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Liquid water from first principles: The importance of exact exchange, dispersion interactions, and nuclear quantum effects[1] ROBERT DISTASIO, ZHAOFENG LI, BISWAJIT SANTRA, Princeton University, XIFAN WU, Temple University, ROBERTO CAR, Princeton University — Quantitative agreement between theory and experiment on the structure of liquid water at ambient conditions has been quite difficult to achieve to date. In this work, we report that highly accurate *ab initio* molecular dynamics simulations of liquid water that account for exact exchange (via the hybrid PBE0 functional [PRB **79**, 085102 (2009)]), dispersion interactions [PRL **102**, 073005 (2009)], and nuclear quantum effects (presently approximated by a 30K increase in the simulation temperature) result in excellent agreement with experiments [PRL **101**, 065502 (2008)]. The importance of each of these effects in the theoretical prediction of the structure of liquid water will be demonstrated by a detailed comparative analysis of the predicted and experimental oxygen-oxygen radial distribution functions. In addition, we will discuss the connection between the experimentally observed scattering intensity, I(k), and the final radial distribution function, g(r), via the structure and form factors.

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Robert DiStasio
Princeton University

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