Charge Compensation and Transfer in Molecular Metal Oxides Special Seminar Date: January 10, 2023 Time: 3:00 pm Remsen Hall 233 Host: Dr. Rebekka Klausen



ABSTRACT: Atomistic understanding of charge transfer processes at redox active transition metal oxide surfaces are central to the development of large-scale energy storage and conversion technologies. Here, we describe our efforts in bridge the conceptual disconnect between molecular and solid-state cation-coupled electron transfer processes through investigation of charge transfer in a family of polyoxovanadate-alkoxide clusters. This talk will highlight recent results from our group, interrogating the interactions of alkali ions and protons with the surface of redox active vanadium oxide assemblies. These studies provide insight into how the manipulation of the surface structure of a cluster can influence mechanism of charge transfer relevant to energy storage and small molecule activation.

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Research Overview: The worldwide push to generate electricity from renewable sources has created a critical need to develop improved energy storage and fuel-production strategies. Recent advances in the conversion of solar and wind energy into electrical energy have been increasingly economical, yet without effective methods for storage, it is impossible to integrate these intermittent resources into the commercial sector without compromising reliability. Research in the Matson Group focuses on using a synthetic inorganic chemistry perspective to address current global issues related to Energy Storage and Production.

An attractive solution to the broad challenge of energy storage is to store chemical energy in molecular bonds by converting inert, abundant molecules into energy-rich chemical fuels. As such, the development of new, carbon neutral fuels is a viable approach for sustainable electricity generation. The development of alternative fuels from secure and sustainable resources would decrease our dependence on fossil fuels, and as a result is among the greatest environmental and economic challenge that society faces today. The development of sustainable methods to convert energy-poor substrates to fuels requires the generation of catalysts that can perform a complex series of multi-electron and multi-proton transformations. The Matson Group is investigating new approaches to catalyst design that applies fundamental knowledge from bioinorganic systems and heterogeneous catalyst-support interactions. We have recently discovered a new class of metal-oxide metalloligands capable of participating in cooperative small molecule activation. The main objectives of this research include (i) determining how the electronic properties and activity of a homogeneous, heterometallic catalyst can be influenced by a reducible metal-oxide support and (ii) revealing the role of metal/metalloligand interactions in the cooperative intramolecular electron and proton transport that enables substrate activation. Insights from these investigations will translate broadly into improved designs for homogeneous catalysts targeting the sustainable production of chemical fuels.