GORDON RESEARCH CONFERENCES

FINAL PROGRESS REPORT
US Department of Energy
Metals in Biology GRC/Bioinorganic Chemistry GRS

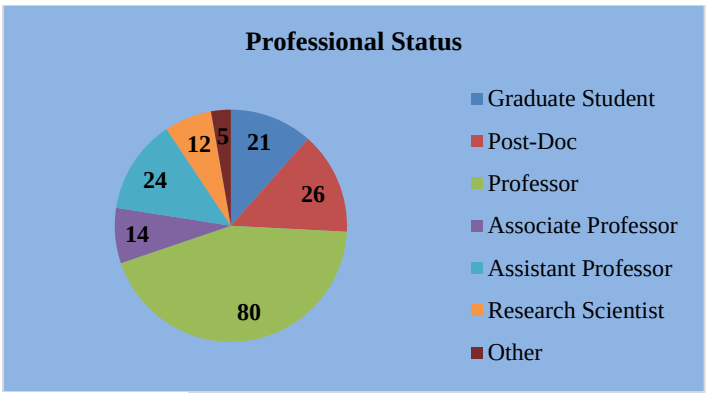
Grant Number DE-SC0016880
January 22-29, 2017

Operational Summary

The Gordon Research Conference (GRC) on Metals in Biology and Gordon Research Seminar (GRS) on Bioinorganic Chemistry were held at the Four Points Sheraton in Ventura, California from January 22-29, 2017. The meeting covered a variety of scientific topics and the content presented was highly rated by participants.

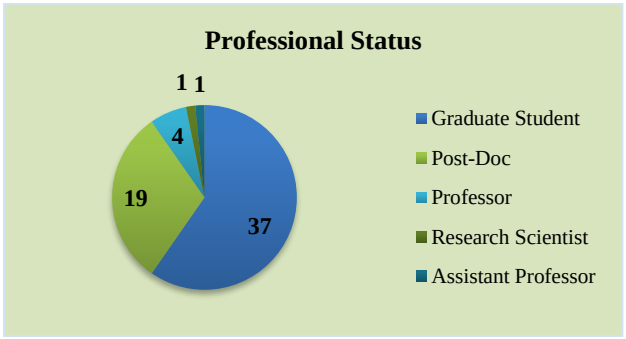
Conference Participants

The Conference was well-attended with 182 participants. Scientists from academia represented 96% of the participants while attendees from government accounted for 3% and those from industry totaled 1%. The meeting also attracted a strong mix of young investigators and senior scientists. Students and post-docs accounted for 26% of all attendees. Approximately 37% of the participants at the 2017 meeting were women.



Seminar Participants

The Seminar was well-attended with 62 participants. Scientists from academia represented 100% of the participants. Approximately 50% of the participants at the 2017 seminar were women.



Conference Program

Biological metal centers assume numerous important structural and functional roles in association with proteins and nucleic acids, adding chemical diversity to the limited number of amino acids and the even smaller number of nucleic acid bases. This augmented chemical diversity is enhanced by the variety of metal centers employed; including both redox-active and non-redox active metals, single metal binding sites, metals bound by organic cofactors, and multinuclear metal clusters. Understanding how metal ions function in these diverse systems requires

multidisciplinary approaches across the broad fields of biology, physics, chemistry/biochemistry, and medicine. The MIB-GRC brought together scientists from diverse backgrounds to foster new collaborations that take advantage of complementary skills. Lectures in the 2017 MIB-GRC covered recent advances in our understanding of the roles of metalloproteins and metal/nucleic acid complexes in cellular signaling, metal ion regulation, and their effects on human health; the evolving biological chemistry of metals from the earth's deep past to the current environment, and metal-centered catalysis by a variety of metalloenzymes, including those crucial in the grand global cycles of hydrogen, nitrogen, and oxygen. In addition to the lectures, poster sessions were held to facilitate discussions in an open atmosphere which was a major highlight of the MIB-GRC.

The Bioinorganic Chemistry GRS, chaired in 2017 by Lauren Rajakovich, served as an extension of the oversubscribed Metals in Biology Gordon Research Conference (GRC) to provide a forum for young scientists to present their work, network, and engage in this vibrant scientific community. The overlapping evening lecture and poster session with the Metals in Biology GRC provided the invaluable opportunity for GRS participants to discuss their research with leaders in the field.

Metals serve in fundamental biological roles that are essential to all life, requiring precise mechanisms for metal acquisition and balance. Nature utilizes metals to achieve chemical conversions that plague synthetic chemists, such as C-H bond activation, hydrogen production and nitrogen fixation. This Gordon Research Seminar (GRS) explored current knowledge of these natural biological roles and strategies to apply these insights to solve problems in the environment and human health.

Conference Budget

Funding provided by the US Department of Energy supported partial registration for 6 graduate students and 4 postdocs at the GRC and partial registration for 7 graduate students and 4 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 the lively discussions, power hour and excellent presentations. Evaluations from the GRS included positive comments regarding the quality of talks and discussion time.

GRC would like to thank the US 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.

