

Comparative application of different approaches for band structure calculations on polyparaphenylene in the Pariser-Parr-Pople model: III. Density functional theories.

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Abstract

We present explicitly and in detail the LSD (local spin d. approxn.) and LSD-SIC (self interaction correction) formalisms for the Hubbard and the PPP model for the π -electrons. The basic formalism (besides the actual expressions for the matrix elements of the potentials) can be used also in ab initio applications. Our numerical results for poly(p-phenylene) indicate that the SIC method meets severe convergency problems for these models, because due to the ZDO approxn. the matrix elements of the potential appear only on the diagonal of the LDA (local d. approxn.) matrix. Since due to symmetry in poly(p-phenylene) the densities at each site are equal (in LDA for the Hubbard case) this has the consequence that the band structure is the same as the one obtained from the one-electron part of the matrix. The same behavior occurs in PPP-LDA, because there in the course of the iterations the densities converge in such a way, that again the electron-electron interaction contributions are the same for all diagonal elements. However, the LDA-SIC total energies as function of a geometry parameter are in good agreement with correlated Hubbard and PPP results.