Soliton trapping and repulsion due to a CO-group in trans-polyacetylene. Foerner, W.; Seel, M.; Ladik, J

Abstract

For a chain of trans-polyacetylene with one CO substitution, the equations of motion of the coupled-electron-phonon system were integrated within the Su-Schrieffer-Heeger model. The calcns. for the time evolution of an end generated kink showed that a -C(:O)- unit presents a trap for both a neutral and a neg. charged kink, and a repulsive barrier for a pos. charged kink. The limitations of the soliton model are discussed.