Dr. R. David Britt, GRC Chair
University of California, Davis

Dr. Lauren Rajakovich, GRS Chair
Pennsylvania State University

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

Metals in Biology

Gordon Research Conference

Biological Metals: Regulation, Catalysis, Medicine, the Environment and Chemical Evolution

January 22-27, 2017

Four Points Sheraton / Holiday Inn Express

Ventura, CA

Chair: R. David Britt / Vice Chair: Yi Lu

Contributors

Gordon Research Conferences

Carl Storm Underrepresented Minority Fellowship

Predominantly Undergraduate Institution Fund (PUI)

BRUKER

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American Chemical Society Division of Biological Chemistry

ACS DIVISION OF INORGANIC CHEMISTRY

Inorganic Chemistry including bioinorganic chemistry

The Ed Stiefel Young Investigator Fund

The Saltman Lecturer Fund

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GRAY FAMILY FUND

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NASA ASTROBIOLOGY INSTITUTE

Metallomics

Dalton Transactions

Chemical Science

SBIC Bringing Inorganic Chemistry To Life

The conference also gratefully acknowledges a contribution from the Sessler Family Charitable Trust.

Final Meeting Program

Sunday	
4:00 pm - 8:00 pm	Arrival and Check-in
6:00 pm	Dinner
7:30 pm - 7:40 pm	Welcome / Introductory Comments by GRC Site Staff
7:40 pm - 9:30 pm	Metals and Biological Signalling
	Discussion Leader: Emily Weinert (Emory University, USA)
7:40 pm - 8:20 pm	Michael Marletta (University of California, Berkeley, USA) "Selective Sensing of Nitric Oxide in Biology"
8:20 pm - 8:35 pm	Discussion
8:35 pm - 9:15 pm	Thomas O'Halloran (Northwestern University, USA) "Zinc Receptors, Fluxes and Switches in Control of Cell Fate Decisions"
9:15 pm - 9:30 pm	Discussion
Monday	
7:30 am - 8:30 am	Breakfast
8:30 am	Group Photo
9:00 am - 12:30 pm	Metal Ion Homostasis, Proteins and Nucleic Acids
	Discussion Leader: Sheila David (University of California, Davis, USA)
9:00 am - 9:30 am	Victoria DeRose (University of Oregon, USA) "Platinum Interactions Across the Cell: New Players and Pathways"
9:30 am - 9:45 am	Discussion
9:45 am - 10:15 am	Lauren Waters (University of Wisconsin-Oshkosh, USA) "Regulation of Mn Metabolism in Bacteria: From a Small RNA to a Small Protein to Riboswitches"
10:15 am - 10:30 am	Discussion
10:30 am - 11:00 am	Coffee Break
11:00 am - 11:30 am	Walter Chazin (Vanderbilt University, USA) "What Are Those Fe-S Clusters Doing in Genome Maintenance Proteins?"
11:30 am - 11:45 am	Discussion
11:45 am - 12:15 pm	David Giedroc (Indiana University, USA)

	"Structural Mechanisms of Transition Metal Homeostasis in Bacteria"
12:15 pm - 12:30 pm	Discussion
12:30 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: Victoria DeRose (University of Oregon, USA) and Lauren Rajakovich (Pennsylvania State University, USA)
4:00 pm - 6:00 pm	Poster Session
6:00 pm	Dinner
7:30 pm - 9:30 pm	Metal Ion Regulation and Human Health
	Discussion Leader: Celia Goulding (University of California, Irvine, USA)
7:30 pm - 8:00 pm	Ashley Bush (Florey Institute of Neuroscience and Mental Health, Australia) "Iron and Ferroptosis in Brain Disease"
8:00 pm - 8:10 pm	Discussion
8:10 pm - 8:40 pm	Guenter Schwarz (University of Cologne, Germany) "New Functions of Molybdenum Enzymes in Neurodegeneration and Nitric Oxide Synthesis"
8:40 pm - 8:50 pm	Discussion
8:50 pm - 9:20 pm	Dianne Newman (California Institute of Technology / Howard Hughes Medical Institute, USA) "Selective Degradation of an Extracellular Electron Shuttle Abrogates Biofilm Development"
9:20 pm - 9:30 pm	Discussion
Tuesday	
7:30 am - 8:30 am	Breakfast
9:00 am - 12:30 pm	Global Chemical Cycles: Nitrogen
	Discussion Leader: Yilin Hu (University of California, Irvine, USA)
9:00 am - 9:30 am	Jonas Peters (California Institute of Technology, USA) "Synthetic Single-Site Fe N_2ases"
9:30 am - 9:45 am	Discussion

9:45 am - 10:15 am	Serena Debeer (Max Planck Institute for Chemical Energy Conversion, Germany) "From FeMoco to FeVco: Heterometal Contributions to Nitrogenase Reactivity"
10:15 am - 10:30 am	Discussion
10:30 am - 11:00 am	Coffee Break
11:00 am - 11:30 am	Leslie Murray (University of Florida, USA) "Towards Understanding How Metal Ions Cooperate to Activate Dinitrogen"
11:30 am - 11:45 am	Discussion
11:45 am - 12:15 pm	Lance Seefeldt (Utah State University, USA) "Light-Driven N_2 Reduction Catalyzed by a CdS-Nitrogenase MoFe Protein Hybrid"
12:15 pm - 12:30 pm	Discussion
12:30 pm	Lunch
1:30 pm - 4:00 pm	Free Time
4:00 pm - 6:00 pm	Poster Session
6:00 pm	Dinner
7:30 pm - 9:30 pm	Global Chemical Cycles: Energy
	Discussion Leader: Anne Jones (Arizona State University, USA)
7:30 pm - 8:00 pm	Fraser Armstrong (University of Oxford, United Kingdom) "New Insights into Hydrogenase Catalysis"
8:00 pm - 8:10 pm	Discussion
8:10 pm - 8:40 pm	Michael Rose (University of Texas at Austin, USA) "Functional Models of Mono-[Fe] Hydrogenase Using an Anthracene-Based Ligand Scaffold"
8:40 pm - 8:50 pm	Discussion
8:50 pm - 9:20 pm	Daniella Goldfarb (Weizmann Institute of Science, Israel) "High Spin Metal Ions as Spin Labels for Structural Studies of Proteins *In-Vitro* and In-Cell"
9:20 pm - 9:30 pm	Discussion
Wednesday	
7:30 am - 8:30 am	Breakfast
9:00 am - 12:30 pm	Metalloenzymes: Mechanisms and Models
	Discussion Leader: Michael Green (University of California, Irvine, USA)
9:00 am - 9:30 am	Steve Yu (Academia Sinica, Taiwan) "Mechanistic Study for the Stereo-Selective Hydroxylation of [2-$^2H_1$,3-$^2H_1$]Butanes Catalyzed

