**2021 Invited Postdoctoral Research Presentation Series**

**Seminar Presenters**

* Indicates on the job market this year

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**Dr. Nadia Léonard***

Research Area: Inorganic  
Institution: University of California, Irvine  
Post-doc Advisor: Jenny Yang

**Electrostatic Effects at Transition Metal Complexes: Tools for Controlling Reactivity**

Reactive transition metals play an important role in mediating or catalyzing a variety of chemical transformations. In enzymes, electrostatics play a crucial role to align the dipoles and net charges of reactants, products, and transition states, leading to enhanced reactivity and greater catalytic efficiency. In contrast, at homogeneous catalysts, electrostatic interactions are rarely given deliberate consideration in synthetic design to rationally control reactivity. However, by synthesizing transition metal complexes with tunable electrostatic interactions, these model complexes can be used to control redox properties, proton affinity, and electronic structure at the transition metal. During my postdoc, I have demonstrated that incorporating a cation of charge 1+, 2+, or 3+ near a transition metal center can install a persistent electrostatic field and applied this strategy to controlling hydrogen atom transfer, spin-state configuration, and electron transfer reactions. The implications for these studies establish correlations between electrostatic effects and kinetic/thermodynamic parameters, advancing our understanding of the importance of electrostatics on controlling reactivity. Thus, by demonstrating the effect of electrostatics on transition metal reactivity, we can better understand how enzymes achieve catalytic efficiency.

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**Dr. Yun Ji Park***

Research Area: Bioinorganic  
Institution: Northwestern University  
Post-doc Advisor: Amy Rosenzweig

**Biosynthesis of a Copper-chelating Natural Product by a Non-heme Diiron Enzyme**

Methanobactins (Mbn) are copper-chelating natural products, first discovered in methanotrophs that utilize copper for their primary metabolic enzyme, copper-dependent particulate methane monooxygenase (pMMO). To meet their high necessity for copper, some methanotrophs developed a specialized system where they produce Mbn to acquire copper from the environment under copper limited conditions. Mbn is ribosomally-synthesized and post-translationally modified peptide that is produced from a precursor peptide, MbnA. MbnA comprises a leader peptide that
is cleaved off eventually and a core peptide that is post-translationally modified to form mature Mbn. The post-translational modifications take place at two specific cysteine residues in MbnA core peptide, resulting in the formation of the copper binding ligands, oxazolone and thioamide groups. Two core Mbn biosynthesis proteins, MbnB and MbnC, form a heterodimeric iron-containing enzyme complex, MbnBC, and catalyze the formations of the oxazolone/thioamide groups from the cysteine residues. This chemistry is believed to occur at the iron active site in MbnB in the presence of O2. In this seminar, my current efforts to identify the structures, functions, and mechanisms of MbnBC using spectroscopic, kinetic, and structural analyses will be discussed. This work will provide insights into novel enzymatic chemistries performed by Mbn biosynthesis enzymes.

**Poster Presenters**

* Indicates on the job market this year

**Dr. Mary Andorfer***
Research Area: Chemical Biology
Institution: Massachusetts Institute of Technology
Post-doc Advisor: Catherine Drennan

**Restoring Activity to Oxygen-Damaged Glycyl Radical Enzymes: Spare Parts for Proteins**

Glycyl radical enzymes perform a wide array of challenging transformations within anaerobic bacteria using a simple glycyl radical cofactor, which is sensitive to oxidative cleavage. We study a unique mechanism of repair of oxidatively cleaved GREs in which a small spare part protein is able to bind to damaged GRE, harbor a new glycyl radical cofactor, and restore catalytic activity.

**Dr. Fang Liu***
Research Area: Materials, Electrochemistry
Institution: Stanford University
Post-doc Advisor: Yi Cui

**Dynamic Behaviors of “Dead Li” in Batteries**

This work focuses on the fundamental understanding of the failure mechanisms in lithium metal batteries, which is one of the most promising candidates for next-generation energy storage systems. In contrast to the common view in the research community that “dead Li” is electrochemically inactive, my research shows that it exhibits significant dynamic responses during battery operations. This discovery shifts how we view the degradation mechanisms in batteries and opens tremendous opportunities for the regeneration and potentially recycling of batteries.
Dr. Anastasia Manesis  
Research Area: Bioinorganic  
Institution: Northwestern University  
Post-doc Advisor: Amy Rosenzweig

Unraveling the Metallomystery Pair: The Role of MbnPH in Microbial Cu Transport

Two copper-regulated genes, mbnP and mbnH, are found both within methanobactin operons and elsewhere in bacterial genomes and are hypothesized to play a role in microbial copper homeostasis. Using optical and magnetic spectroscopies coupled with electrochemistry and biochemical assays, we can begin to uncover the function of this metallomystery protein pair.

Dr. Olja Simoska*  
Research Area: Analytical, Physical  
Institution: The University of Utah  
Post-doc Advisor: Shelly Minteer

Understanding the Properties and Mechanism of Phenazine-based Mediated Electron Transfer in *Escherichia coli*

Using electrochemical experimental approaches in combination with computational strategies to understand the properties of phenazine mediators that facilitate extracellular electron transfer in the model microorganism E. coli during glucose metabolism. The findings from this research provide impetus for the future development of mediated microbial-based bioelectrocatalytic systems, such as microbial fuel cells and biosensors.

Dr. Minjung Son  
Research Area: Physical  
Institution: University of Wisconsin-Madison  
Post-doc Advisor: Martin Zanni

Mapping and Controlling the Pathways of Energy Flow in Light-harvesting Systems using 2D White-light Spectroscopy

In natural and artificial light-harvesting systems, sunlight is absorbed and transferred through a network of coupled chromophores whose transitions span a wide energy range. I will describe the elucidation of previously hidden pathways of energy transfer in the photosynthetic protein of green plants using 2D white-light spectroscopy that maps excited-state dynamics across the visible, and how energy flow can be controlled by strong light-matter coupling in a model artificial light-harvesting system containing semiconducting carbon nanotubes.