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Entropy of Liquid Water from Ab Initio Molecular Dynamics LEONARDO SPANU, CUI ZHANG, Chemistry Department University of California Davis, GIULIA GALLI, Chemistry Department and Physics Department University of California Davis — The debate on the structural properties of water has been mostly based on the calculation of pair correlation functions. However, the simulation of thermodynamic and spectroscopic quantities may be of great relevance for the characterization of liquid water properties. We have computed the entropy of liquid water using a two-phase thermodynamic model and trajectories generated by ab initio molecular dynamics simulations [1]. In an attempt to better understand the performance of several density functionals in simulating liquid water, we have performed ab initio molecular dynamics using semilocal, hybrid [2] and van der Waals density functionals [3]. We show that in all cases, at the experimental equilibrium density and at temperatures in the vicinity of 300 K, the computed entropies are underestimated, with respect to experiment, and the liquid exhibits a degree of tetrahedral order higher than in experiments. We also discuss computational strategies to simulate spectroscopic properties of water, including infrared and Raman spectra.

[1] C.Zhang, L.Spanu and G.Galli, *J.Phys.Chem. B* 2011 (in press)
[2] C.Zhang, D.Donadio, F.Gygi and G.Galli, *J. Chem. Theory Comput.* 7, 1443 (2011)
[3] C.Zhang, J.Wu, G.Galli and F.Gygi, *J. Chem. Theory Comput.* 7, 3061 (2011)

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