Electronic-band-structure calculations and soliton dynamics for polyketene and related compounds. Foerner, Wolfgang; Ladik, Janos J.

Abstract

Minimal-basis-set ab initio band-structure calcns. on trans-polyacetylene (I) and polyketene (II) are performed. In agreement with exptl. findings, the fundamental gap of the polymer does not change due to substitution of H by OH. Soliton dynamics within the Su-Schrieffer-Heeger Hamiltonian in II shows a moving soliton in this system, however, with a reduced velocity compared to I. Together with the previous results that a C:O group in a I chain behaves as a soliton trap and the fact that ≈30% of the CO groups in II are in the keto form instead of the enol form, the exptl. findings of both localized and mobile spins in this material are explained.