Nonlinear charge carriers in organic conjugated polymers. Forner, Wolfgang

Abstract

In this work, a procedure for the prediction of the nature, stability, thermal behavior and mobility of charge carriers in org. polymers exhibiting π conjugation is descried on the basis of a simple semi-empirical π-electron model. These charge carriers are assumed to be charged solitons in polymers with degenerate ground state and charged polarons in those with non-degenerate ground state. On the basis of calcns. on the dynamics of polyenes, we explain in detail how the parameters of the model Hamiltonian can be detd. It is shown that energy levels in the gap due to the nonlinear quasiparticles can be calcd., at least qual. correctly. Further, a short review of simulations of the dynamics of the charge carriers in trans-polyacetylene is provided. For the first time, we show theor. spectra, calcd. including electron correlations of neg. charge solitons in trans-polyacetylene (t-PA). Also the first time an exact soln. for the Su-Schrieffer-Heeger Hamiltonian is derived in the adiabatic limit, exhibiting explicitly the dynamics of the electrons. From the results obtained with this procedure, the temp. dependence of the mobility of neutral solitons in t-PA is discussed, which is shown to start around 10K, while at 100K the solitons we found to be completely mobilized, in agreement with expt. Further, for the first time the theor. expressions are derived for the calcn. of vibrational spectra from dynamic simulations. Finally, it is shown how the procedure can be extended to other polymers, and how the stability of such polymers against oxygen can be studied with the help of more sophisticated methods.