

## **Department of Chemistry**



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Correlation of Electronic Structure to Reactivity in Organometallic Catalysis and Polynuclear Small Molecule Activation

Research interests encompass the development of polynuclear coordination complexes has given rise to structurally and electronically well-defined species possessing redox-flexibility with the potential to perform multi-electron transformations. The successful construction of these materials has allowed researchers to understand their redox behavior and target small molecule activation pathways reminiscent of naturally occurring enzymatic function.

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## Abstract

Electronic structure considerations dictate the stability and/or reactivity of both mono- and polynuclear complexes. The utilization of weak-field ligands have enabled (1) the development of reactive iron-based reagents to catalyze C-H bond functionalization, and (2) directly control M-M interactions in polynuclear clusters to unveil a host of new physical properties. In the latter context, the close proximity of the metal ions within the polynuclear architectures enforce direct metal-orbital overlap, giving rise to fully delocalized electronic configurations. Within this delocalized framework, ligand alterations allows for tuning of the resultant electronic structure from low-spin to high-spin configurations. Within both bodies of chemistry, obtaining high-spin electronic configurations are necessary to achieve catalysis or small molecule activation.