BALANCED DESCRIPTION OF GROUND-STATE PROPERTIES, VALENCE EXCITATIONS, AND CHARGE-TRANSFER EXCITATIONS WITH LONG-RANGE CORRECTED DENSITY FUNCTIONALS

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Time-dependent density functional theory's favorable scaling properties make it an attractive technique for the study of large, condensed-phase systems. However, in such systems conventional generalized gradient approximation functionals are plagued by spurious, low-energy charge transfer (CT) excitations. Long-range corrected (LRC) functionals, which asymptotically turn on full Hartree-Fock exchange at long range, push these CT states to higher energies. Until recently it has seemed impossible to find a long-range corrected functional that performed acceptably well for both ground- and excited-state properties. We have constructed an implemented a LRC hybrid functional that not only performs reasonably well in a battery of tests on ground-state properties and valence excitations, but also achieves reasonable accuracy for a small database of CT excitations.