	by Cytochrome P450 BM3 Variants"
9:30 am - 9:45 am	Discussion
9:45 am - 10:15 am	Joseph Martin Bollinger (The Pennsylvania State University, USA) "Emerging Diversity in the Chemistry of Non-Heme Diiron Oxidases and Oxygenases"
10:15 am - 10:30 am	Discussion
10:30 am - 11:00 am	Coffee Break
11:00 am - 11:30 am	Judith Klinman (University of California, Berkeley, USA) "Lipoxygenase: An Enzyme for All Seasons"
11:30 am - 11:45 am	Discussion
11:45 am - 12:15 pm	John Peters (Washington State University, USA) "New Insights into the Mechanism of Electron Bifurcating NADH-Dependent Reduced Ferredoxin:NADP Oxidoreductase"
12:15 pm - 12:30 pm	Discussion
12:30 pm	Lunch
1:30 pm - 4:00 pm	Free Time
4:00 pm - 6:00 pm	Poster Session
6:00 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	Metals and the Environment, from the Deep Past to Today Discussion Leader: William Casey (University of California, Davis, USA)
7:30 pm - 8:00 pm	Alison Butler (University of California, Santa Barbara, USA) "Biological Wet Adhesion to Mineral Surfaces: Mussels, Siderophores and the Catechol-Cation Synergy"
8:00 pm - 8:10 pm	Discussion
8:10 pm - 8:40 pm	Dan Rothman (Massachusetts Institute of Technology, USA) "Nickel-Driven Methanogenic Burst Accompanying Earth's Greatest Extinction"
8:40 pm - 8:50 pm	Discussion
8:50 pm - 9:20 pm	Thomas Spiro (University of Washington, USA) "How Bacteria Use a Multicopper Oxidase to Close the Environmental Mn Cycle by Producing MnO_2 Biomineral"

9:20 pm - 9:30 pm	Discussion
Thursday	
7:30 am - 8:30 am	Breakfast
9:00 am - 12:30 pm	Water Oxidation/Oxygen Evolution
	Discussion Leader: Richard Debus (University of California, Riverside, USA)
9:00 am - 9:30 am	Woodward Fischer (California Institute of Technology, USA) "A Geobiological Perspective on the Role of Mn in the Evolution of Photosynthesis"
9:30 am - 9:45 am	Discussion
9:45 am - 10:15 am	Victor Batista (Yale University, USA) "Studies of Oxomanganese Complexes for Natural and Artificial Photosynthesis"
10:15 am - 10:30 am	Discussion
10:30 am - 11:00 am	Coffee Break
11:00 am - 11:30 am	Nicholas Cox (Australian National University, Australia / Max Planck Institute for Chemical Energy Conversion, Germany) "High-Field Pulse EPR - A Biophysical Toolbox for the Study of the Oxygen Evolving Complex"
11:30 am - 11:45 am	Discussion
11:45 am - 12:15 pm	Petra Fromme (Arizona State University, USA) "New Insights into the Water Splitting Mechanism of Photosystem II by Time-Resolved Femtosecond Nanocrystallography"
12:15 pm - 12:30 pm	Discussion
12:30 pm	Lunch
1:30 pm - 4:00 pm	Free Time
4:00 pm - 6:00 pm	Poster Session
6:00 pm	Dinner
7:30 pm - 9:30 pm	Oxygen, Life in the Balance
	Discussion Leader: Kara Bren (University of Rochester, USA)
7:30 pm - 7:40 pm	Jennifer Kan (California Institute of Technology, USA) "Directed Evolution of Cytochrome c for Carbon-Silicon Bond Formation: Bringing Silicon to Life"
7:40 pm - 7:45 pm	Discussion
7:45 pm - 7:55 pm	Kyle Lancaster (Cornell University, USA)

	"Cytochrome P460: A 'New' Leak in the Biogeochemical Nitrogen Cycle"
7:55 pm - 8:00 pm	Discussion
8:00 pm - 8:10 pm	Hannah Shafaat (The Ohio State University, USA) "Unraveling the Mn/Fe Lipid-Binding Oxidases: An Investigation of Metal Specificity and Cofactor Assembly in R2lox"
8:10 pm - 8:15 pm	Discussion
8:15 pm - 9:15 pm	Harry Gray (California Institute of Technology, USA) "Living with Oxygen"
9:15 pm - 9:30 pm	Discussion
Friday	
7:30 am - 8:30 am	Breakfast
9:00 am	Departure

This material is based upon work supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under award number DE-SC0016880. This 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 United States 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.

