Abstract Submitted
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Accelerating Hybrid Density Functional Theory Molecular Dynamics[1] WILLIAM DAWSON, FRANCOIS GYGI, UC Davis — For many systems, accurate First-Principles Molecular Dynamics (FPMD) simulations require the use of hybrid density functional theory. Molecular Dynamics requires short wall clock times and thus highly scalable parallel algorithms. The Qbox[1] code implements the recursive subspace bisection algorithm[2,3] which accelerates hybrid density functional theory calculations by creating a set of localized orbitals to reduce the number of exchange integrals computed. This approach allows for controlled accuracy and requires no a priori assumptions about localization. We discuss heuristic algorithms for improving the scalability and performance of this approach. We then demonstrate these improvements in applications to aqueous solutions and water-metal interfaces.
[1] http://eslab.ucdavis.edu/software/qbox
[2] F. Gygi, Phys. Rev. Lett. **102**, 166406 (2009).
[3] F. Gygi and I. Duchemin, J. Chem. Theory Comput. **9**, 582 (2012).

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