Efficient and Accurate Propagator Methods for Calculating Electron Binding Energies

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Abstract

Tests on the predictive ability and computational efficiency of a variety of electron–propagator methods disclose their advantages in determining electron binding energies of various kinds, including ionization energies of large organic molecules and carbon clusters, electron detachment energies of anions and electron affinities of organic acceptors. The extrapolation of basis–set trends reveals the favorable intrinsic characteristics of several, highly efficient approximations which deserve more widespread use. Among these approximations are the diagonal second–order, partial third order, extended partial third order and nondiagonal renormalized second–order methods. Composite models in which basis–set and self–energy corrections are estimated in a sequence of calculations and schemes for the correction of spin–contamination in calculations based on unrestricted spin–orbitals facilitate reliable predictions of electron binding energies for large anionic clusters of carbon and boron.