Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Computational photoelectron spectroscopy of liquid water[1] ALEX P. GAIDUK, University of Chicago, TUAN ANH PHAM, Lawrence Livermore National Laboratory, MARCO GOVONI, University of Chicago and Argonne National Laboratory, FRANCESCO PAESANI, University of California, San Diego, GIULIA GALLI, University of Chicago and Argonne National Laboratory — We present an extensive computational study of the electronic properties of liquid water simulated with MB-pol potential [1]. Electronic properties were determined using density-functional and many-body perturbation theory methods. We find that the G_0W_0 approximation starting from wavefunctions obtained with dielectric-dependent hybrid functionals [2] provides the best agreement of computed photoelectron spectra with experiment. The inclusion of nuclear quantum effects softens the structure of water, broadens the lines in the spectra and yields narrower band gaps; the use of different methods for modeling water in the absence of quantum effects, such as density-functional approximations [3–4], has a weaker effect on the liquid electronic properties. Remarkably, the positions of the valence band maximum and conduction band minimum are rather sensitive to the presence of the air/liquid interface, underlining the importance of modeling realistic systems for comparison with experiment.

[1] G. R. Medders, V. Babin, F. Paesani, JCTC 10, 2906 (2014); [2] J. H. Skone, M. Govoni, G. Galli, PRB 89, 195112 (2014); [3] T. A. Pham, C. Zhang, E. Schwegler, G. Galli, PRB 89, 060202 (2014); [4] A. P. Gaiduk, M. Govoni, R. Seidel, J. Skone, B. Winter, G. Galli, JACS 138, 6912 (2016)

[1]This work was supported by MICCoM center funded through DOE/BES 5J-30161-0010A and by NSERC Postdoctoral Fellowship

Alex Gaiduk
University of Chicago

Date submitted: 09 Nov 2016 Electronic form version 1.4