

MAR11-2010-002474

Abstract for an Invited Paper
for the MAR11 Meeting of
the American Physical Society

Exploring hydration at the nanoscale¹

PETER ROSSKY, University of Texas at Austin

It is widely appreciated that water molecules contribute a critical element to the forces governing chemical processes in an aqueous environment, and the purported differences in water structure induced by the presence of confining surfaces are correspondingly likely to play a role in interfacial chemistry. The development of a detailed understanding of the organization of fluid water at the interface with real materials 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 surface character on water structure and energetics. Further, we emphasize the extension of studies to temperatures and pressures well outside the conventional realm of the ambient solvent thermodynamic state. The interface examples to be considered in this presentation emphasize systematic studies designed to elucidate guiding principles. These include extended and nanoscale hydrophobic and hydrophilic crystalline surfaces and interfaces with systematically patterned hydrophobicity.

¹This work is the result of support for Collaborative Research by the US National Science Foundation.