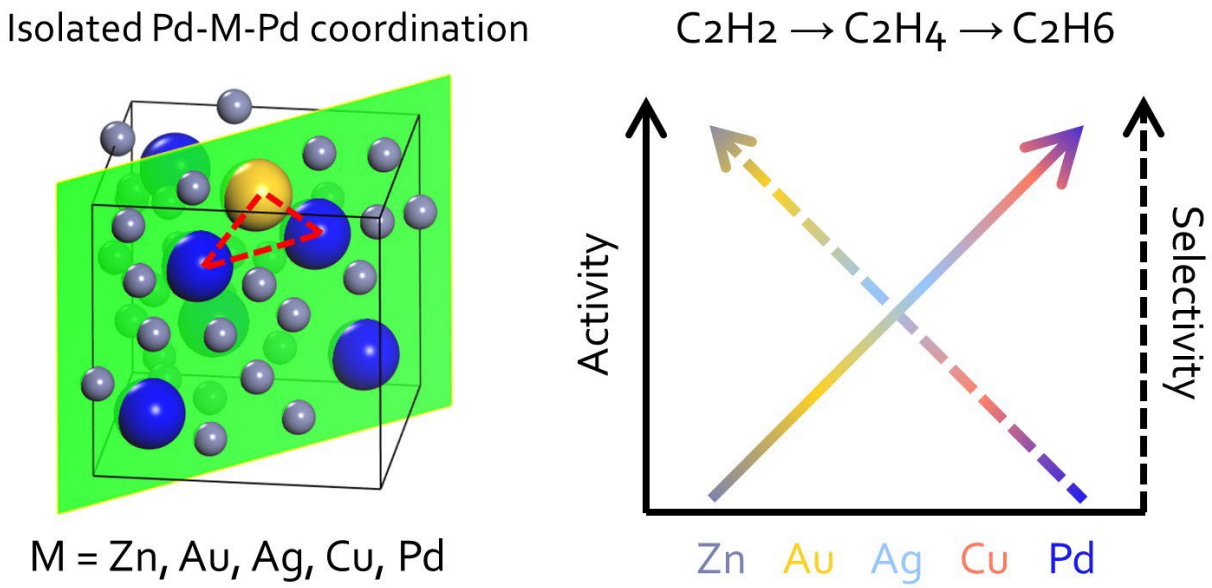
Intermetallic catalysts enable determination of active site requirements

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 machine learning approaches, computational chemistry, and experimental synthesis, characterization, and catalytic testing to define active site requirements for selective hydrogenation catalysis. The combination of density functional theory methods, microkinetic modeling, and experimental studies will be used to demonstrate catalytic differences between isolated Pd monomer, Pd_3 trimer, and Pd-M-Pd (M=Cu, Ag, Au) sites exposed in gamma-brass intermetallic systems. Following detailed analysis of this system, the development of a computational workflow to predictively design sites selective for a range of hydrogenation reactions will be discussed.



Bio

Dr. Michael Janik is a Professor and Associate Head of Chemical Engineering 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 concentrate on electrocatalysis within fuel cells and electrolysis, intermetallic and single-atom catalysis, and organic electronics. Research methods emphasize atomistic simulation using quantum chemical methods and kinetic modeling. The Janik group currently includes 12 graduate students and 5 undergraduate students. 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. He has co-authored approximately 180 peer reviewed papers, and co-edited the book "Computational Catalysis" (with Aravind Asthagiri), published by the Royal Society of Chemistry in 2013.