

Effects of disorder on soliton dynamics. Part 2. Solitons in trans-polyacetylene within the Pariser-Parr-Pople model. Foerner, Wolfgang

Abstract

Numerical calcns. are presented on the interactions of solitons with impurities in trans-polyacetylene using a PPP Hamiltonian in the mean field approxn. To remove spin contaminations inherent in the UHF Slater determinant the major contaminating component is annihilated in each SCF iteration cycle. A conjugation break (e.g. a CH₂ group instead of CH) and isoelectronic chem. substitutions (B, N, NH⁺, O⁺) for CH are considered as impurities. Further random sequences. Random sequences in all parameters along the chain, most probably present in the real system owing to its disordered structure, are also considered.