

Abstract Submitted
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Hybrid DFT First-Principles Study of the Properties of Water¹

MARTIN SCHLIPF, FRANCOIS GYGI, UC Davis — Water plays a crucial role in many chemical and biological reactions. Hence, an accurate description of the properties of water is imperative for a detailed understanding of these reactions. In recent years, hybrid density functionals such as PBE0 and HSE06 have improved the accuracy of DFT calculations for many insulators and semiconductors, as well as for aqueous solutions[1]. However, the evaluation of the Hartree Fock (HF) exchange energy makes these functionals computationally very demanding. We present a comparison of the structural and electronic properties of water obtained using the PBE0 and HSE06 density functionals. Simulations were performed using the Qbox code[2], and a recursive bisection scheme[3] reducing the computational cost of HF integrals. We discuss the effect of this approximation on the accuracy and the computation time, and compare our results to related work[4-5].

[1] C. Zhang, *et al.*, J. Chem. Phys. **138**, 181102 (2013).

[2] <http://eslab.ucdavis.edu/software/qbox>

[3] F. Gygi and I. Duchemin, J. Chem. Theory Comput. **9**, 582 (2012).

[4] T. Todorova, *et al.*, J. Phys. Chem. B **110**, 3685 (2006).

[5] M. Guidon, *et al.*, J. Chem. Phys. **128**, 214104 (2008).

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Francois Gygi
UC Davis

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