Approximations in Local Hybrid Density Functionals

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Local hybrid density functionals combine semilocal density functional approximations with a position-dependent admixture of exact (Hartree-Fock-type) exchange. This ansatz can, in principle, provide combine the nondynamical correlation corrections of semilocal functionals with an exact treatment of asymptotic and one-electron regions. A critical parameter is the choice of exact-exchange mixing function. We present investigations of a similarity metric that provides a useful ingredient for local hybrid mixing functions. The metric locally compares the Kohn-Sham one-particle spin-density matrix used to construct exact exchange, and the uniform electron gas model density matrix used in semilocal DFT exchange. The metric is computationally tractable, bound between 0 and 1, and is sensitive to fractional occupancy of molecular (sub)systems. We also present preliminary results for approximate density functionals that incorporate some of the desirable properties of local hybrids, without requiring explicit evaluation of exact exchange. These provide novel insights into existing semilocal density functionals, and show promise for applications to large systems.