



Uncovering and Capitalizing on the Chemistry of Metals in Biology

January 25 - 28, 2018

Chair

John Nicoludis

Four Points Sheraton / Holiday Inn Express

1050 Schooner Drive

Ventura, CA, US

Conference Description

GRS Speaker Abstract Deadline: *Although applications will be accepted until the date noted above, any applicants who wish to be considered for an oral presentation should submit their application by **October 27, 2017**.*

Meeting Description

From controlling the transport of metals into, out of and around the cell to positioning metals in active sites to do chemical transformations that inspire synthetic chemists, biology still has unparalleled mastery that bioinorganic chemists seek to understand. A variety of diseases, from cancer to nutrient imbalances, involve processes of metal transport and reactivity within the body, making our goal of understanding the role of metals in biology an important biomedical direction. This Gordon Research Seminar presents the most novel research in the field of bioinorganic chemistry, providing a current view into our knowledge of the roles of metal in biology and our progress in emulating this chemistry. In addition to experimental investigations, this conference will highlight the emerging roles that computational tools, such as molecular dynamics, quantum mechanical calculations, bioinformatics and RNA-seq analysis, have in understanding bioinorganic chemistry.

Now in its 22nd year, the Bioinorganic Chemistry GRS was established in 1996 to supplement the routinely oversubscribed Metals in Biology Gordon Research Conference (GRC). The GRS provides a platform for young scientists to hear novel research and take part in a dynamic scientific community. The breadth of the bioinorganic chemistry field creates a collaborative environment for scientists from a variety of fields that are united by an interest in biology and inorganic chemistry. A joint session with the Metals in Biology GRC and a focus on connecting young scientists looking for their next career move with senior researchers provides exceptional networking opportunities.

We encourage prospective attendees to apply early as the GRS has been consistently oversubscribed due to the unique format of this GRS. Any scientist at the graduate student or postdoc level in the field of bioinorganic chemistry is welcome to apply. Preference will be given to those who submit poster or talk abstracts. Please contact the 2018 Chair, Jack Nicoludis, if you have any questions.

The seminar will consist of the following sessions:

- Metal homeostasis: moving metals into, out of, and around the cell
- Inspired by nature: designing metalloproteins and inorganic catalysts
- Spectroscopic methods to study metal reactivity and the flow of electrons in the cell
- Emerging computational tools for bioinorganic chemistry
- Structure-function relationships in bioinorganic macromolecules

Related Meeting



This GRS will be held in conjunction with the "Metals in Biology" Gordon Research Conference (GRC). Those interested in attending both meetings must submit an application for the GRC in addition to an application for the GRS. Refer to the [associated GRC program page](#) for more information.

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	Keynote Session: Metals, Water, Light, O₂, Camera and Action! <i>Joint session with the Metals in Biology Gordon Research Conference.</i> 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	Jan Kern (Lawrence Berkeley National Laboratory, USA) "Taking Snapshots of the Water Oxidation Reaction in Photosystem II Using Crystallography and Spectroscopy at an XFEL"
8:10 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
9:30 pm - 11:00 pm	Poster Session <i>Joint Poster Session with the Metals in Biology GRC</i>

Friday

7:30 am - 8:30 am	Breakfast
8:30 am - 9:00 am	Group Photo
9:00 am - 12:30 pm	Spectroscopic Methods to Study Metal Reactivity and the Flow of Electrons in the Cell Discussion Leader: Kara Bren (University of Rochester, USA)
9:00 am - 9:15 am	Introduction by Discussion Leader
9:15 am - 9:35 am	Levi Ekanger (California Institute of Technology, USA) "Nitric Oxide Modulates DNA Repair Enzyme Conformation and DNA-Bound Redox Activity Through Nitrosylation of a [Fe ₄ S ₄] Cluster"
9:35 am - 9:40 am	Discussion
9:40 am - 10:00 am	Md. Mahbbat Ali (University of Wisconsin-Milwaukee, USA) "A Mechanistic View of Cytochrome c Nitrite Reductase (ccNiR)-Catalyzed Reduction of Nitrite to Nitric Oxide"

