



SCHOOL OF
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College of Engineering, Architecture and Technology

CHE SEMINAR SERIES

Intermetallics for catalytic active site design

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Catalysis research seeks to connect the composition and structure of active sites to the catalytic activity and selectivity to desired products. Intermetallics – multi-metal systems with a well-defined arrangement of the metal atom – offer a platform to control active site structure and composition. In this talk, I will detail our combined use of density functional theory (DFT) and microkinetic modeling (MKM), high throughput and machine learning approaches, together with experiment to design active sites for selective hydrogenation reactions. The combination of DFT, MKM, and experimental studies will be used to show control of active site geometric structure, electronic structure, and exposed surface configurations towards optimizing activity and selectivity. Detailed kinetic analysis of binary and ternary intermetallics will be discussed, as well as the development of a high throughput, machine learning enabled computational workflow to predictively design sites selective for a range of hydrogenation reactions.

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Dr. Michael Janik is a Professor of Chemical Engineering and Associate Director of the Institute of Energy and the Environment at Pennsylvania State University. 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, intermetallic and single-atom catalysis, and organic electronics. Research methods emphasize atomistic simulation using quantum chemical methods and kinetic modeling. Dr. Janik also holds the title of Visiting Professor at Dalian University of Technology. 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. Dr. Janik leads a highly collaborative research program of 15 graduate students, has co-authored over 220 peer reviewed papers, and co-edited the book "Computational Catalysis" (with Aravind Asthagiri).

