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Ab initio **liquid water from PBE0 hybrid functional simulations**[1]
ZHAOFENG LI, XIFAN WU, ROBERTO CAR, Princeton University — For reasons of computational efficiency, so far most *ab initio* molecular dynamics simulations of liquid water have been based on semi-local density functional approximations, such as PBE and BLYP. These approaches yield a liquid structure that, albeit qualitatively correct, is overstructured compared to experiment, even after nuclear quantum effects have been taken into account.[2] A major cause of this inaccuracy is the delocalization error associated to semi-local density functional approximations, which, as a consequence, overestimate slightly the hydrogen bond strength in the liquid. In this work we adopt the PBE0 hybrid functional approximation, which, by mixing a fraction of exact (Hartree-Fock) exchange, reduces significantly the delocalization error of semi-local functionals. Our approach is based on a numerically efficient order-N implementation of exact exchange.[3] We find that PBE0 systematically improves the agreement of the simulated liquid with experiment. Our conclusion is substantiated by the calculated radial distribution functions, H-bond statistics, and molecular dipole distribution.

[1]National Energy Research Scientific Computing Center
[2]J. A. Morrone and R. Car, Phys. Rev. Lett. **101**, 017801(2008)
[3]X. Wu, A. Selloni, and R. Car, Phys. Rev. B **79**, 085102(2009)

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