Nonlinear Quasiparticles as Charge Carriers in Conjugated Organic Polymers on the Example of Doped

and Photoconducting Polyacetylene. Förner, W..

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Abstract

Conjugated organic polymers are intrinsically semiconductors but become conducting upon doping and

photoconducting after optical excitation. In the low doping regime they show usually conduction without an

associated spin transport. Thus as charge carriers in this regime nonlinear quasiparticles are assumed, such as

charged solitons in materials with a degenerate ground state like e.g. trans-polyacetylene or pernigraniline. In

the case of materials with a non-degenerate ground state the situation is often less clear but it is assumed that

charged polarons or bipolarons are the charge carriers in them.

We present a theoretical model for the description of the dynamics of such quasiparticles which yields also

informations on their mobility, their nature and stability, as well as on their spectral properties. The model is

based on a π-electron Hamiltonian including electron-electron interactions. On the basis of the prototype

material polyacetylene it is discussed that such a model has to be reparametrized with the help of correlated

ab initio or density functional calculations and how it can be applied. We show in some detail the dynamics of

the pristine material, as well as of doped and of electronically excited polyene chains. With the help of these

dynamics a scenario for the conduction mechanism assumed for polyacetylene is given. Further we calculate

optical spectra from the dynamics for charged solitons and for excited chains which are in fair agreement with

experiments. The thermal mobility of neutral solitons is also studied.

Further we show how the model can be extended for applications to polymers different to polyacetylene.

Such modifications could yield informations about the nature of nonlinear quasiparticles involved in the

process of charge transport in cases where the question is not completely solved. This is the case in cis-poly-

acetylene where recent literature suggests that bipolarons should be instable. However, we could show that both

charged polarons and bipolarons are stable in the material with bipolarons favored over charged polarons.

Due to the fact that the model can be extended to other polymers, also to chemical structures not yet

synthesized it could gain also predictive power after further development.