Bioinorganic Chemistry (GRS)

Gordon Research Seminar

Biological Roles of Metals and Harnessing Their Chemical Power

January 26-29, 2017

Four Points Sheraton / Holiday Inn Express

Ventura, CA

Chair: **Lauren J. Rajakovich** / Vice Chair: **Jack Nicoludis**

Contributors

Final Meeting Program

Thursday	
4:00 pm - 8:00 pm	Arrival and Check-in
6:00 pm	Dinner
7:30 pm - 9:30 pm	**Keynote Session: Oxygen, Life in Balance**
	Discussion Leader: **Kara Bren** (University of Rochester, USA)
7:30 pm - 7:40 pm	**Jennifer Kan** (California Institute of Technology, USA) "Directed Evolution of Cytochrome c for Carbon-Silicon Bond Formation: Bringing Silicon to Life
7:40 pm - 7:45 pm	Discussion
7:45 pm - 7:55 pm	**Kyle Lancaster** (Cornell University, USA) "Cytochrome P460: A 'New' Leak in the Biogeochemical Nitrogen Cycle"
7:55 pm - 8:00 pm	Discussion
8:00 pm - 8:10 pm	**Hannah Shafaat** (The Ohio State University, USA) "Unraveling the Mn/Fe Lipid-Binding Oxidases: An Investigation of Metal Specificity and

	Cofactor Assembly in R2lox"
8:10 pm - 8:15 pm	Discussion
8:15 pm - 9:15 pm	**Harry Gray** (California Institute of Technology, USA) "Living with Oxygen"
9:15 pm - 9:30 pm	Discussion
9:30 pm	Joint Poster Session with Metals in Biology GRC
Friday	
7:30 am - 8:30 am	Breakfast
8:30 am	Group Photo
9:00 am - 12:30 pm	**Metals in Pathogenesis, Disease and Medicine**
	Discussion Leader: **Celia Goulding** (University of California, Irvine, USA)
9:00 am - 9:10 am	Opening Remarks
9:10 am - 9:20 am	Introduction by Discussion Leader
9:20 am - 9:40 am	**Toshiki Nakashige** (Massachusetts Institute of Technology, USA) "Metal Sequestration of the Host-Defense Protein Human Calprotectin "
9:40 am - 9:50 am	Discussion
9:50 am - 10:10 am	**Daisy Wong** (Western University, Canada) "Mass Spectrometric Studies of Human Metallothionein and Glutathione Binding to the Anti-Tumour Complex, Dirhodium Tetraacetate"
10:10 am - 10:20 am	Discussion
10:20 am - 10:35 am	**Patricia Feliciano** (Massachusetts Institute of Technology, USA) "Fe-S Cluster-Containing Fumarate Hydratase Enzyme as a Drug Target Against Neglected Tropical Diseases"
10:35 am - 10:40 am	Discussion
10:40 am - 11:05 am	Coffee Break
11:05 am - 11:25 am	**Julia Martin** (Indiana University Bloomington, USA) "Perturbation of Manganese Metabolism Disrupts Cell Division in *Streptococcus pneumoniae*"
11:25 am - 11:35 am	Discussion
11:35 am - 11:55 am	**Sarah Harris** (University of Minnesota, USA) "Altering the Selectivity of Luminescent Terbium Probes for Copper over Zinc via the Number of Sensitizing Phenanthridine Moieties"

11:55 am - 12:05 pm	Discussion
12:05 pm - 12:25 pm	**Edmund Chun Ming Tse** (California Institute of Technology, USA) "Tracking DNA Damage via a Key Electron Transfer Mechanism Involving Iron-Sulfur Cluster Proteins
12:25 pm - 12:30 pm	Discussion
12:30 pm	Lunch
1:30 pm - 4:00 pm	Free Time
4:00 pm - 6:00 pm	Poster Session
6:00 pm	Dinner
7:30 pm - 9:30 pm	**Metallocofactor Assembly and Enzyme Mechanisms**
	Discussion Leader: **Markus Ribbe** (University of California, Irvine, USA)
7:30 pm - 7:40 pm	Introduction by Discussion Leader
7:40 pm - 8:00 pm	**Amanda Byer** (Montana State University, USA) "[FeFe]-Hydrogenase Maturase HydF"
8:00 pm - 8:10 pm	Discussion
8:10 pm - 8:20 pm	**Soo Ro** (Northwestern University, USA) "Understanding Particulate Methane Monooxygenase in a Native-Like Environment"
8:20 pm - 8:25 pm	Discussion
8:25 pm - 8:45 pm	**Noah Dunham** (The Pennsylvania State University, USA) "Mechanistic Insight into Desaturation Reactions by Two Fe(II)/2-(Oxo)glutarate-Dependent Oxygenas
8:45 pm - 8:55 pm	Discussion
8:55 pm - 9:05 pm	**Derek Gagnon** (University of California, Davis, USA) "An Intermediate in the Radical Addition of S-Adenosyl-L-Methionine to S-VOBA in MqnE"
9:05 pm - 9:10 pm	Discussion
9:10 pm - 9:25 pm	**Elizabeth Blaesi** (Pennsylvania State University, USA) "Insights into the Mechanism of PhnZ, a Peculiar, Mixed-Valent Oxygenase"
9:25 pm - 9:30 pm	Discussion

