

Understanding and Harnessing the Power of Metalloregulators and Metalloenzymes for Applications in Energy, Environment and Medicine

January 21 - 26, 2018

Chair

Yi Lu

Vice Chair

J. Martin Bollinger

Four Points Sheraton / Holiday Inn Express

1050 Schooner Drive Ventura, CA, US

Conference Description

Metal ions play vital roles in regulation and catalytic transformation in numerous biological processes, including photosynthesis, respiration, global nitrogen, hydrogen and carbon cycles, biosynthesis of natural products such as antibiotics, genetic control, and neurotransmission. At the same time, many biological systems are exposed to toxic metal ions in the environment. Understanding both beneficial and detrimental effects of these metal ions in biology will allow us to harness the power of many metalloregulators and metalloenzymes and to design artificial proteins or synthetic models for many applications, such small molecular activation and transformation in sustainable energies and pharmaceuticals, environmental monitoring, bioremediations, and metal-based drugs. To achieve the goals, we need multiple disciplinary approaches to develop new methods to characterize the structures of metal-binding sites in proteins and nucleic acids and their regulation or reaction mechanisms, and then apply insights gained from the study to harness power of the native systems or design artificial systems.

The Metals in Biology GRC is the annual premier conference that brings scientists from diverse backgrounds and expertise in chemistry, physics, biochemistry, molecular biology, cellular biology and medicinal science to discuss recent progress in this field. To stimulate new directions of research and foster new collaborations among participants with complementary interests and skills, the conference has scheduled ample time after each lecture and during poster sessions to facilitate discussions in an open atmosphere.

The Gordon Research Seminar (GRS) in Bioinorganic Chemistry is closely associated with the MIB GRC. This meeting typically draws graduate and postdoctoral students from a variety of laboratories studying metals in biology. The GRS overlaps with the MIB GRC meeting for one evening session on Thursday, including a poster session that allows students to meet and interact with established scientists. We specifically encourage graduate students and postdocs to take advantage of these unique educational opportunities and to participate in either the MIB GRC conference or the Bioinorganic Chemistry GRS or both.

Related Meeting



This GRC will be held in conjunction with the "Bioinorganic Chemistry (GRS)" Gordon Research Seminar (GRS). Those interested in attending both meetings must submit an application for the GRS in addition to an application for the GRC. Refer to the <u>associated GRS program page</u> for more information.

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	Keynote Session: Metalloenzymes in Solar Fuels Discussion Leader: Junko Yano (Lawrence Berkeley National Laboratory, USA)
7:40 pm - 8:20 pm	Jian-Ren Shen (Okayama University, Japan) "Mechanism of Photosynthetic Water-Splitting Catalyzed by the Mn ₄ CaO ₅ Metal Cluster in Photosystem II"
8:20 pm - 8:35 pm	Discussion
8:35 pm - 8:55 pm	Jan Kern (Lawrence Berkeley National Laboratory, USA) "Taking Snapshots of the Water Oxidation Reaction in Photosystem II Using Crystallography and Spectroscopy at an XFEL"

8:55 pm - 9:05 pm	Discussion
9:05 pm - 9:25 pm	James Birrell (Max Planck Institute for Chemical Energy Conversion, Germany) "The Catalytic Cycle of [FeFe] Hydrogenase: A Tale of Two Sites"
9:25 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	Design and Engineering of Functional Metalloproteins Discussion Leader: Vincent Pecoraro (University of Michigan, USA)
9:00 am - 9:30 am	Thomas Ward (University of Basel, Switzerland) "Endowing Metal-Based Catalysts with a Genetic Memory: Artificial Metalloenzymes"
9:30 am - 9:40 am	Discussion
9:40 am - 10:10 am	John Hartwig (University of California, Berkeley, USA) "Platinum-Group Organometallic Enzymes from Heme Proteins for Abiological Transformations"
10:10 am - 10:20 am	Discussion
10:20 am - 10:35 am	Ross Anderson (University of Bristol, United Kingdom) "Catalytic Versatility in a Heme-Dependent <i>De Novo</i> Enzyme"
10:35 am - 10:40 am	Discussion
10:40 am - 11:10 am	Coffee Break
11:10 am - 11:40 am	Jiangyun Wang (Institute of Biophysics, Chinese Academy of Sciences, China) "Metalloprotein Design Using Genetic Code Expansion"
11:40 am - 11:50 am	Discussion

