Formulation of the coupled cluster theory with localized orbitals in correlation calculations on polymers. Foerner, Wolfgang

Abstract

In the framework of coupled cluster theory both the correlation energy per unit cell and quasi-particle band structures of polymers can be computed directly from matrix elements of the excitation operator and the 2-electron integrals calcd. in localized orbital basis. Further, it is described how to take advantage of the localized nature of the orbitals applied. Ab initio test calcns. on a finite model system similar to the PPP Hamiltonian are presented.