Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Ab initio Simulations of Fluid and Superionic Water in the Interiors of Uranus and Neptune BURKHARD MILITZER, SHUAI ZHANG, University of California, Berkeley — Water is one of the most prevalent substances in our solar system. Large quantities are assumed to be stored in the interiors of ice giant planets. Water has an unusually rich phase diagram with 15 solid phases that were determined experimentally and 6 additional ones that were predicted theoretically at high pressure. Water is predicted to assume a superionic state where the oxygen ions remain confined to specific lattice sites while the hydrogen ions move through the crystal structure like a fluid. In our recent article [Physical Review Letters 110 (2013) 151102], we predicted the oxygen sub-lattice to assume a face-centered cubic structure at pressures above 1 Mbar. For this presentation, we extended our density functional molecular dynamics simulations in order to determine the equation of state of fluid and superionic water. We employed a thermodynamics integration technique to derive the entropy and the Gibbs free energy of both phases. We discuss how a novel superionic state could be identified in high pressure experiments and talk about the implications for the interiors of Uranus and Neptune.

Burkhard Militzer
University of California, Berkeley

Date submitted: 15 Nov 2013 Electronic form version 1.4