Strong Correlation Effects in Electron Propagator Calculations on Large Molecules

J. V. Ortiz

Department of Chemistry and Biochemistry
Auburn University
Auburn, Alabama 36849-5312

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Abstract

Algorithmic improvements in *ab initio* electron propagator calculations now permit the identification and assignment of correlation states in the photoelectron spectra of large molecules such as fullerenes and phthalocyanines. Previous theoretical treatments based on orbital energies that emerge from Hartree–Fock or Kohn–Sham equations are incapable of describing such effects. Numerous correlation states with low pole strengths may lie between final states which are well described in a qualitative sense by the Koopmans approximation. Renormalized self–energy approximations that are especially effective in the discovery of correlation states and the computational techniques that accompany them are described in detail. The advantage of this approach is illustrated by calculations on fullerenes and metallocyclic compounds with phthalocyanine and porphyrin ligands.