

Coupled-cluster studies. II. The role of localization in correlation calculations on extended systems. Foerner, W.; Ladik, J.; Otto, P.; Cizek, J

Abstract

Calcns. of correlation energies by using localized orbitals (C., et al., 1983) were done with the previously developed (F., et al., 1985) program for the soln. of the coupled-cluster doubles (CCD) equations. This enabled a substantial redn. of the no. of necessary excitations in correlation calcns. performed for metallic and mol. hydrogen rings and for a medium size mol. in a min. basis set. For the mol. hydrogen rings and the medium size mol., the scheme was successfully applied, reproducing more than 90% of the correlation energy in the given basis set. In the case of metallic hydrogen rings, the scheme was not applicable. The correlation energies were calcd. for the four nucleotide bases of DNA with a min. basis, and for cytosine with an extended basis. In this way, .apprx.50% of the estd. total valence-correlation energy for cytosine was obtained, which is to be expected for a valence-split basis set.