

Comparative application of different approaches for band structure calculations on polyparaphenylene in the Pariser-Parr-Pople model: I. The mean field (Hartree-Fock) approximation and localized Wannier functions. Forner, Wolfgang

Abstract

An investigation on the calcn. of the band structure of polyparaphenylene using the one-particle Hartree-Fock method is presented. In the ab initio case there are many calcns. on this level published which are all based on different Hartree-Fock (HF) program packages and thus use different cutoff schemes for the interactions and different basis sets. Therefore the results of these studies are not directly comparable and a through study of different approaches based on one and the same ref. is highly desirable. A similar study on the same system using conventional correlation methods and d. functional schemes, esp. self interaction cor. ones, is forthcoming. The PPP or the Hubbard model are well suited for such a purpose, since the correlation methods on top of HF use exactly the same formalisms as the corresponding ab initio applications, however, the numerical calcns. are much cheaper. The formalism of the PPP and Hubbard models and its relation to the full ab initio theory are presented in full detail. Obtaining localized Wannier functions from the delocalized canonical Bloch orbitals is described. Localized Orbitals are of utmost importance both for conventional correlation methods and for the self-interaction correction in d.-functional theory. Expressions for transition dipole moments in polymer calcns. are derived and applied to the spectrum of polyparaphenylene.