Saturday

7:30 am - 8:30 am	Breakfast
9:00 am - 12:30 pm	**Artificial Protein and Molecular Design**
	Discussion Leader: **Jared Lewis** (University of Chicago, USA)
9:00 am - 9:10 am	Introduction by Discussion Leader

9:10 am - 9:30 am	**Gozde Ulas** (University of California, San Francisco, USA) "Designed Metalloproteins to Control Radicals"
9:30 am - 9:40 am	Discussion
9:40 am - 10:00 am	**Anastasia Manesis** (Ohio State University, USA) "Developing Nickel-Substituted Azurin as a Model for Acetyl CoA Synthase"
10:00 am - 10:05 am	Discussion
10:05 am - 10:15 am	**Ariel Schuelke** (University of Vermont, USA) "Spectroscopy-Guided Design of Synthetic Selective Nickel Chelatases from CbiXS"
10:15 am - 10:20 am	Discussion
10:20 am - 10:50 am	Coffee Break
10:50 am - 11:10 am	**Jan Paulo Zaragoza** (Johns Hopkins University, USA) "Direct Observation of Oxygen Rebound in a Synthetic Iron(Hydroxo) Complex"
11:10 am - 11:20 am	Discussion
11:20 am - 11:40 am	**Victoria Oswald** (University of California, Irvine, USA) "Ligand Design to Support High Valent Metal Oxido/Hydroxido Complexes"
11:40 am - 11:50 am	Discussion
11:50 am - 12:00 pm	**Ruixi Fan** (Carnegie Mellon University, USA) "Characterization of a Novel Fe(V)=O Species Using Mossbauer Spectroscopy"
12:00 pm - 12:05 pm	Discussion
12:05 pm - 12:25 pm	**Kazuki Tanifuji** (University of California, Irvine, USA) "Synthesis, Characterization, and Reactivity of an Asymmetric Synthetic Mimic of the Nitrogenase M-Cluster"
12:25 pm - 12:30 pm	Discussion
12:30 pm	Lunch
1:30 pm - 4:00 pm	Free Time
4:00 pm - 6:00 pm	Poster Session
6:00 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	**Biological Electron Transfer and Applications in Renewable Energy**

Discussion Leader: **James Mayer** (Yale University, USA)

7:30 pm - 7:40 pm Introduction by Discussion Leader

7:40 pm - 8:00 pm **Chang Cui** (University of Illinois at Urbana-Champaign, USA)
"A Designed Metalloenzyme Achieving the Catalytic Rate of a Native Enzyme"

8:00 pm - 8:10 pm Discussion

8:10 pm - 8:30 pm **S. Garrett Williams** (Arizona State University, USA)
"Electrochemical Comparison of the [FeFe]-Hydrogenases from *Clostridium pasteurianum*"

8:30 pm - 8:35 pm Discussion

8:35 pm - 8:55 pm **Suzanne Adam** (Johns Hopkins University, USA)
"Reactions of o-Catechols with a Heme-Peroxo-Cu Complex Occur via a pKa-Dependent Mechanism:
Insights into the Nature of PCET in O_2 Reduction"

8:55 pm - 9:05 pm Discussion

9:05 pm - 9:25 pm **Mioy Huynh** (University of Illinois at Urbana-Champaign, USA)
"Bioinspired [NiFe]- and [FeFe]-Hydrogenase Models for Hydrogen Production"

9:25 pm - 9:30 pm Discussion

Sunday

7:30 am - 8:30 am Breakfast

9:00 am - 12:30 pm **Functional Insights from Structure and Spectroscopy**

Discussion Leader: **Petra Fromme** (Arizona State University, USA)

9:00 am - 9:10 am Introduction by Discussion Leader

9:10 am - 9:30 am **Franklin Fuller** (Lawrence Berkeley National Laboratory, USA)
"High Throughput Transient X-Ray Crystallography and Emission Spectroscopy on the Metalloenzymes at an X-Ray Free Electron Laser"

9:30 am - 9:40 am Discussion

9:40 am - 10:00 am **Ruchira Chatterjee** (Lawrence Berkeley National Laboratory, USA)
"Room Temperature Femtosecond X-Ray Crystallography of Photosystem II"

10:00 am - 10:10 am Discussion

10:10 am - 10:30 am **Adam Offenbacher** (University of California, Berkeley, USA)

	"Towards an Understanding of the Origins of Enzymatic Catalysis in Nature"
10:30 am - 10:35 am	Discussion
10:35 am - 11:05 am	Coffee Break
11:05 am - 11:25 am	**Rebeca Gomez Castillo** (Max Planck Institute for Chemical Energy Conversion, Germany) "XAS Investigation of the Q Intermediate of sMMO"
11:25 am - 11:35 am	Discussion
11:35 am - 11:55 am	**Elizabeth Onderko** (Pennsylvania State University, USA) "Effect of the Axial Ligand on Cytochrome P450 Catalysis"
11:55 am - 12:05 pm	Discussion
12:05 pm - 12:25 pm	**Cindy Pham** (University of California, Davis, USA) "Terminal Hydride Species in Wild-Type and Variant FeFe Hydrogenases Characterized by Nuclear Resonance Vibrational Spectroscopy"
12:25 pm - 12:30 pm	Discussion
12:30 pm	Lunch
1:30 pm	Departure

This material is based upon work supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under award number DE-SC0016880.

