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Performance and Accuracy of Recursive Subspace Bisection for Hybrid DFT Calculations[1] WILLIAM DAWSON, FRANCOIS GYGI, Univ of California - Davis — The high cost of computing the Hartree-Fock exchange has resulted in limited use of Hybrid Functionals in DFT calculations. Approximations based on transformation to localized orbitals provide one way to reduce this cost. One such method is the recursive subspace bisection method (RSB)[1]. Such localization methods involve truncation of localized orbitals, which introduces an additional approximation. We take advantage of our ability to systematically reduce the error in RSB calculations through a single parameter to study this approximation. We present the errors in ground state energy, forces, and relative energy differences between configurations for a variety of systems, including tungsten oxide, a silicon-water interface, and liquid water including the calculation of empty states.
[1] F.Gygi, Phys. Rev. Lett. 102, 166406 (2009).
[2] Qbox code, http://eslab.ucdavis.edu/software/qbox/

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