana University Department of Chemistry	Poster Presenter
Waskell, Lucy A	University of Michigan	Attendee
Weinert, Emily E	Emory University	Poster Presenter
Wilcox, Dean E	Dartmouth College	Poster Presenter
Wilcoxen, Jarett M	University of California, Davis	Poster Presenter
Wilks, Angela	University of Maryland	Poster Presenter
Winkler, Jay R	California Institute of Technology	Attendee
Yang, Yang	California Institute of Technology	Poster Presenter
Yang, Jenny Y	University of California, Irvine	Speaker
Yazdani, Syed Shams	International Centre for Genetic Engineering and Biotechnology	Speaker
Yu, Steve S.-F.	Academia Sinica	Poster Presenter
Yu, Chung-Jui	Northwestern University	Poster Presenter
Zaragoza, Jan Paulo T	University of California Berkeley	Poster Presenter
Zhang, Shiyu	Ohio State University	Poster Presenter
Zhang, Limei	University of Nebraska-Lincoln	Poster Presenter
Zhang, Juner	California Institute of Technology	Poster Presenter
Zhao, Jing	Nanjing University	Poster Presenter
Zheng, Peng	Nanjing University	Poster Presenter

## Bioinorganic Chemistry GRS Registration List

Name	Organization	Participation
Ali, Md. Mahbbat	University of Wisconsin-Milwaukee	Poster Presenter
Alvarez-Hernandez, Jose	University of Rochester	Speaker
Alwan, Katherine B	Oregon Health and Science University	Poster Presenter
Arias, Renee	Oregon Health and Science University	Poster Presenter
Bahrami-Dizicheh, Zahra	Arizona State University	Speaker
Bower, Jamey K.	The Ohio State University	Speaker
Britt, R. David	University of California, Davis	Discussion Leader
Burger, Richard M	Brooklyn College of CUNY	Poster Presenter
Butz, Zachary	Colorado State University	Speaker
Campecino, Julius	Michigan State University	Poster Presenter
Carpenter, Jessica M	Dartmouth College	Poster Presenter
Caruso, Alessio	Princeton University	Poster Presenter
Chacon, Kelly N	Reed College	Discussion Leader
Cohen, Steven E	Massachusetts Institute of Technology	Speaker
Confer, Alex M	Johns Hopkins University	Poster Presenter
Corrigan, Patrick S	Penn State	Poster Presenter
Deng, Yunling	Dartmouth College	Poster Presenter
Dong, Hai T	University of Michigan	Poster Presenter
Dwaraknath, Sudharsan	University of Illinois at Urbana-Champaign	Attendee
Fernandez, Rebeca L	University of Wisconsin Madison	Poster Presenter
Fu, Wen	University of California Davis	Poster Presenter
Gomez Castillo, Rebeca	Max Planck Institute for Chemical Energy Conversion	Poster Presenter
Gordon, Jesse	Johns Hopkins University	Speaker
Greenhalgh, Elizabeth	University of Wisconsin-Madison	Poster Presenter
Hardy, Clifford D	University of California, Santa Barbara	Speaker
Jones, Thomas	University of Alabama in Huntsville	Poster Presenter
Kiernicki, John J.	University of Michigan	Poster Presenter
Koehn, Eric M	University of California, Berkeley	Speaker
Kwon, Yubin M	University of Montana	Poster Presenter
Lancaster, Kyle M	Cornell University	Discussion Leader
Ledray, Aaron P	University of California, Irvine	Speaker
Li, Yan	University of Montana	Poster Presenter
Llases, Maria-Eugenia	Instituto de Biología Molecular y Celular de Rosario	Speaker
MacArdle, Siobhan G	California Institute of Technology	Poster Presenter
Manesis, Anastasia C	Ohio State University	Chair
Mann, Samuel I	UCSF	Poster Presenter
Marquez, Melissa D	Boston University	Speaker
Mazzotta, Michael G	Woods Hole Oceanographic Institution	Speaker
Mehmood, Rimsha	Massachusetts Institute of Technology	Poster Presenter
Miller, Kelsey R	University of California, Irvine	Speaker
Neugebauer, Monica E	UC Berkeley	Poster Presenter

Ng, Tai L	Harvard University	Poster Presenter
Nguyen, Chi H	Massachusetts Institute of Technology	Speaker
Ok, Kiwon	University of Maryland School of Pharmacy	Poster Presenter
Oyala, Paul H	California Institute of Technology	Poster Presenter
Palacios, Philip	University of Texas-Arlington	Poster Presenter
Palowitch, Gavin	The Pennsylvania State University	Poster Presenter
Parker, Mackenzie J	New England Biolabs	Poster Presenter
Pence, Natasha	Washington State University	Speaker
Purohit, Rahul	California Institute of Technology	Speaker
Ragsdale, Stephen W.	University of Michigan Medical School	Discussion Leader
Riskowski, Ryan A	Colorado State University	Speaker
Rivera, Shannon	Emory University	Speaker
Rodriguez, Kyle J	Adolphe Merkle Institute, University of Fribourg	Chair
Rodriguez Macia, P	Max Planck Institute for Chemical Energy Conversion	Speaker
Rose, Hannah R	Pennsylvania State University	Speaker
Ross, Matthew O	Northwestern University	Speaker
Rush, Katherine W	Oregon Health and Science University/Reed College	Poster Presenter
Sabuncu, Sinan	Oregon Health and Science University	Poster Presenter
Sarkar, Anindita	University of Michigan	Speaker
Sayler, Richard I	University of California, Davis	Speaker
Sen, Sambuddha	The Ohio State University	Speaker
Sestok, Alexandrea E	University of Maryland, Baltimore County	Poster Presenter
Speina, Kevin J	Princeton University	Poster Presenter
Steck, Viktoria C	University of Rochester	Speaker
Stevenson, Michael J	University of California, Davis	Speaker
Tezcan, Akif	University of California, San Diego	Discussion Leader
Thompson, Zechariah	The Ohio State University	Poster Presenter
Tutol, Jasmine N	University of Texas at Dallas	Speaker
Van Stappen, Casey M	Max-Planck Institute for Chemical Energy Conversion	Speaker
Walsh, Brenna J.C.	Indiana University Department of Chemistry	Poster Presenter
Yu, Chung-Jui	Northwestern University	Speaker
Zaragoza, Jan Paulo T	University of California Berkeley	Poster Presenter
Zhang, Juner	California Institute of Technology	Speaker