Soliton dynamics in trans-polyacetylene using the full Pariser-Parr-Pople Hamiltonian.

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Abstract

Soliton dynamics applying the full PPP Hamiltonian is presented for a (CH)29 model chain. These first calcns. in the PPP Hamiltonian show that the best expression for the electron-electron interaction is the Ohno formula with an on-site Hubbard term U = 11.08 eV for carbon. The kinetic mass of the soliton is roughly twice the value obtained from Su-Schrieffer-Heeger (SSH) calcns. The soliton velocity is smaller than that in the SSH model; its half-width is reduced from 7 to ≈ 3 upon inclusion of electron-electron interaction. This value compares well with modified neglect of differential overlap results found in the literature. Analytic gradients are used and tested in the simulations.