State University of New York Binghamton University Department of Chemistry

THE NINETEENTH BIANNUAL Eisch Lectureship in Inorganic/Organometallic Chemistry

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Oxo Metal Clusters in Water Splitting and Bond Activations

The conversion of solar energy into a useful chemical fuel represents a major goal in the drive towards a society fully powered by renewable energy. Several potential fuels are of interest, including hydrogen from proton reduction, and various hydrocarbons from carbon dioxide reduction. To achieve meaningful rates of fuel production, the potential reduction reactions must be coupled to an oxidative reaction that generates electrons and protons. The most reasonable candidate to provide these electrons and protons is water, which can be chemically decomposed to 4 protons, 4 electrons, and oxygen (the oxygen evolution reaction, OER). For solar fuel applications, this water-splitting half reaction must be catalyzed to make it energetically efficient, as accomplished in nature's photosynthesis by a tetra-manganese oxo cluster (the oxygen-evolving complex, OEC). Indeed, related transition-metal oxo cubane clusters represent intriguing model systems and catalyst design motifs for development of new water-splitting catalysts based on the most abundant metals. Molecularly derived catalysts of this type offer a number of potential advantages, including the synthetic tunability of structure-activity relationships and chemical properties. Also, the study of model, high-valent molecular species can provide key insights into the mechanism of water oxidation, and thereby help bridge the gap between solid-state and molecular systems to allow for more rational design of catalysts. This presentation will describe highvalent tetracobalt oxo cubane clusters, and the experimental determination of a well-defined mechanism for cubane-catalyzed oxygen evolution via water oxidation. The systematic variation of electronic properties for these clusters, and strategies for their stabilization, will be described. The synthesis and study of clusters doped by another transition metal, and linked bis-cubane complexes, are further topics to be discussed.

> Friday, April 25, 2025 4:00pm - 5:30pm Fountain Room Smart Energy Building All Are Welcome