Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

First-principles simulation of water on graphene using different levels of theory[1] P. GANESH, P.R.C. KENT, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, TN, DE-EN JIANG, Chemical Sciences Division, Oak Ridge National Laboratory, TN — We show results from molecular-dynamics simulations of water confined between flat graphene sheets using different levels of theory. DFT simulations using PBE exchange-correlation show strong layering near the graphene sheet, with the hydrogens closer to the graphene surface. Correlations die off to bulk values after $\sim$10Å from the surface. Inclusion of an empirical Grimme-type van der Waals potential has a small effect on the interfacial C-H distance but a seemingly large effect from the second coordination shell onwards from the surface. Existing reactive force-fields for water, e.g. ReaxFF, do not capture the structure of water on graphene accurately and require refitting to more closely reproduce the DFT results. Molecular dynamics results with available self-consistent vDW-DFx kernels and contrasts with existing classical water models will also be presented.

[1]Work supported by the FIRST Cneter, an EFRC funded by U.S. DOE under award ERKCC61.

P. Ganesh
Center for Nanophase Materials Sciences,
Oak Ridge National Laboratory, TN

Date submitted: 23 Nov 2010 Electronic form version 1.4