Cluster-in-molecule local correlation approach: Recent developments and applications

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The "Cluster-in-Molecule" (CIM) local correlation approach for post-Hartree-Fock calculations in a basis of orthogonal occupied and virtual localized molecular orbitals (LMOs) is reviewed and some recent developments and applications are shown. The main idea of the CIM approach is that significant excitation amplitudes can be approximately obtained by solving the coupled cluster (CC) (or Møller-Plesset perturbation theory (MPPT)) equations of a series of "clusters", each of which contains a subset of occupied and virtual LMOs.[1-5] Recently, we proposed two refined CIM schemes[6,7] for predicting the relative energies, in which two new strategies for building clusters are introduced. Our results show that the present CIM scheme can reproduce more than 99% of conventional correlation energies for a wide variety of systems. Furthermore, the present CIM scheme can give satisfactory descriptions for conformation energy differences of quite large systems. In general, CIM can be considered as an effective framework for extending electron structure methods to large systems.

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