

Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Density and Structure of Water under Confinement as Determined using Monte Carlo Simulations SUMIT SHARMA, SANAT K. KUMAR, Columbia University — The structure and local density of water is thought to play an important role in phenomena such as protein adsorption. These properties of water under confinement between surfaces can be significantly different from those of bulk water. A change in the water's structure, which is coupled to a change in the local density of the confined water in equilibrium with the bulk water, can create an attractive or repulsive force between the planar surfaces. This force itself can dominate the mechanism of adsorption when adsorbing molecules are within close proximity from adsorbent. In order to probe the effects of confinement further, Grand Canonical ensemble Monte Carlo (GCMC) simulations of Single Point Charge Enhanced (SPC/E) water confined between two planar surfaces of differing hydrophobicity, ranging from hydrophobic to hydrophilic, have been performed. The dependence of the water's structure and local density on the hydrophobicity and distance between the two planar surfaces has been determined. Further, the effect of surface curvature will also be examined.

Sumit Sharma
Columbia University

Date submitted: 05 Dec 2006

Electronic form version 1.4