Metals in Biology (2017)

Name	Organization	Participation
Ackerson, Christopher	Colorado State University	Poster Presenter
Adam, Suzanne M	Johns Hopkins University	Poster Presenter
Almo, Steven C	Albert Einstein College of Medicine	Attendee
Angerhofer, Alexander	University of Florida	Poster Presenter
Armstrong, Fraser A	University of Oxford	Speaker
Aron, Allegra T	UC Berkeley	Poster Presenter
Austin, Rachel N	Barnard College, Columbia University	Poster Presenter
Bahrami-Dizicheh, Z	Arizona State University	Poster Presenter
Baldwin, Michael J	University of Cincinnati	Poster Presenter
Barondeau, David P	Texas A&M University	Poster Presenter
Basu, Partha	Indiana University-Purdue University Indianapolis	Poster Presenter
Batista, Victor S	Yale University	Speaker
Blaesi, Elizabeth J	Pennsylvania State University	Poster Presenter
Bollinger, Joseph M	The Pennsylvania State University	Speaker
Boralugodage, Nilusha	Pacific Northwest National Laboratory	Poster Presenter
Bowler, Bruce E	University of Montana	Poster Presenter
Bren, Kara L	University of Rochester	Discussion Leader
Britt, R. David	University of California, Davis	Chair
Brumaghim, Julia L	Clemson University	Poster Presenter
Burger, Richard M	Brooklyn College of CUNY	Attendee
Burgmayer, Sharon	Bryn Mawr College	Poster Presenter
Bush, Ashley I	Florey Institute of Neuroscience and Mental Health	Speaker
Butch, Susan	Wilmad-Labglass	Poster Presenter
Butler, Alison	University of California, Santa Barbara	Speaker
Casey, William H	University of California, Davis	Discussion Leader
Chacon, Kelly	Reed College	Poster Presenter
Chazin, Walter J	Vanderbilt University	Speaker
Chen, Hao	Nanjing University	Poster Presenter

Cotruvo, Joseph A	Pennsylvania State University	Poster Presenter
Cox, Nicholas J	Australian National University, Australia	Speaker
Cramer, Stephen P	UC Davis	Poster Presenter
Cui, Chang	University of Illinois at Urbana-Champaign	Poster Presenter
Cutsail, George E	Max Planck Institute for Chemical Energy Conversion	Poster Presenter
Darensbourg, Marcetta	Texas A&M University	Poster Presenter
David, Sheila	University of California, Davis	Discussion Leader
Dawson, John H	Univ of South Carolina	Attendee
Deane, Caitlin D	Nature Chemical Biology	Attendee
Debeer, Serena	Max Planck Institute for Chemical Energy Conversion	Speaker
Debus, Richard J	University of California, Riverside	Discussion Leader
DeRose, Victoria J	University of Oregon	Speaker
Do, Loi	University of Houston	Poster Presenter
Dubois, Jennifer L	Montana State University	Poster Presenter
Dunham, Noah P	The Pennsylvania State University	Poster Presenter
Elliott, Sean J	Boston University	Poster Presenter
Farquhar, Erik R	Case Western Reserve University	Poster Presenter
Fischer, Woodward	California Institute of Technology	Speaker
Fromme, Petra	Arizona State University	Speaker
Fuller, Franklin D	Lawrence Berkeley National Laboratory	Poster Presenter
Gagnon, Derek M	University of California, Davis	Poster Presenter
Ghiladi, Reza A	North Carolina State University	Poster Presenter
Ghirlanda, Giovanna	Arizona State University	Poster Presenter
Giedroc, David P	Indiana University	Speaker
Gilbertson, John D	Western Washington University	Poster Presenter
Gizzi, Anthony S	Albert Einstein College of Medicine	Poster Presenter
Glover, Starla D	University of Pennsylvania	Poster Presenter
Goldberg, David P	Johns Hopkins University	Poster Presenter
Goldfarb, Daniella	Weizmann Institute of Science	Speaker
Gomez Castillo, R	Max Planck Institute for Chemical Energy Conversion	Poster Presenter

Goodin, David B	Department of Chemistry	Poster Presenter
Goulding, Celia W	University of California, Irvine	Discussion Leader
Gray, Harry B	California Institute of Technology	Speaker
Green, Michael T	University of California, Irvine	Discussion Leader
Greene, Brandon L	Harvard University	Poster Presenter
Grove, Tyler L	Albert Einstein College of Medicine	Poster Presenter
Groves, John T	Princeton University	Attendee
Guo, Yisong	Carnegie Mellon University	Poster Presenter
Guo, Yirui	UC Berkeley	Poster Presenter
Harman, William H	University of California, Riverside	Poster Presenter
Harris, David	Northwestern University	Poster Presenter
Heffern, Marie C	University of California, Berkeley	Poster Presenter
Hegg, Eric L	Michigan State University	Poster Presenter
Hellwig, Petra	University of Strasbourg-CNRS	Poster Presenter
Henthorn, Justin	Max-Planck-Institute	Poster Presenter
Hoffman, Brian M	Northwestern University	Attendee
Hu, Yilin	University of California, Irvine	Discussion Leader
Hu, Jian	Michigan state university	Poster Presenter
Hughes, Philippa	Royal Society of Chemistry	Attendee
Ikeda-Saito, Masao	Tohoku University	Attendee
Ishimori, Koichiro	Hokkaido University	Poster Presenter
Ivanovic-Burmazovic, I	University Erlangen-Nuernberg	Poster Presenter
Jollie, David R	National Institutes of Health	Attendee
Jones, Anne K	Arizona State University	Discussion Leader
Kan, Jennifer	California Institute of Technology	Speaker
Kern, Jan	Lawrence Berkeley National Lab	Poster Presenter
Kieber-Emmons, M	University of Utah	Poster Presenter
King, Paul W	National Renewable Energy Lab	Poster Presenter
Kirk, Martin L	The University of New Mexico	Poster Presenter
Klinman, Judith	University of California, Berkeley	Speaker

