Abstract Submitted
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The Effect of van der Waals Interactions on the Structure of Liquid Water.[1] ROBERT DISTASIO JR., ZHAOFENG LI, ROBERTO CAR, Princeton University — In this work, we demonstrate the importance of including van der Waals (vdW) interactions in the theoretical prediction of the structure of liquid water. These effects are investigated by computing and analyzing the oxygen-oxygen, oxygen-hydrogen, and hydrogen-hydrogen radial distribution functions (RDFs) obtained from highly accurate *ab initio*molecular dynamic simulations that explicitly account for vdW interactions. In particular, we utilize an efficient order(N) algorithmic implementation of the self-consistent energy and analytical forces of the density functional based vdW correction proposed by Tkatchenko and Scheffler (PRL 102, 073005 (2009)) to demonstrate the importance of vdW interactions in obtaining RDFs that are in close agreement with experiment. In addition, we also provide an analysis of finite size effects in vdW-based liquid water simulations as well as a comparison to several other competitive theoretical methods for treating vdW interactions.

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