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How do hybrid functionals, dispersion interactions and quantum nuclei affect the structure of liquid water? ZHAOFENG LI, ROBERT A. DISTASIO JR., ROBERTO CAR, Princeton University, XIFAN WU, Temple University — We report *ab-initio* molecular dynamics simulations of liquid water at STP and at the volume corresponding to experimental equilibrium density. These simulations are based on the hybrid functional PBE0 for the electrons and include approximate dispersion interactions according to Ref ¹. Nuclear quantum corrections were included as estimated by Ref ². We find that all of these components are important to significantly improve the agreement of the simulated structure with recent experimental analyses based on neutron and X-ray diffraction³ and on NMR experiments. ⁴

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