

Numerical application of the coupled cluster theory with localized orbitals to polymers. I. Total correlation energy per unit cell. Ye, Yuan-Jie; Foerner, Wolfgang; Ladik, Janos

Abstract

The orbital invariant Moeller-Plesset perturbation theory of second order (LMP2), the coupled-cluster doubles theory, and its linear approxn. are applied to compute total correlation energies per unit cell in different polymers, using localized orbitals. The involved approxns. are numerically checked against calcns. with the canonical MP2 (CMP2) method. The major aim of this work is to det. numerically, whether the localization properties of Wannier functions are sufficient to make a localized orbital approxn. possible or not. Calcns. were performed on H chains, water chains, polyacetylene, and polyethylene applying different at. basis sets. Also the correlation energy as a function of the geometry of some of the polymers is compared to the CMP2 results. The localization of the Wannier functions is sufficient for the application of the authors' approxn. in nonbonded chains, but not in polymers with chem. bound unit cells.