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The effects of long-range exact exchange in hybrid-functional methods

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Over the past several years, hybrid density functional theory, which mixes a fraction of exact exchange into conventional semilocal exchange-correlation functionals, has become the dominant method used in molecular electronic structure calculations. While hybrid functionals are responsible for many successes of modern Kohn-Sham theory, they suffer from several drawbacks as well. The rapid decay of semilocal exchange causes errors in describing many phenomena, including charge transfer and Rydberg excitations, polarizabilities of long chains, and several others. Further, different properties seem to require different amounts of exact exchange; calculations near equilibrium, for example, appear to require less exact exchange than do calculations far from equilibrium. Including long-range exact exchange in finite systems improves accuracy in quantities sensitive to the long-range potential and makes it possible to treat systems both near and away from equilibrium on a fairly even footing. This talk discusses the motivations for including long-range exact exchange, as well as some remarkable successes and notable failures caused by doing so. Alternatives which attempt to retain most of the successes while eliminating most of the failures are also discussed.