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Ab-inito **liquid water with hybrid functionals and dispersion interactions**[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.[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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[2]A. Tkatchenko and M. Scheffler, Phys. Rev. Lett. **102**, 073005 (2009).

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