

Spin contamination, disorder effects, and soliton dynamics in the Pariser-Parr-Pople model of trans-polyacetylene. Foerner, Wolfgang

Abstract

Numerical calcns. on the interactions of solitons with impurities in trans-polyacetylene are described. The PPP Hamiltonian in mean-field form is used. To remove spin contaminations inherent in the UHF-Slater determinant, the major contaminating component is annihilated in each self-consistent-field iteration cycle (annihilated UHF method). As impurities a conjugation break (e.g., a CH₂ group instead of CH) and isoelectronic chem. substitutions (B,N,NH⁺,O⁺) for CH are considered. Further, a random sequence in all parameters along the chain is introduced. Such a random sequence is probably present in the system due to its disordered structure. For reasonable disorder strength the soliton is able to move through the chain.