11:50 am - 12:20 pm	Jenny Yang (Georgia State University, USA) "Designing Metalloproteins for Precision Diagnosis and Medicine"
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: Rachel Austin (Barnard College / Columbia University, USA) and Kara Bren (University of Rochester, USA)
4:00 pm - 6:00 pm	Poster Session
6:00 pm - 7:00 pm	Dinner
7:30 pm - 9:30 pm	Roles of Metal Ions and Metal Clusters in Nucleic Acids- Based Catalysis and Signaling Discussion Leader: Victoria DeRose (University of Oregon, USA)
7:30 pm - 8:00 pm	Jacqueline Barton (California Institute of Technology, USA) "DNA Signaling by Metalloproteins"
8:00 pm - 8:10 pm	Discussion
8:10 pm - 8:40 pm	Roland Sigel (University of Zurich, Switzerland) "Tweaking Structure and Function - Metal lons in the Core of Single Ribozymes and Riboswitches"
8:40 pm - 8:50 pm	Discussion
8:50 pm - 9:20 pm	Peng Chen (Peking University, China) "Transition Metal-Mediated Signal Transduction at the Host-Pathogen Interface"
9:20 pm - 9:30 pm	Discussion

Tuesday	
7:30 am - 8:30 am	Breakfast
9:00 am - 12:30 pm	Metalloenzymes and Their Models in Global Hydrogen, Oxygen and Nitrogen Cycles Discussion Leader: J. Martin Bollinger (The Pennsylvania State University, USA)
9:00 am - 9:30 am	Kyle Lancaster (Cornell University, USA) "Bacterial Nitrification, Revised"
9:30 am - 9:40 am	Discussion
9:40 am - 9:55 am	Molly O'Hagan (Pacific Northwest National Laboratory, USA) "Controlling the Reactivity of Molecular Catalysts Using the Medium and Protein Scaffolds"
9:55 am - 10:00 am	Discussion
10:00 am - 10:15 am	Jaeheung Cho (Daegu Gyeongbuk Institute of Science and Technology, South Korea) "Unprecedented Nitrile Reactivity Mediated by a Peroxocobalt(III) Intermediate"
10:15 am - 10:20 am	Discussion
10:20 am - 10:35 am	Yilin Hu (University of California, Irvine, USA) "CO ₂ Activation by Nitrogenase Iron Proteins"
10:35 am - 10:40 am	Discussion
10:40 am - 11:10 am	Coffee Break
11:10 am - 11:40 am	Marcetta Darensbourg (Texas A&M University, USA) "Actor Ligands in Bioinspired HER Catalysts: NO as Electron Buffer and Guide of Hemi-Lability in Metallodithiolates"
11:40 am - 11:50 am	Discussion
11:50 am - 12:20 pm	William Tolman (University of Minnesota, USA) "Formally Cu(III) Complexes Relevant to Proposed Enzyme 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	Metalloenzymes and Their Models in Biological Electron Transfer and Catalysis Discussion Leader: James Kincaid (Marquette University, USA)
7:30 pm - 8:00 pm	Kara Bren (University of Rochester, USA) "Metalloprotein Catalysts for Energy Storage"
8:00 pm - 8:10 pm	Discussion
8:10 pm - 8:40 pm	Yong Zhang (Stevens Institute of Technology, USA) "Mechanisms of Heme-Based Carbene Transfer Reactions"
8:40 pm - 8:50 pm	Discussion
8:50 pm - 9:05 pm	Thomas Makris (University of South Carolina, USA) "Aberrant Reactivity of Enzyme Metal-Oxo Species"
9:05 pm - 9:10 pm	Discussion
9:10 pm - 9:25 pm	Abhishek Dey (Indian Association for the Cultivation of Science, India) "H-Atom Transfer Reactivity of Dioxygen Adducts of Iron Porphyrins"
9:25 pm - 9:30 pm	Discussion
Wednesday	
7:30 am - 8:30 am	Breakfast
9:00 am - 12:30 pm	Metalloenzymes and Their Models in Global Carbon Cycles and Chemical Transformations Discussion Leader: Lawrence Que (University of Minnesota, USA)

