Title: Nanoarchitecture and Catalyst Designs for Fuel Cell and Water Splitting Applications

Abstract

A variety of novel composite materials have been used/tested for next-generation energy conversion devices. However, in many cases little is known about their properties and performance, although such fundamental understanding is essential for further advances in energy conversion technologies. Experiments may yield many clues to the behavior of those materials, but the interpretations are often controversial due largely to the difficulty of direct characterization. Under such circumstances, first principles-based computational approaches have emerged as one of the most powerful tools for design and development of new energy materials. This talk will focus on introducing our ongoing efforts in first principles modeling of energy conversion materials. In the first part of my talk, I will discuss the properties and performance of Pt-based nanomaterials and composites PEMFCs, particularly the dissolution mechanisms of Pt-based nanomaterials near the surface and interface, with comparisons to those in bulk Pt, as well as the surface and interface effects on the anode and cathode performance, such as oxidation/reduction reaction rate and stability. In the second part, I will present recent progress in our collaborative theoretical and experimental efforts to explore electrolysis catalysts with the stability, costs, and abundance for electro-powered hydrogen/oxygen production.