

Chemistry and Biochemistry Department Seminar

Thursday, October 8, 2020 12:15pm See Chem/Biochem Canvas site for Zoom link

Tuning the Reactivity of First-Row Transition Metals for C–H Bond Functionalization

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Efficient conversion of simple hydrocarbon feedstocks into value-added products remains a major synthetic target. To this end, seeking to emulate the aerobic C–H hydroxylation function of cytochrome P450, metal-ligand multiple bond constructs have been extensively targeted for C–H bond functionalization. The Betley group has reported C–H amination catalysis using highspin iron dipyrrinato complexes, ascribing this reactivity to the unique electronic configuration of an isolated high-spin ferric iminyl. Our studies also highlighted the access to a di-iron bridging imido that can catalytically transfer the *N*-group into allylic and benzylic C–H bonds, emphasizing the importance of establishing a correlation between electronic structure and reactivity. With an interest in further expanding the avenues for C–H bond functionalization, my research group seeks to leverage metal-metal and metal-ligand cooperativity using both synthetic and biological scaffolds to manipulate the electronic structure and reactivity of earthabundant, first-row transition metals. We aim to target bimetallic complexes to (1) explore a polarization-induced mechanism for C–H cleavage and (2) fundamentally understand electronic structure requirements of bioinspired dimeric oxo motifs for C–H hydroxylation.