Knapp, Michael J	University of Massachusetts Amherst	Poster Presenter
Koehn, Eric	University of California, Berkeley	Poster Presenter
Koppenol, Willem H	Swiss Federal Institute of Technology	Attendee
Korendovych, Ivan V	Syracuse University	Poster Presenter
Krebs, Carsten	Penn State University	Attendee
Lancaster, Kyle M	Cornell University	Speaker
Lanzilotta, William N	University of Georgia	Poster Presenter
Lee, Chi-Chung	University of California, Irvine	Poster Presenter
Lindahl, Paul A	Texas A&M University	Poster Presenter
Lippard, Stephen J.	Massachusetts Institute of Technology	Attendee
Liptak, Matthew D	University of Vermont	Poster Presenter
Liu, Aimin	University of Texas at San Antonio	Poster Presenter
Lu, Yi	University of Illinois	Vice Chair
Magyar, John S	California Institute of Technology	Poster Presenter
Majumder, Erica L-W	University of Missouri	Poster Presenter
Manesis, Anastasia C	Ohio State University	Poster Presenter
Marchiori, David	University of California, Davis	Poster Presenter
Marletta, Michael A	University of California, Berkeley	Speaker
Maroney, Michael J	University of Massachusetts	Poster Presenter
Mathies, Guinevere	Massachusetts Institute of Technology	Poster Presenter
Mayer, James M	Yale University	Poster Presenter
McGarry, Jennifer M	University of Wisconsin - Milwaukee	Poster Presenter
Michel, Sarah L	University of Maryland	Poster Presenter
Morrow, Janet R	University at Buffalo, SUNY	Poster Presenter
Mukherjee, Anusree	University of Alabama in Huntsville	Poster Presenter
Munck, Eckard	Carnegie Mellon University	Attendee
Murray, Leslie J	University of Florida	Speaker
Nakashige, Toshiki G	Massachusetts Institute of Technology	Poster Presenter
Newman, Dianne K	California Institute of Technology	Speaker
Nicoludis, Jack	Harvard University	Attendee

Niklas, Jens	Argonne National Laboratory	Poster Presenter
Nolan, Elizabeth M	Massachusetts Institute of Technology	Poster Presenter
O'Connor, Joseph M	UCSD	Poster Presenter
O'Halloran, Thomas V	Northwestern University	Speaker
Offenbacher, Adam R	University of California, Berkeley	Poster Presenter
Olshansky, Lisa	University of California, Irvine	Poster Presenter
Onderko, Elizabeth	Pennsylvania State University	Poster Presenter
Pacheco, A. Andrew	University of Wisconsin-Milwaukee	Poster Presenter
Pecoraro, Vincent L	University of Michigan	Attendee
Peters, Jonas C	California Institute of Technology	Speaker
Peters, John W	Washington State University	Speaker
Poulos, Thomas L	Univ. Ca. Irvine	Attendee
Prisic, Sladjana	University of Hawaii	Poster Presenter
Que, Emily L	University of Texas at Austin	Poster Presenter
Rajakovich, Lauren J	Pennsylvania State University	Poster Presenter
Rao, Guodong	University of California	Poster Presenter
Raven, Emma	University of Leicester	Poster Presenter
Reddi, Amit R	Georgia Institute of Technology	Poster Presenter
Ribbe, Markus	University of California, Irvine	Attendee
Rivera, Shannon	Emory University	Poster Presenter
Ro, Soo	Northwestern University	Poster Presenter
Rodriguez, Kyle J	University of New Hampshire	Poster Presenter
Romano, Christine A	Oregon Health & Science University	Poster Presenter
Rose, Michael J	University of Texas at Austin	Speaker
Rothman, Dan	Massachusetts Institute of Technology	Speaker
Roy, Lisa	Max Planck Institute for Chemical Energy Conversion	Poster Presenter
Schwarz, Guenter	University of Cologne	Speaker
Seefeldt, Lance C	Utah State University	Speaker
Shafaat, Hannah S	The Ohio State University	Speaker
Shearer, Jason M	University of Nevada, Reno	Poster Presenter

