

Chain-end effects in Su-Schrieffer-Heeger-type models of alternating trans-polyacetylene.
Foerner, Wolfgang

Abstract

Finite chain-length effects on soliton dynamics in Su-Schrieffer-Heeger models for trans-polyacetylene are reported and indicate that for the frequently used value of 0.1 Å for the dimerization const., the results depend strongly on the chain length. An equation for the potential due to σ -electrons is reformulated so that no addnl. linear terms to avoid chain shrinkage are necessary. Second-neighbor resonance integrals of a magnitude suggested by exptl. findings had no influence on soliton dynamics.