COLLEGE OF ENGINEERING

Research Seminar Series

University of Nebraska-Lincoln
Department of Chemical and Biomolecular Engineering

Development of Electrocatalytic Materials Guided by Computational Chemistry: Fuel Cells and Electrolysis

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Host: Dr. Vitaly Alexandrov

Friday, November 9, 2018

Time: 10:00 a.m. - 11:00 a.m.
Othmer Hall, Room 205
**Refreshments provided*

Abstract

Our group applies computational chemistry techniques to a range of catalyst and materials design challenges in energy technology. This presentation will concentrate on our work in electrocatalysis. Electrocatalysts are an essential component of fuel cells, electrolyzers, and some battery technologies. The development of composition-structure-functional relationships guides rational design of electrocatalytic materials. Quantum mechanics based computational techniques, such as density functional theory methods, are a useful tool in guiding catalyst design. Density functional theory (DFT) methods are widely used to evaluate surface catalytic reaction mechanisms and to predict the relative performance of various catalyst formulations or structures. Translation of DFT approaches to the electrocatalytic environment requires additional methodological choices due to additional complexities offered by the electrified catalyst-electrolyte interface. This talk will provide an overview of the challenges to atomistic modeling of electrochemical interfaces and describe the various DFT approaches used to model electrocatalytic systems. The use of DFT to determine electrocatalytic reaction mechanisms and guide the design of catalytic materials will be discussed using examples from our group's research; hydrogen fuel cells, borohydride fuel cells, carbon dioxide and nitrogen reduction to fuels and chemicals.

Biography

Dr. Janik is a Professor of Chemical Engineering at Pennsylvania State University. He began his appointment at Penn State in August, 2006. His research interests are in the use of computational methods to understand and design materials for alternative energy conversion systems. Current activities address a wide-range of energy technologies including fuel cells and electrolysis, heterogeneous catalysis, organic electronics, and CO_2 capture and utilization. Research methods emphasize atomistic simulation using quantum chemical methods and kinetic modeling. Janik is affiliated with the Penn State Energy Institute, PSU-Dalian University of Technology Joint Center for Energy Research, the PSU Institutes of Energy and the Environment, and the Battery and Energy Storage Technology Center. He also holds the title of Visiting Professor at Dalian University of Technology. The Janik group currently includes 8 graduate students, 8 undergraduate students, and a post-doctoral research associate. Dr. Janik is all the Undergraduate Program Coordinator for the Chemical Engineering Department at Penn State. Dr. Janik received his B. S. in Chemical Engineering from Yale University. He completed his doctoral studies at the University of Virginia under the advisement of Bob Davis and Matt Neurock. He has co-authored approximately 130 peer reviewed papers, and co-edited the book "Computational Catalysis" (with Aravind Asthagiri), published by the Royal Society of Chemistry in 2013.