10:00 am - 10:10 am	Discussion
10:10 am - 10:30 am	Avery Vilbert (Cornell University, USA) "Influences of the Heme-Lysine Crosslink in Cytochrome P460 over Redox Catalysis and Nitric Oxide Sensitivity"
10:30 am - 10:35 am	Discussion
10:35 am - 11:05 am	Coffee Break
11:05 am - 11:25 am	Brandon Greene (Harvard University, USA) "Shedding Light on Conformational Dynamics in Ribonucleotide Reductase"
11:25 am - 11:35 am	Discussion
11:35 am - 11:55 am	Alex Confer (Johns Hopkins University, USA) "Investigations of Nitroxyl (NO-/HNO) Reactivity at Mononuclear Nonheme Iron"
11:55 am - 12:00 pm	Discussion
12:00 pm - 12:20 pm	Derek Rice (University of Kansas, USA) "Tuning the Proton-Coupled Electron-Transfer Reactivity of Mn(III)-OH Complexes via Ligand Perturbations and Addition of Lewis Acids"
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	Computational Tools for Bioinorganic Chemistry Discussion Leader: Yong Zhang (Stevens Institute of Technology, USA)
7:30 pm - 7:40 pm	Introduction by Discussion Leader

7:40 pm - 7:55 pm	Matthew Conger (University of Vermont, USA) "1H and 13C NMR of Azide-Inhibited IsdG Reveals Spin Density Delocalization"
7:55 pm - 8:00 pm	Discussion
8:00 pm - 8:20 pm	Zachary Reitz (University of California, Santa Barbara, USA) "Genomics-Based Expansion of a Natural Combinatoric Library of Siderophores"
8:20 pm - 8:25 pm	Discussion
8:25 pm - 8:40 pm	Anne Fischer (Marquette University, USA) "Synthesis and Spectroscopic Characterization of Nonheme Iron Dioxygenases and Reactive Intermediates"
8:40 pm - 8:45 pm	Discussion
8:45 pm - 9:05 pm	David Stevens (Yale University, USA) "Exploring the Role of the Third Active Site Metal Ion in DNA Polymerase Eta with Quantum Mechanical/Molecular Mechanical Free Energy Simulations"
9:05 pm - 9:10 pm	Discussion
9:10 pm - 9:25 pm	Laura Cunningham (Boston University, USA) "O ₂ Activation at a Non-Heme Iron Center: A Kinetic and Spectroscopic Investigation of Catalytic C-H Bond Oxidation"
9:25 pm - 9:30 pm	Discussion
Saturday	
7:30 am - 8:30 am	Breakfast
9:00 am - 12:30 pm	Inspired by Nature: Designing Metalloproteins and Inorganic Catalysts Discussion Leader: Robert Scarrow (Haverford College, USA)
9:00 am - 9:10 am	Introduction by Discussion Leader

9:10 am - 9:30 am	Charles Arnett (California Institute of Technology, USA) "Site-Differentiated, High Spin Tetranuclear Iron Clusters that Reversibly Bind CO in Four Redox States"
9:30 am - 9:40 am	Discussion
9:40 am - 10:00 am	Xiongyi Huang (California Institute of Technology, USA) "Cytochrome c-Mediated Chiral Organoborane Synthesis via Iron-Heme-Carbene Insertion into B-H Bonds"
10:00 am - 10:10 am	Discussion
10:10 am - 10:30 am	Joel John Rempillo (Syracuse University, USA) "Design of Mononuclear Non-Heme Enzyme for Oxygen Activation"
10:30 am - 10:35 am	Discussion
10:35 am - 11:05 am	Coffee Break
11:05 am - 11:25 am	Allyssa Massie (University of Kansas, USA) "Influences of Structural Perturbations on Hydrogen Atom Transfer Reactivity by Oxomanganese(IV) Complexes"
11:25 am - 11:35 am	Discussion
11:35 am - 11:55 am	Evan Mirts (University of Illinois at Urbana-Champaign, USA) "Engineering Heteronuclear Metal Centers from Iron-Sulfur and Heme-Copper Sulfite Reductases in Cytochrome c Peroxidase"
11:55 am - 12:05 pm	Discussion
12:05 pm - 12:25 pm	Monica Sanchez (Emory University, USA) "FeFe Hydrogenase Biorod Conjugate by Electrochemistry and Transient Absorption"
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

