2018-19

Joseph O. Hirschfelder Lectures in Theoretical Chemistry

Professor Peter Rossky

Rice University

"Exploring Hydrophobicity at the Nanoscale"

Monday, October 8 3:30 p.m. Room 1315 Chemistry

It is widely appreciated that water is an essential player in the organizational forces associated with biological self-assembly, and efforts to harness corresponding interactions for assembly of synthetic advanced materials are widespread. The development of a detailed understanding of the organization of fluid water at the interface with real materials and its consequences is therefore of great interest.

In this presentation, results obtained from fully atomistic computer simulations of water in the presence of confining interfaces will be discussed, with the goal of elucidating the molecular level influence of interface chemistry on water structure and energetics and, further, extending this knowledge outside the conventional realm of the ambient solvent thermodynamic state. The interface examples to be considered emphasize systematic studies designed to elucidate guiding principles, beginning more than thirty years ago. These include simple small molecule solutes, evolving to extended and nanoscale idealized hydrophobic and hydrophilic crystalline surfaces, to interfaces with systematically patterned hydrophobicity, and finally to surfaces involved in protein subunit assembly.

"Translating the Message in Spectroscopic Probes of Conjugated Molecular Materials"

Tuesday, October 9 11:00 a.m. Room 1315 Chemistry

Refreshments prior to seminar at 10:45 a.m. in the Shain Atrium

Over recent decades, there have been a steadily increasing number of studies on electronically conjugated materials for use in solar photovoltaic cells, organic transistors, and fluorescent probes. Progress in using semiconducting polymers has been limited by a fundamental lack of knowledge about the nanoscale organizational structure underlying variations in electro-optical behavior in these highly amorphous materials. Hence, in contrast to familiar silicon-based technology, there is a dearth of principles to drive the bottom-up design of molecular material building blocks. In the case of fluorescent probes of biological systems, molecular engineering is well ahead of the science.

Experimental scientists probe such materials by their response to light, i.e., spectroscopically. The challenge is to interpret the observations in physical and structural terms. Computational modeling based on the physics of atomistic details and explicit electronic structure is ideally suited to enabling this connection of spectra to structure, since the connection in modeling is unambiguous while the experiment provides a strong constraint on the validity of the model. In this presentation, I will discuss examples of conjugated molecular material systems studied by theoretical, modeling, and experimental approaches that elucidate both atomistic and electronic structure and dynamics in a way inaccessible to either theory or experiment alone. Examples from the area of conjugated polymers and also from biosensors based on GFP will be presented.