

## **Synthetic Cluster Models of Protein Active Sites**

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Complex inorganic active sites perform challenging catalytic transformations in biological systems, such as water oxidation by Photosystem II and nitrogen reduction in Nitrogenase. These conversions are of interest in the context of artificial photosynthesis. The effect of cluster structure on the physical and chemical properties of the protein active sites is not well understood. We have developed methodologies for the rational synthesis of tetra- and pentanuclear homo- and hetero-metallic cluster models of protein active sites, which allow for systematic structure-property studies. Distal redox changes have been demonstrated to have a substantial effect on the reactivity and binding of ligands relevant to small molecule conversions. Upon incorporation of second coordination sphere hydrogen bonding interactions, water oxidation catalysis was observed. Spectroscopic studies of models with structures or redox states relevant to the protein active site provide benchmarking for the biological systems. Implications for function will be discussed.

### **Theodor Agapie, Biographical Sketch:**

Originally from Bucharest, Romania, Agapie received his B.S. degree from Massachusetts Institute of Technology in 2001 and his Ph.D. from California Institute of Technology in 2007. He was a Miller Postdoctoral Fellow at University of California, Berkeley. Agapie returned to Caltech in 2009 to start his independent career as Assistant Professor of Chemistry. He has been Professor of Chemistry since 2014. His research focuses on synthetic inorganic and organometallic chemistry on topics related to energy conversion, catalysis, and upgrading readily available chemical precursors. He has ~120 scientific publications and has presented over 100 invited lectures at international and US universities, companies, and conferences. Selected awards include the ACS Award in Pure Chemistry (2013), Presidential Early Career Award for Scientists and Engineers (PECASE, 2014), Dreyfus Teacher-Scholar Award (2014), and Humboldt Foundation's Bessel Research Award (2022).