Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Accurate calculation of the x-ray absorption spectrum of water via the GW/Bethe-Salpeter equation[1] KEITH GILMORE, Soochow University, JOHN VINSON, National Institute of Standards and Technology, JOSH KAS, FERNANDO VILA, JOHN REHR, University of Washington — We calculate x-ray absorption spectra (XAS) of water within the OCEAN code, which combines plane-wave, pseudopotential electronic structure, PAW transition elements, GW self-energy corrections, and the NIST BSE solver [1]. Due to the computational demands of this approach, our initial XAS calculations were limited to 17 molecule super cells [2]. This lead to unphysical, size dependent effects in the calculated spectra. To treat larger systems, we extended the OCEAN interface to support well-parallelized codes such as QuantumESPRESSO. We also implemented an efficient interpolation scheme of Shirley. We applied this large-scale GW/BSE approach to 64 molecule unit cell structures of water obtained from classical DFT/MD and PIMD simulations [3]. In concurrence with previous work [4], we find the calculated spectrum both qualitatively and quantitatively reproduces the experimental features. The agreement implies that structures based on PIMD, which are similar to the traditional distorted tetrahedral view, are consistent with experimental observations.

[1] J. Vinson et al., PRB 83, 115106 (2011); J. Vinson and J.J. Rehr, PRB 86, 195135 (2012). [2] J. Vinson et al., PRB 85, 045101 (2012). [3] J.A. Morrone and R. Car, PRL 101, 017801 (2008). [4] L. Kong et al., PRB 86, 134203 (2012).

[1]Supported by the DOE CMCSN through DOE award DE-SC0005180 (Princeton University) and in part by DOE Grant No. DE-FG03-97ER45623 (JJR) with computer support from NERSC.

Keith Gilmore
Soochow University

Date submitted: 14 Nov 2013 Electronic form version 1.4