9:00 am - 9:30 am	Rachel Austin (Barnard College / Columbia University, USA) "Catalytic Activity of Non-Heme Diiron Monooxygenases"
9:30 am - 9:40 am	Discussion
9:40 am - 10:10 am	Sharon Hammes-Schiffer (Yale University, USA) "Proton-Coupled Electron Transfer and the Catalytic Role of Iron in Soybean Lipoxygenase"
10:10 am - 10:20 am	Discussion
10:20 am - 10:35 am	Kenichi Yokoyama (Duke University Medical Center, USA) "Radically Novel Mechanism in Natural Product and Cofactor Biosynthesis"
10:35 am - 10:40 am	Discussion
10:40 am - 11:10 am	Coffee Break
11:10 am - 11:40 am	Seigo Shima (Max Planck Institute for Terrestrial Microbiology, Germany) "An Astonishing CO_2 Fixation Mechanism Involved in Biological Methanogenesis"
11:40 am - 11:50 am	Discussion
11:50 am - 12:20 pm	Alison Fout (University of Illinois at Urbana-Champaign, USA) "Bioinspired Iron Catalysts for Nitrate and Perchlorate Reduction"
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	Metal Ions in Astrobiology, Evolution Biology, Marine Biochemistry and the Environment Discussion Leader: Joan Valentine (University of California, Los Angeles, USA)
7:30 pm - 8:00 pm	Ariel Anbar (Arizona State University, USA) "Elements and Evolution"
8:00 pm - 8:10 pm	Discussion
8:10 pm - 8:40 pm	Paul Falkowski (Rutgers University, USA) "Life's Legos: The Structural Modules Responsible for Electron Transfers Across the Tree of Life"
8:40 pm - 8:50 pm	Discussion
8:50 pm - 9:05 pm	Jennifer Glass (Georgia Institute of Technology, USA) "Ironing Out the Impact of Metal-Microbe Interactions on Ancient Atmospheres"
9:05 pm - 9:10 pm	Discussion
9:10 pm - 9:25 pm	Can Xie (Peking University, China) "MagR: Dual Faceted Nature of Animal Magnetoreception"
9:25 pm - 9:30 pm	Discussion
Thursday	
7:30 am - 8:30 am	Breakfast
9:00 am - 12:30 pm	Metal Ion Homeostasis, Imaging and Therapeutics Discussion Leader: Amy Barrios (University of Utah, USA)
9:00 am - 9:30 am	Jonathan Sessler (University of Texas at Austin, USA) "Texaphyrin-Based Theranostics - An Update"
9:30 am - 9:40 am	Discussion
9:40 am - 10:10 am	Thomas Meade (Northwestern University, USA) "Opening the Proteome to MR Imaging Analysis: Possible?"
10:10 am - 10:20 am	Discussion

10:20 am - 10:35 am	Emily Que (University of Texas at Austin, USA) "Exploiting First Row Transition Metals for Magnetic Resonance Biosensing"
10:35 am - 10:40 am	Discussion
10:40 am - 11:10 am	Coffee Break
11:10 am - 11:40 am	Katherine Franz (Duke University, USA) "Metals, Drugs and Fungal Pathogens"
11:40 am - 11:50 am	Discussion
11:50 am - 12:05 pm	Jun-Long Zhang (Peking University, China) "Bioinspired Approach to Design of Lanthanide Probes for NIR Imaging"
12:05 pm - 12:10 pm	Discussion
12:10 pm - 12:25 pm	Sarah Michel (University of Maryland, USA) "Translational Bioinorganic Chemistry: Tracking Iron in Blood Plasma After Infusion with Intravenous Iron Nanoparticles"
12:25 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	Keynote Session: Metals, Water, Light, O ₂ , Camera and Action! Joint session with the Bioinorganic Chemistry Gordon Research Seminar. Discussion Leader: Harry Gray (California Institute of Technology, USA)
7:30 pm - 7:40 pm	Starla Glover (University of Pennsylvania, USA) "Unraveling the Role of Local and Global Protein Properties on the Redox Behavior of Tryptophan and Tyrosine"

7:40 pm - 7:45 pm	Discussion
7:45 pm - 7:55 pm	Kelly Chacon (Reed College, USA) "Trapping Intermediates in Metal Transfer Reactions of the CusCBAF Export Pump of <i>E. coli</i> "
7:55 pm - 8:00 pm	Discussion
8:00 pm - 8:10 pm	Huangen Ding (Louisiana State University, USA) "Electron Transfer Activity of mitoNEET via Its [2Fe-2S] Clusters"
8:10 pm - 8:15 pm	Discussion
8:15 pm - 9:15 pm	Gary Brudvig (Yale University, USA) "Progress Towards a Molecular Mechanism of Water Oxidation in Photosystem II"
9:15 pm - 9:30 pm	Discussion
Friday	
7:30 am - 8:30 am	Breakfast
9:00 am	Departure

Contributors









Sessler Family Charitable Trust



















The Saltman Lecturer Fund































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