MAR05-2004-005382

Abstract for an Invited Paper
for the MAR05 Meeting of
the American Physical Society

Fast methods for evaluating molecular electron correlation energies

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Some of the issues associated with developing fast methods for the wavefunction- based description of electron correlation will be re-examined in this talk, after a brief introductory overview of standard methods for treating electron correlation in molecules. The first main topic is the description of so-called dynamic correlation effects that are closely related to atomic correlations. Local correlation methods that describe two and three-body correlations at reduced computational cost, while still ensuring continuous potential energy surfaces will be described and their performance assessed in terms of accuracy and computational cost. The second main topic is describing strong correlations associated with near-degeneracies, such as occur in diradicaloid molecules and transition metal compounds. Simplified coupled cluster methods appropriate for such problems will be described, along with examples of their application to several molecules believed to have significant diradical character.