

Abstract Submitted
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**van der Waals density functional comparison for water monomers,
dimers and clusters and the implications on the dynamics of liquid water¹**

ADRIAN SOTO, MARIVI FERNANDEZ-SERRA, Department of Physics and Astronomy, Stony Brook University, DEYU LU, Center for Functional Nanomaterials, Brookhaven National Laboratory — The appearance of van der Waals (vdW) density functionals has allowed the efficient ab initio molecular dynamics (AIMD) study of systems for which dispersion forces are critical. Despite the great improvement over GGA functionals, the errors in the simulations are still too large for some applications of interest. Furthermore, different vdW functionals can produce qualitatively different results. In particular, for liquid water at ambient conditions there is a discrepancy of approximately 20% in the yielded $P(\rho)$ “equations of state”; the radial distribution functions (RDF) disagree substantially with experiment, giving an overstructured liquid mainly due to an overbinding of the hydrogen bond; the self-diffusion coefficients can vary over 75% [J. Chem Phys. 139, 194502(2013)]. In this study we focus on the role of the electronic polarizabilities, responsible for the vdW dispersion forces using two very different vdW functionals. In particular we study how 1-body, 2-body and 3-body terms modify the molecular polarizabilities and how these effects are linked to the many-body decomposition of the total energy of the systems.

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