Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Alumina(0001)/water interface structure and infrared spectra from first-principles molecular dynamics simulations[1] ERIC SCHWEGLER, Lawrence Livermore National Laboratory, TUAN ANH PHAM, Lawrence Livermore National Laboratory and Department of Chemistry UC Davis, PATRICK HUANG, Lawrence Livermore National Laboratory, GIULIA GALLI, Department of Chemistry and Department of Physics UC Davis — Knowledge of the interaction of water with solid oxide surfaces is of fundamental importance for the stability of solid oxides in aqueous environments. We studied the atomic structure and infrared (IR) spectra of the alumina(0001)/water interface, using molecular dynamics simulations and the Qbox code. We found that the structural properties of the interface, as described within the generalized gradient approximation, are in good agreement with synchrotron X-ray scattering experiments. In addition, a detailed analysis of the computed IR spectra of interfacial water reveals two types of water molecules at the solid-liquid interface: one type participating in strong "ice-like" hydrogen bonding with the oxide surface, and one type of water molecules involved in weak "liquid-like" hydrogen bonding at the interface. Our results provide a molecular interpretation of the "ice-like" and "liquid-like" peaks observed in sum-frequency vibrational spectroscopy experiments.

[1]Work at LLNL was performed under Contract DE-AC52-07NA27344. DOE-CMSN Grant DE- SC0005180 is gratefully acknowledged.

Tuan Anh Pham
Lawrence Livermore National Laboratory and
Department of Chemistry UC Davis

Date submitted: 09 Nov 2012 Electronic form version 1.4