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Density, structure and dynamics of water: the effect of Van der Waals interactions[1] MARIVI FERNANDEZ-SERRA, JUE WANG, Stony Brook University, GUILLERMO ROMAN, Universidad Autonoma de Madrid, EMILIO ARTACHO, University of Cambridge, JOSE SOLER, Universidad Autonoma de Madrid — We present a DFT AIMD study of liquid water using several GGA functionals as well as the van der Waals density functional (vdW-DF) of Dion et al. [PRL 92, 246401(2004)]. As expected, we find that the density of water is grossly underestimated by GGA functionals. When a vdW-DF is used, the density improves drastically and the experimental diffusivity is reproduced without the need of thermal corrections. We analyze the origin of the density differences between all the functionals. We show that the vdW-DF increases the population of non-H-bonded interstitial sites, at distances between the first and second coordination shells. However, it excessively weakens the H-bond network, collapsing the second coordination shell. This structural problem is partially associated to the choice of GGA exchange in the vdW-DF. We show that a different choice for the exchange functional is enough to achieve an overall improvement both in structure and diffusivity. Jue Wang et al. J. Chem. Phys, 133, (2010).

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