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Van der Waals Density Functional Simulations of Liquid Water¹ JUN WU, CUI ZHANG, GIULIA GALLI, FRANCOIS GYGI, University of California Davis, Davis, CA95616 — We compare two versions of van der Waals density functionals (DRSLL [1], LMKLL [2]) in electronic structure computations of weakly bonded systems. The functionals are implemented in the Qbox code [3] and are verified by reproducing published binding energies and equilibrium separations of several weakly bonded dimers. Vibrational frequencies of the water monomer and dimer computed using the above van der Waals functionals are not improved compared to PBE results. We present results of molecular dynamics simulations of liquid water using the DRSLL and LMKLL functionals and compare radial distribution functions with corresponding results obtained with GGA functionals.

[1] M. Dion et al. Phys. Rev. Lett. 92, 246401 (2004).

[2] K. Lee et al. Phys. Rev. B 82, 081101 (2010).

[3] http://eslab.ucdavis.edu/software/qbox

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