Analysis of the Heyd-Scuseria-Ernzerhof Density Functional Parameter Space

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The Heyd-Scuseria-Ernzerhof (HSE) density functionals are popular for their ability to improve the accuracy of standard semilocal functionals such as Perdew-Burke-Ernzerhof (PBE), particularly for semiconductor band gaps. They also have a reduced computational cost compared to hybrid functionals, which results from the restriction of Fock exchange calculations to small inter-electron separations. These functionals are defined by an overall fraction of Fock exchange and a length scale for exchange screening. We systematically examine this two-parameter space to assess the performance of hybrid screened exchange (sX) functionals and to determine a balance between improving accuracy and reducing the screening length, which can further reduce computational costs. Three parameter choices emerge as useful: "sX-PBE" is an approximation to the sX-LDA screened exchange density functionals based on the local density approximation (LDA); "HSE12" minimizes the overall error over all tests performed; and "HSE12s" is a range-minimized functional that matches the overall accuracy of the existing HSE06 parameterization but reduces the Fock exchange length scale by half. Analysis of the error trends over parameter space produces useful guidance for future improvement of density functionals.

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