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The Structure, Density, and Local Environment Distribution in *Ab Initio* Liquid Water[1] BISWAJIT SANTRA, ROBERT A. DISTASIO, JR., Princeton University, XIFAN WU, Temple University, ROBERTO CAR, Princeton University — We have performed extensive *ab initio* molecular dynamics (AIMD) simulations of liquid water at ambient conditions in the canonical (NVT) and isothermal-isobaric (NPT) ensembles to understand the individual and collective importance of exact exchange, van der Waals interactions, and nuclear quantum effects on the structural properties of liquid water. AIMD simulations which include these effects result in oxygen-oxygen radial distribution functions which are in excellent agreement with experiments and a liquid water structure having an equilibrium density within 1% of the experimental value of 1 g/cm^3. A detailed analysis of the distribution of local structure in ambient liquid water has revealed that the inherent potential energy surface is bimodal with respect to high- and low-density molecular environments, consistent with the existence of polymorphism in the amorphous phases of water. With these findings in mind, the methodology presented herein overcomes the well-known limitations of semi-local density functional theory (GGA-DFT) providing a detailed and accurate microscopic description of ambient liquid water.

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