Professor Janik's group utilizes atomistic modeling techniques, mainly first principles based electronic structure methods, to probe the relationship between the structure/composition of catalytic materials and their activity and selectivity. Specific emphasis is placed on catalytic processes of relevance to alternative energy conversion technologies, and current research concentrates on electro-catalytic systems such as fuel cell electrodes.

Electronic structure methods allow us to probe the fundamental relationship between the composition and structure of a catalytic site and its activity and selectivity for a given reaction. Using the first-principles based algorithms, we construct a reaction energy diagram over the catalyst surface, and then apply transition state theory and statistical mechanics to translate reaction energetics into elementary rate constants and equilibrium constants. Kinetic models then allow us to predict observable values such as the apparent reaction barrier, the overall rate of reaction, or, for an electro-catalytic system, the current produced. These macroscopic properties are predicted directly from first-principles. Therefore, once our approximations and assumptions are validated against comparable experimental data, we can extend our work to the predictive design of improved catalytic materials.

Current research topics include:
Solid Oxide Fuel Cells
Borohydride Based Fuel Cell Systems
Effects of electrode/electrolyte interfacial structure on oxygen reduction kinetics

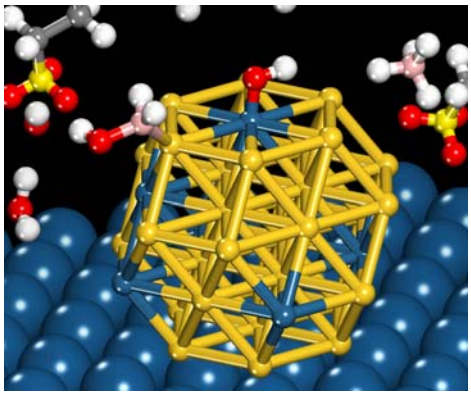
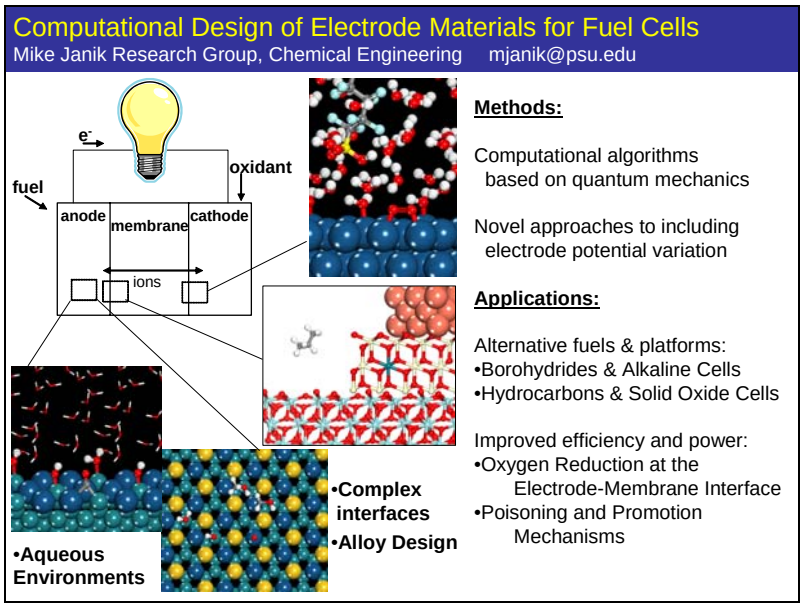


Figure Caption: An atomistic model of a supported bimetallic particle in an electrochemical system.



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8. **M. J. Janik**, R. J. Davis, M. Neurock. "A Quantum Chemical Study of Tertiary Carbenium-Ions in Acid Catalyzed Hydrocarbon Conversions Over Phosphotungstic Acid" *Catalysis Today* 116 (2006) 90-98.

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3. K. A. Campbell, **M. J. Janik**, M. Neurock, R. J. Davis. "Ab Initio and Microcalorimetric Investigations of Alkene Adsorption on Phosphotungstic Acid" *Langmuir* 21 (2004) 4738-4745.

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