Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Nuclear Quantum Effects in Liquid Water: A Highly Accurate *ab initio* Path-Integral Molecular Dynamics Study[1] ROBERT A. DISTASIO JR., BISWAJIT SANTRA, HSIN-YU KO, ROBERTO CAR, Princeton University — In this work, we report highly accurate *ab initio* path-integral molecular dynamics (AI-PIMD) simulations on liquid water at ambient conditions utilizing the recently developed PBE0+vdW(SC) exchange-correlation functional, which accounts for exact exchange and a self-consistent pairwise treatment of van der Waals (vdW) or dispersion interactions, combined with nuclear quantum effects (*via* the colored-noise generalized Langevin equation[2]). The importance of each of these effects in the theoretical prediction of the structure of liquid water will be demonstrated by a detailed comparative analysis of the predicted and experimental oxygen-oxygen (O-O), oxygen-hydrogen (O-H), and hydrogen-hydrogen (H-H) radial distribution functions as well as other structural properties. In addition, we will discuss the theoretically obtained proton momentum distribution, computed using the recently developed Feynman path formulation,[3] in light of the experimental deep inelastic neutron scattering (DINS) measurements.

[1]DOE: DE-SC0008626, DOE: DE-SC0005180
[2]M Ceriotti, DE Manolopoulus Phys. Rev. Lett., **109**, 100604 (2012).
[3]L Lin, JA Morrone, R Car, M Parrinello Phys. Rev. Lett., **105**, 110602 (2010).

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Date submitted: 15 Nov 2013 Electronic form version 1.4