

Interchain coupling in trans-polyacetylene: dynamic simulations. Ottschofski, Edgar; Foerner, Wolfgang; Ladik, Janos.

Abstract

Using Su-Schrieffer-Heeger-type Hamiltonians for trans-polyacetylene in calcns. of soliton dynamics, computations were performed taking into account effects of neighboring chains. The time simulations for a soliton showed that for large interchain coupling, the soliton was localized on the chain end, in agreement with previous results. Geometry optimization showed that the out-of-phase bond alternation of the chains was energetically preferred. Two solitons on neighboring chains were simulated.