

Investigation of soliton dynamics in excited polyacetylene. Rubner, Oliver; Foerner, Wolfgang; Ladik, Janos

Abstract

The predictions concerning the existence and properties of solitons in excited alternating trans-polyacetylene are studied numerically. The computations include electron-electron interaction on a PPP level. To approx. the gradient of the potential energy with respect to the geometrical variables, 1st-order perturbation theory is used. As found in earlier studies which used the Heuckel-type Su-Schrieffer-Heeger Hamiltonian, soliton formation occurs in excited polyacetylene. Electron-electron interactions have qual. a smaller than expected influence on soliton dynamics.