Ab-initio liquid water with hybrid functionals and dispersion interactions\textsuperscript{1} ZHAOFENG LI, Princeton University, XIFAN WU, Temple University, ROBERT DISTASIO JR., ROBERTO CAR, Princeton University — We report ab-initio molecular dynamics simulations of liquid water using the hybrid PBE0 functional plus self-consistent dispersion forces based on the scheme of Ref.\textsuperscript{2} Simulations were performed at $T=300K$ and at $T=330K$ to approximately account for nuclear quantum effect on the oxygen-oxygen(O-O) RDF, as suggested by previous path integral simulations. Focusing on O-O RDF, we find that the combined effect of the hybrid functional and of the dispersion interactions significantly improves the agreement of the simulated structure with experiment.

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