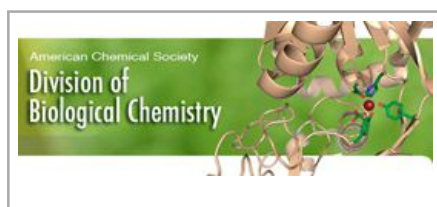
6:00 pm - 7:00 pm	Dinner
7:00 pm - 7:30 pm	Evaluation Period <i>Fill in GRS Evaluation Forms</i>
7:30 pm - 9:30 pm	Metal Homeostasis: Moving Metals into, out of, and Around the Cell Discussion Leader: Emily Que (University of Texas at Austin, USA)
7:30 pm - 7:40 pm	Introduction by Discussion Leader
7:40 pm - 8:00 pm	Amanda Vo (Boston University, USA) "Identifying Protein-Protein Interactions Required for Iron-Sulfur Cluster Protein Recognition"
8:00 pm - 8:05 pm	Discussion
8:05 pm - 8:20 pm	Anastassia Gallo (Temple University, USA) " <i>Rhodococcus ruber</i> GIN-1 Titanium Incorporation via Cell-Oxide Interactions"
8:20 pm - 8:25 pm	Discussion
8:25 pm - 8:45 pm	Julian Rees (Lawrence Berkeley National Laboratory, USA) "Prevention and Treatment of Internal Gadolinium Contamination from MRI Contrast Agents"
8:45 pm - 8:50 pm	Discussion
8:50 pm - 9:05 pm	Ananya Rakshit (Tata Institute of Fundamental Research, India) "Cu(II) Selective Cell-Permeable Chelators Relieve Metal-Overload Induced Oxidative Stress"
9:05 pm - 9:10 pm	Discussion
9:10 pm - 9:25 pm	Gayani Petersingham (Western Sydney University, Australia) "Characterisation of Metal-Ligand Interactions and the Effect of Metal Ions on the Gene Expression of Amyloid Precursor Protein"
9:25 pm - 9:30 pm	Discussion

Sunday

7:30 am - 8:30 am	Breakfast
9:00 am - 12:30 pm	<p>Structure-Function Relationships in Bioinorganic Chemistry</p> <p>Discussion Leader: Christina Zimanyi (New York Structural Biology Center, USA)</p>
9:00 am - 9:10 am	Introduction by Discussion Leader
9:10 am - 9:30 am	<p>Rakshya Gorkhali (Georgia State University, USA)</p> <p>"Role of Metal Ions in Calcium Sensing Receptor (CaSR) Mediated Extracellular Signaling"</p>
9:30 am - 9:40 am	Discussion
9:40 am - 10:00 am	<p>Oriana Fisher (Northwestern University, USA)</p> <p>"A Novel Copper Center in an Uncharacterized Protein from Methanotrophs"</p>
10:00 am - 10:05 am	Discussion
10:05 am - 10:25 am	<p>Angela Picciano (Cornell University, USA)</p> <p>"Characterization of a Complete Nitric Oxide Synthase from <i>Synechococcus</i>"</p>
10:25 am - 10:30 am	Discussion
10:30 am - 11:00 am	Coffee Break
11:00 am - 11:20 am	<p>Elizabeth Wittenborn (Massachusetts Institute of Technology, USA)</p> <p>"Redox-Dependent Metal Migration in the Ni-Fe-S Cluster of Carbon Monoxide Dehydrogenase"</p>
11:20 am - 11:30 am	Discussion
11:30 am - 11:50 am	<p>Russell Lewis (California Institute of Technology, USA)</p> <p>"Crystallographic Studies of a Silicon-Carbon Bond-Forming Enzyme"</p>
11:50 am - 12:00 pm	Discussion

12:00 pm - 12:20 pm	Emily Thompson (University of California, Berkeley, USA) "Linking Specific Macromolecular Motions to Enzyme Rate Acceleration in the TIM Barrel Superfamily of Proteins"
12:20 pm - 12:30 pm	Discussion
12:30 pm - 1:30 pm	Lunch
1:30 pm	Departure

Contributors



This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Science under award number DE-SC0018031. This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the U.S. 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

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