Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

A Molecular Dynamics Study of Water Confined Between Hydrophobic Plates JOSH LAYFIELD, DIEGO TROYA, Virginia Tech — The interactions between water and hydrophobic surfaces are ubiquitous in nature and have warranted a wealth of research effort studying their properties. We present a molecular dynamics (MD) simulation of the behavior of water molecules when confined between two hydrophobic self-assembled monolayers of varying size. We have performed MD simulations with simulation times >10ns in an effort to understand the nature of water in hydrophobic environments. Analysis of the water between the hydrophobic plates elucidates the role that hydrogen bonding, water structuring, and orientation play in hydrophobic interactions. We compare the simple point charge-extended (SPC/E) and TIP5P molecular-mechanics force fields and their ability to model the water in a hydrophobic environment. We also present the preliminary results from an investigation into the role that dissolved gases have in the ordering of water between hydrophobic plates.

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Date submitted: 20 Nov 2009 Electronic form version 1.4