IOWA STATE UNIVERSITY
Department of Mechanical Engineering

Integrated Experimental and Computational Studies of Energy-Relevant Interfaces

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Seminar on August 25, 2015 at 11:00 am in 2004 Black
Seminar host: Ganesh Balasubramanian

Abstract

Interfaces are ubiquitous in energy-relevant systems. Examples include the subterranean mineral-fluid interfaces that govern carbon sequestration, the electrode-fluid interfaces in batteries and supercapacitors, and the fluid-solid interfaces at which heterogeneous catalysis takes place. For many years, we have studied mineral-fluid interfaces with a combination of molecular (e.g., X-ray reflectivity, quasi-elastic neutron scattering and neutron spin echo) and bulk (e.g., titration) experimental probes closely integrated with molecular dynamics simulations using fluid-solid forcefields derived from ab initio calculations. Recently, as part of the activities of the Fluid Interface Reactions Structure and Transport (FIRST) Engineering Frontier Research Center (EFRC), we have extended this approach to the study of interfaces encountered in batteries, supercapacitors, and heterogeneous catalysis. The FIRST Center performs fundamental research on fluid-solid interfaces based on the premise that the next generation of electrical storage devices with superior performance will require a fundamental knowledge of the nanoscale architecture of the interface, the effect of nanotexture on interfacial properties, and the structural and dynamic changes that occur during charge and discharge cycles. In this presentation, we will provide an overview of our research on the molecular-level modeling and experimental characterization of interfaces relevant to supercapacitors composed of nanostructured carbon electrodes and ionic liquid electrolytes. Our work in this area was the subject of a recently published invited review.

Peter T. Cummings is the John R. Hall professor of chemical engineering at Vanderbilt University. He also holds the position of Associate Dean for Research in the Vanderbilt University School of Engineering. For 20 years (1994-2013), he was associated with Oak Ridge National Laboratory (ORNL) at levels of effort ranging from 40 to 50%. Most recently (2007-2013), he served as the chief scientist (with title Principal Scientist) in the ORNL's Center for Nanophase Materials Sciences (CNMS); previous to this, he was the founding director of the Nanomaterials Theory Institute, the theory program within the CNMS, and one of the four principal investigators who wrote the proposal to establish the CNMS. His research interests include statistical mechanics, molecular simulation, computational materials science, computational and theoretical nanoscience, and computational biology. He is the author of over 380 refereed journal publications and the recipient of many awards, including the 1998 Alpha Chi Sigma award given annually to the member of the American Institute of Chemical Engineers (AIChE) with the most outstanding research contributions over the pr evious decade, the 2007 AIChE Nanoscale Science and Engineering Forum Award, the 2010 AIChE Founders Award for Outstanding Contributions to the Field of Chemical Engineering in recognition of his "outstanding contributions through research, service to the Institute, and national leadership on behalf of the profession," the 2012 Yeram S. Touloukian Award from the American Society of Mechanical Engineers and the 2013 John Prausnitz award, the most prestigious research award – presented every three years – in chemical engineering thermodynamics. He has been elected fellow of the American Physical Society, of the American Association for the Advancement of Science (AAAS), and of the American Institute of Chemical Engineers.

This seminar counts towards the ME 600 seminar requirement for Mechanical Engineering graduate students. www.me.iastate.edu