Shelake, Rahul M	Proteo-Science Center, Ehime University	Poster Presenter
Silakov, Alexey	Pennsylvania State University	Poster Presenter
Soldatova, Alexandra	University of Washington	Poster Presenter
Spiro, Thomas G	University of Washington	Speaker
Stich, Troy A	University of California	Poster Presenter
Streit, Bennett R	Montana State University	Poster Presenter
Suess, Daniel	University of California, Davis	Poster Presenter
Szymczak, Nathaniel K	University of Michigan	Poster Presenter
Tao, Lizhi	University of California, Davis	Poster Presenter
Tebo, Bradley M	OHSU	Attendee
Tezcan, Akif	University of California, San Diego	Attendee
Tomat, Elisa	University of Arizona	Poster Presenter
Tommos, Cecilia I	University of Pennsylvania	Poster Presenter
Trogler, William C	University of California San Diego	Poster Presenter
Tse, Edmund Chun M	California Institute of Technology	Poster Presenter
Ulas, Gozde	University of California, San Francisco	Poster Presenter
Utschig, Lisa M	Argonne National Laboratory	Poster Presenter
Valentine, Joan S	University of California Los Angeles	Poster Presenter
Van Stappen, Casey M	Max-Planck Institute for Chemical Energy Conversion	Poster Presenter
Wang, Jiangyun	Institute of Biophysics, Chinese Academy of Sciences	Poster Presenter
Waskell, Lucy A	University of Michigan	Poster Presenter
Waters, Lauren S	University of Wisconsin-Oshkosh	Speaker
Weinert, Emily E	Emory University	Discussion Leader
Wilcox, Dean E	Dartmouth College	Poster Presenter
Wilcoxen, Jarett M	University of California, Davis	Poster Presenter
Wilks, Angela	University of Maryland	Poster Presenter
Williams, S. Garrett	Arizona State University	Poster Presenter
Wilson, Justin J	Cornell University	Poster Presenter
Wong, Daisy	Western University	Poster Presenter
Yatsunyk, Liliya	Swarthmore College	Poster Presenter

Yu, Steve S.F.	Academia Sinica	Speaker
Zaragoza, Jan Paulo	Johns Hopkins University	Poster Presenter
Zhao, Jing	Nanjing University	Poster Presenter
Ziegler, Christopher J	University of Akron	Poster Presenter

Bioorganic Chemistry (GRS) (2017)

Name	Organization	Participation
Bak, Daniel W	Boston College	Poster Presenter
Balogh, Dora	Technische Universitat Munchen	Poster Presenter
Bechtel, Tyler	Boston College	Discussion Leader
Bienick, Matthew	University of Arizona	Poster Presenter
Blom, Antoinette	California Institute of Technology	Speaker
Buckton, Laura K	University of New South Wales	Poster Presenter
Cabral, Charles	Federal Bureau of Investigation	Speaker
Cai, Xiaochuan	Memorial Sloan Kettering Cancer Center	Speaker
Cao, Jian	Southern Methodist University	Poster Presenter
Csizmar, Clifford M	University of Minnesota	Poster Presenter
Davis, Tony D.	University of California, San Diego	Poster Presenter
Deibler, Kristine	Northwestern University	Poster Presenter
DeMeester, Kristen E	University of Delaware	Discussion Leader
Eising, Selma	Radboud University Nijmegen	Poster Presenter
Elsohly, Adel M	University of California, Berkeley	Poster Presenter
Eubanks, Christopher	Duke University Chemistry	Poster Presenter
Furst, Ariel L	University of California, Berkeley	Poster Presenter
Gee, Clifford T	University of Minnesota	Chair
Gober, Isaiah N	University of North Carolina at Chapel Hill	Poster Presenter
Halford, Bethany	Chemical and Engineering News	Speaker
Hallenbeck, Kenneth K	University of California, San Francisco	Poster Presenter
Haney, Conor M	University of Pennsylvania	Poster Presenter
Hill, Zachary B	University of California, San Francisco	Discussion Leader
Huang, Mia	University of California, San Diego	Discussion Leader
Johnson, Oleta T	University of Michigan	Poster Presenter
Jradi, Fadi M	Howard Hughes Medical Institute	Poster Presenter
Kaiser, Christine E	AstraZeneca	Speaker
Kinarivala, Nihar S	Texas Tech University Health Science Center	Poster Presenter

Kulkarni, Rhushikesh	National Cancer Institute, NIH	Speaker
Lorenz, Daniel A	University of Michigan	Poster Presenter
Maini, Rumit	The University of Tokyo	Discussion Leader
Matikonda, Siddharth	University of Otago	Discussion Leader
Milosevich, Natalia H	University of Victoria	Poster Presenter
Mix, Kalie	University of Wisconsin-Madison	Discussion Leader
Modell, Ashley	New York University	Chair
Morgan, Brittany S	Duke University	Speaker
Padilla-Salinas, R	University of Colorado Boulder BioFrontiers Institute	Poster Presenter
Parker, Christopher G	The Scripps Research Institute	Speaker
Pham, Grace	The Genomics Institute of the Novartis Foundation	Poster Presenter
Pyzocha, Neena K	Broad Institute of MIT and Harvard	Speaker
Schultz, Peter G	The Scripps Research Institute	Speaker
Spek, Erik	Vedanta Biosciences	Speaker
Steinauer, Angela	Yale University	Poster Presenter
Stover, James	Aegis Sciences Corporation	Speaker
Tan, Zhi Wei	Harvard Medical School HIM	Poster Presenter
Thomas, Nicole C	University of Wisconsin, Madison	Poster Presenter
Wang, Yuanyou	Texas A&M University	Poster Presenter
Weeks, Amy M	University of California, San Francisco	Poster Presenter
West, Harrison T	University of Minnesota	Poster Presenter
Wu, Mingxuan	Johns Hopkins University School of Medicine	Poster Presenter
Wuo, Michael G	New York University	Poster Presenter
Yim, Joshua	Stanford University School of Medicine	Speaker
Zhang, Chi	Massachusetts Institute of Technology	Poster Presenter
Zhou, Effie	University of Illinois at Urbana-Champaign	Poster Presenter