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Title: Retrofit of the HSE density functional

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A recent trend in density functional theory (DFT) is the concept of range-separation, where the Coulomb interaction is split into a sum of multiple components and a different treatment of exchange and correlation is applied to each. A particularly popular range-separated functional is HSE, which treats correlation and long-range exchange with a semi-local form but computes short-range exchange exactly. Restricting the calculation of Fock exchange to a short range reduces the computational cost relative to full Fock exchange while retaining most of the empirical benefits. The empirical success of short-range Fock exchange can be attributed to its crude approximation of the material-dependent screened Fock exchange found in more sophisticated quasiparticle theories. We thoroughly explore the two-parameter space (a minimum screening value and a screening length) that defines the HSE functional to empirically determine a best "one size fits all" screening form. Our tests include properties of molecules (the G3/99 test set) and semiconductors (the SC/40 test set) in an effort to balance the relative errors in approximating localized and delocalized electronic states. Such a balance is beneficial for the study of defect level alignment in semiconductors. In addition, the new HSE parameters result in an even shorter ranged Fock exchange term that may further reduce computational costs. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.