Performance of Long-Range Corrected Functionals MARY
ROHRDANZ, JOHN HERBERT, The Ohio State University — Popular general-
ized gradient approximations (GGA) to the exchange-correlation functional are ac-
curate and useful in many different physical systems. However they have several
well-documented shortcomings, including the incorrect asymptotic behavior. One
manifestation of this is that linear response time-dependent density functional calcu-
lations of vertical excitation energies with GGA functionals sharply underestimate
charge-transfer excitations in large systems. Consequently, such functionals are not
reliable for calculations in such situations, for example, biomolecules in solution. To
circumvent this problem, a number of long-range-corrected functionals (based on
GGAs) have recently been developed, which posses the correct asymptotic form by
construction. We analyze the performance of some of these functionals through a
battery of tests, and demostrate that there exists a functional form and parame-
ter set that provide reasonable results for both ground-state properties and verti-
cal excitation energies. We find these functionals suitable for general use in large
condensed-phase systems.

Mary Rohrdanz
The Ohio State University