Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

First-Principles Investigation of Water Properties at Functionalized Silicon surface[1] DONGHWA LEE, ERIC SCHWEGLER, Lawrence Livermore National Laboratory, YOSUKE KANAI, The University of North Carolina, Chapel Hill — Numerous experimental and theoretical investigations have been made to understand the behavior of water molecules under various conditions. Interfacial water behavior at semiconductor interfaces is one of the most important areas of investigation for diverse industrial applications such as crystal growth, lubrication, catalysis, electrochemistry and sensors. Although the terms, hydrophobic and/or hydrophilic, are often used to describe the properties of water in this context at macroscopic level, the effect of hydrophobicity on water behavior at nano-scale interfaces is still not well understood. Computational simulations could offer atomistic basis to build a better foundation for understanding this important dynamics. In this study, first principles molecular dynamics is employed to investigate the water behavior at silicon surfaces that are functionalized with several different molecules. In particular, various analysis methods are used to elucidate the effect of surface polarity on structural and dynamical properties of interfacial water. Our studies show that properties of interfacial water are not always governed by surface polarity alone but also by other atomistic factors.

[1]This work is Prepared by LLNL under Contract DE-AC52-07NA27344.

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Date submitted: 20 Nov 2012 Electronic form version 1.4