Abstract Submitted
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Density Functional Theory study of the equilibrium density of water at normal conditions[1] JUE WANG, Stony Brook University, GUILLERMO ROMAN-PEREZ, JOSE M. SOLER, Universidad Autonoma de Madrid, EMILIO ARTACHO, University of Cambridge, MARIVI FERNANDEZ-SERRA, Stony Brook University — *Ab initio* molecular dynamics of liquid water with the use of density functional theory (DFT) currently underperform experimental equilibrium density 1g/cm^3 under room temperature. At constant density, not much is known about the equilibrium density of commonly used GGA functionals in liquid water simulations. We present a DFT-based AIMD study of liquid water at different densities and analyze the structure and diffusivity of water with different exchange and correlation functionals. We show that all current GGA functionals fail to reproduce experimental density, however, the explicit description of long range correlations through a Van der Walls density functional (DRSLL)[2] can potentially transform our current understanding of the structure of liquid water. Our results shows that this new functional improves density, with only 2% error to experiment. But it underperforms GGA functionals in terms of structure.

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[2]M. Dion, H. Rydberg, E. Schröder, D. C. Langreth, and B. I. Lundqvist, *Phys. Rev. Lett.* **92**, 246401 (2004)

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