Other

Molecular Modeling of Interfacial Systems: Environmental and Nanomaterials Applications

Francisco Hung, LSU

Material World Adjunct Professor Presentation

Johnston Hall 338
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Abstract:

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 investigate the adsorption of several organic molecules on atmospheric air/water and air/ice interfaces (e.g., water droplets, rain, fog, ice, snow). These organic molecules can come from different sources (plants, car emissions, the 2010 Deepwater Horizon oil spill), and can adsorb into water drops 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 investigate the properties of these hydrocarbons 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 carbon 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 carbon 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 crucial for the rational design of materials for the applications mentioned before. The structure and dynamics of ILs inside nanoporous carbons are investigated using classical MD simulations, and the effects of variables such as pore size, pore geometry and electrical charges are analyzed and discussed.

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Speaker's Bio:

Francisco Hung is currently an Assistant Professor in the Cain Department of Chemical Engineering 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, where he worked under the direction of Professor Keith Gubbins. After working two years as a postdoctoral researcher in the group of Professor Juan de Pablo in the Department of Chemical and Biological Engineering at the University of Wisconsin-Madison, he joined the faculty at LSU in Fall 2007. 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: (1) ionic liquids confined in nanoporous materials (energy storage, nanomaterials); and (2) adsorption of organic contaminants and oxygen species on atmospheric air/water and air/ice interfaces (environmental chemistry).

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