

Influence of substitutional impurities on soliton dynamics in trans-polyacetylene.

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Abstract

For different chains of trans-polyacetylene with various substituents the equations of motion of the coupled electron-phonon system were integrated within the Su-Schrieffer-Heeger model. NH^+ , N, and O^+ as isoelectronic substitutions for a CH group as well as the effect of an NH and a CO group were investigated. The calcns. for the time evolution of an end-generated kink show that neutral solitons can pass a N atom and an O ion, but not an NH^+ , NH, or CO group. The neg. charged soliton is not able to pass any of the investigated substitutions. The CO unit, which is of special interest in the light of recent exptl. results for acetylene-CO-copolymers with similar properties as trans-polyacetylene, represents a trap for both neutral and neg. charged kinks and a repulsive barrier for a pos. charged kink. The limitations of the soliton model are discussed.