

**Numerical application of the coupled cluster theory with localized orbitals to polymers. II. Optimal localization of Wannier functions and the correlation energy in different approximations.** Knab, Reinhard; Foerner, Wolfgang; Cizek, Jiri; Ladik, Janos

**Abstract**

An iterative method is presented for obtaining localized Wannier functions, needed in the framework of correlation energy calcns. on polymers with different size-consistent methods using a localized orbital basis. Test calcns. using different possible localization schemes are performed on alternating all-trans polyacetylene (t-PA), which is an example for polymers with covalently bound unit cells. The improvement of the localization is compared with respect to the total correlation energy per unit cell at the level of second order orbital invariant Moeller-Plesset perturbation theory (LMP2) to the canonical MP2 (CMP2) method, and also results of the calcn. of the correlation energy with the coupled cluster doubles theory (CCD) and its linear approx. (LCCD) are shown. The coupled cluster expansions failed to converge for systems contg. the Wannier functions belonging to two interacting unit cells if their interactions are too large. This is probably due to linear dependences in the systems of equations for such a highly sym. system. Such a behavior can be made plausible with the help of a very simple model. Possibilities to overcome this problem are discussed. A comparison of the influence of the localization approxn. on the correlation energy obtained with the corresponding canonical procedure is made for Clementi's minimal and double zeta basis sets on the MP2 level and, in addn., the localized Wannier functions of larger systems and the effects of the localized orbital approxn. on a potential curve for t-PA are discussed.