College of Engineering
Department of
Mechanical & Industrial Engineering

The Sidney E. Fuchs Seminar Series

3:30-4:20pm, Friday, March 7, 2014
Frank H. Walk Design Presentation Room

Molecular Modeling of Interfacial Systems: Environmental and NanoMaterials Applications

by Francisco Hung*

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In this talk I will give an overview of recent research efforts in my group, where molecular modeling was used to investigate different interfacial systems relevant to environmental and materials applications.
In the first part of my talk, we investigated the adsorption of several organic molecules on atmospherically-relevant interfaces (e.g., the surface of water droplets from rain or fog, or those generated from breaking waves at the sea surface). These organic molecules can come from different sources (plants, car emissions, the 2010 Deepwater Horizon oil spill), and can adsorb into water droplets and react with atmospheric oxidants, producing compounds that can contribute to the formation of secondary organic aerosols. These aerosols are a portion of particulate matter that is poorly understood at present, and can have negative effects on the climate and human health. Using classical molecular dynamics (MD) simulations and potential of mean force (PMF) calculations, we investigated the properties of several organic molecules at these atmospheric interfaces.
In the second part of my talk, we report classical MD simulations of typical ionic liquids (ILs) confined inside different nanoporous materials. ILs are organic salts that are in liquid state at room temperature, and can be used as electrolytes for energy storage in the nanoporous electrodes of electrochemical double-layer capacitors. Furthermore, inserting ILs inside nanoporous materials is one step in the synthesis of optically-active (fluorescent) and magnetic nanomaterials based on ILs. A fundamental understanding of the behavior of ILs inside nm-sized pores is therefore crucial for the rational design of materials for the applications mentioned before. The structure and dynamics of ILs inside different nanoporous materials are investigated using classical MD simulations, and the effects of variables such as pore size, pore geometry and electrical charges are analyzed and discussed.

* Francisco R. Hung is currently the Paul M. Horton Associate Professor in the Cain Department of Chemical Engineering, and an Adjunct in the Center for Computation and Technology at Louisiana State University. He has an undergraduate degree in Chemical Engineering from Universidad Simón Bolívar in Caracas, Venezuela, and a PhD in Chemical Engineering from North Carolina State University. After working two years as a postdoctoral researcher in the Department of Chemical and Biological Engineering at the University of Wisconsin-Madison, he joined the faculty at LSU in Fall 2007. Honors include a CAREER Award from the National Science Foundation in 2013, and the Ralph E. Powe Junior Faculty Enhancement Award from Oak Ridge Associated Universities in 2008. His research program is focused on investigating different interfacial systems using molecular simulation and computational modeling. Current research areas of interest in his group include ionic liquids and nanoporous materials, organic contaminants at atmospheric water and ice interfaces, and oil dispersion using surface-active proteins. His research is relevant to applications in energy storage, nanomaterials and nanotechnology, and environmental studies.