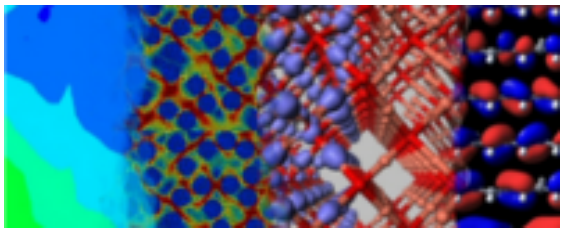

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Modeling of Electrochemical Interfaces in Polymer Electrolyte Fuel Cells

Friday, November 9, 2012 9:00 AM (45 minutes)

The deployment of cost-competitive, highly efficient, and environmentally benign energy conversion and storage technologies is a major global challenge. In spite of excellent technological prospects, commercialization of advanced electrochemical energy systems, such as Polymer Electrolyte Fuel Cells (PEFCs) and metal-air batteries in transportation, electronics, and stationary power generation is far from being guaranteed.

For the commercialization of PEFC technology, the concomitant reduction in Pt loading would be the decisive breakthrough, meeting rigorous targets of the DOE (reduce Pt loading by factor > 10, improve stability by factor > 2.5 by 2010). Critical progress hinges on new concepts in the design of advanced materials as well as fundamental understanding of basic (electro) chemical processes. In particular, material morphologies and processes at the nanoscale are decisive for maximizing the ratio of power density to Pt loading. As pointed out by fuel cell industry leaders, automakers, and experts; fundamental understanding of electrode-electrolyte interfaces is key and of vital importance for lowering the cost and improving fuel cell performance and durability. Current trends in fuel cell research activities indicates that phenomenological concepts are slowly transformed into a discipline that will be able to address many challenges, opportunities and research needs in the areas of basic science of fuel cell materials.

This presentation focuses on multi-scale modeling and molecular-level understanding of interfacial structure and interfacial processes at catalyst-support, catalyst-electrolyte, and support-electrolyte interfaces in catalyst layers (CL) of Polymer Electrolyte Fuel Cells (PEFC). Recent results in experiment and modeling indicate that catalyst activity and utilization could be improved by substantial factors. The fundamental understanding of relevant catalyst systems is, however, inept for guiding the design of electrodes with optimized structures, processes and overall performance. This challenge will be addressed. Initially, we focus on modeling of morphology, electronic structure, and electrochemical processes at various interfaces in supported catalyst nanoclusters. Physical properties will be studied by applying multi-scale molecular simulations. Thereafter, we will utilize this insight in view of developing physical models for microstructure and electrokinetic performance in catalyst layers of PEFC. Anticipated structure vs. property relations will provide enhanced capabilities for the rational design of advanced catalytic nanoarchitectures for PEFC.

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