

Abstract Submitted
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Exponential supercell convergence of the exact exchange energy via truncated coulomb potentials¹ RAVISHANKAR SUNDARARAMAN, T. A. ARIAS, Department of Physics, Cornell University, Ithaca, NY — Hybrid density functionals have become increasingly popular as a solution to mitigate the self-interaction error in semi-local density functionals, but widespread application to periodic systems has been limited by computational cost. This cost is exacerbated by poor k -point convergence due to the $G \rightarrow 0$ singularity in the exact exchange energy, in spite of several singularity correction methods such as auxiliary function integration,^{2,3} image subtraction,⁴ and spherical truncation of the coulomb potential.⁵ We analyze these rather disparate methods in an intuitive formalism based on Wannier function localization, which naturally suggests the truncation of the Coulomb potential on the superlattice Wigner-Seitz cell. We demonstrate that this scheme systematically exhibits the best k -point convergence, comparable to that of semi-local functionals, even for low-symmetry and reduced-periodicity systems where previous methods fail.

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