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The role of middle-range Hartree-Fock-type exchange in hybrid functionals THOMAS HENDERSON, ARTUR IZMAYLOV, GUSTAVO SCUSE-RIA, Rice University, ANDREAS SAVIN, Universite Pierre et Marie Curie — While hybrid functionals are responsible for many successes in modern Kohn-Sham theory, they have several drawbacks. The slow decay of nonlocal exchange makes hybrids computationally demanding in extended systems with small bandgaps, while in finite systems the rapid decay of semilocal exchange causes errors in quantities sensitive to the long-range potential. Both problems can be addressed by range-separated hybrids which include nonlocal exchange only for some values of the interelectronic separation. Excluding long-range nonlocal exchange in extended systems improves computational efficiency without loss of accuracy, while including full long-range nonlocal exchange in finite systems improves accuracy without loss of efficiency. Both approaches use a significant fraction of nonlocal exchange for intermediate electronic separations. We show that a hybrid functional that uses nonlocal exchange only for this middle range has many advantages, properly describing thermochemistry, reaction barriers, and bandgaps in the same framework.

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