CHEMISTRY & BIOCHEMISTRY SEMINAR: Electrostatic Effects at Transition Metal Complexes: Tools for Controlling Reactivity

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Date:
11/12/2021

Time:
10:30 AM- 11:50 AM

Location:
COB1 265

About the Speaker:

Nadia Léonard received her PhD in chemistry from Princeton University and was an NSF Graduate Fellow under the guidance of Professor Paul Chirik. Her graduate research focused on developing earth-abundant transition metal catalysts for site-selective hydrofunctionalization of hindered alkenes. Outside of lab work, Nadia is passionate about mentorship and cultivating an inclusive scientific environment. She was a Diversity Fellow with the Graduate School, Office of Diversity and Inclusion during her PhD. Nadia is currently a UC President's Postdoctoral Fellow with Professor Jenny Yang at the University of California, Irvine where she is investigating electric field effects at transition metal complexes.

Abstract:

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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