DREXEL UNIVERSITY
Materials Science and Engineering
College of Engineering

# Spring Seminar Series

# Turning a cheap, poor catalyst into a cheap, excellent catalyst. Optimizing layered MnO-based materials for water oxidation using experiment and theory.

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**Abstract:** Efficient catalytic water oxidation is an important reaction for the development of solar hydrogen as a source of green energy. Extraction of high energy electrons from water for the preparation of fuel leaves O2 as a byproduct. Nature boasts the only truly effective catalyst for this reaction, the oxygen evolving complex (OEC), a tetramanganese-calcium-oxo cluster. The exploration of solid-state manganese oxides inspired by (or possibly a primordial precursor to) this inorganic cluster is of interest for the chemical and electrochemical oxidation of water, and while promising catalysts have been discovered, an understanding of their active site structures and mechanisms has been elusive, precluding incremental improvements in design. This lecture is focused on the birnessite phase of MnO2, typically viewed as a poor water oxidation catalyst. The Center for the Computational Design of Functional Layered Materials at Temple University is undertaking a combined experimental and theoretical approach where Density Functional Theoretical (DFT), and Molecular Dynamics (MD) computations inform and guide experimental approaches as to understand the functioning of, and thereby identify ways to improve the catalytic activity of these materials. Modification of birnessite by enrichment with Mn(III) defect sites, intercalated interlayer Co or Ni ions, and alloying of the layers with Co(III) have turned this relatively poor catalyst into one competitive with excellent IrO-, cobalt-oxide-, and double-layer-hydroxide-based catalysts. The discoveries have been guided by MD simulations which show enhanced geometric frustration of water enhances electron transfer rates, and DFT calculations which describe geometric features that optimize band structure for beneficial electronic conductivity and charge separation.


**Bio:** Prof. Michael Zdilla is an inorganic chemist at the Department of Chemistry at Temple University in Philadelphia PA. A native of Lancaster County, PA, Prof. Zdilla attended Millersville University for his Bachelors in Science in biochemistry, and studied synthesis of biologically inspired molybdenum complexes for his thesis research under the direction of R. Edward Rajaseelan. In addition to academic pursuits, while at MU, Zdilla participated in the marching band, concert band, and Jazz Band. Zdilla attended graduate school and obtained his Ph.D in inorganic chemistry at Princeton University under the supervision of Sonny C. Lee, performing inorganic synthesis of iron-nitrogen cluster mimics of the nitrogenase iron-molybdenum cofactor. As a postdoctoral fellow, he studied catalysis and mechanistic bioinorganic chemistry on the chlorite dismutase enzyme and on synthetic models of metalloporphyrin redox enzymes and under the supervision of Mahdi M. Abu-Omar. Since starting his independent career at Temple in 2009 he has published 55 papers on the topics of synthetic and mechanistic inorganic chemistry, catalysis, materials science, nanoscience, energy science, and crystallography. He has been the recipient of the NSF Career Award, the Office of Naval Research Young Investigator Award, the Camille Dreyfus Teacher Scholar award, and was named the inaugural Robert L. Smith Early Career Chair in Chemistry at Temple University.