# Cluster Models of the Nitrogenase Active Site

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Complex inorganic active sites perform challenging catalytic transformations in biological systems, such as water oxidation in Photosystem II and nitrogen reduction in Nitrogenase. The effect of cluster structure on the physical and chemical properties of these active sites is not well understood. We have developed methodologies for the rational synthesis of homo- and hetero-metallic models for these protein active sites which allow for systematic structure-property studies. Di- and tetranuclear complexes that mimic various structural aspects of Nitrogenase active site have been prepared. Site-differentiated tetranuclear complexes have been employed to address the effect of the oxidation state of remote metals on small molecule binding and activation; internal redox reorganization was shown to influence ligand binding. Relatedly, the impact of bridging carbyne ligands on reactivity and physical properties have been investigated. Carbyne bridged diiron complexes show $N_2$ activation chemistry. Cubane clusters with chelating carbyne ligands are significantly more reducing that S and N analogs. Potential implications for function will be discussed.