Abstract Submitted
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Acceleration of Hartree-Fock Exchange Computations using Recursive Subspace Bisection[1] IVAN DUCHEMIN, Department of Applied Science, University of California Davis, Davis CA 95616, FRANCOIS GYGI, Department of Computer Science, University of California Davis, Davis CA 95616 — We use the recursive subspace bisection algorithm [1] to accelerate the computation of the Hartree-Fock exchange operator in electronic structure computations involving hybrid density functionals. This approach leads to a reduction of the computational cost of the exchange operator from $O(N^3 \log N)$ to $O(N^2 \log N)$ and allows for controlled accuracy through a threshold parameter. The subspace bisection method is extended to invariant subspaces including excited states. Applications to molecular dynamics simulations and computations of energy band gaps in large systems using the PBE0 hybrid functional will be presented.

[1] F. Gygi, Phys. Rev. Lett. 102, 166406 (2009).

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