

## Calculation of Electronic Spectra of Trans-Polyacetylene. Förner, W..

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### Abstract

We present in this work theoretically calculated electronic spectra of charged trans-polyacetylene chains

containing solitons. These calculations are based on the random phase and rotating wave approximation.

Further we use correlation corrected energy levels computed in the framework of the Pariser-Parr-Pople (PPP)

Hamiltonian. The geometries of the chains as function of time have been taken from simulations within the Su-

Schrieffer-Heeger (SSH) model. The spectra obtained for many time steps within a simulation are subsequently

superimposed and averaged. The Su-Schrieffer-Heeger model was chosen for the simulation because it is often

stated, that this one-particle model is based on renormalized parameters which essentially contain already the

effects of electron-electron interactions. Further at least for charged solitons the theory gives quite correct

soliton widths as compared to Pariser-Parr-Pople calculations. Thus the present study is also aimed as a first

step to investigate whether the SSH model is really able to yield reliable geometries in time simulations. We

found that our spectra reproduce the experimentally known peaks of the solitons and band to band excitations

well within an uncertainty of 0.3 – 0.5 eV. Further, the ratio of intensities of the two peaks as obtained in our

calculations agrees quite well with the corresponding experimental ones. The remaining small error in

intensities should be due to our use of transition dipole moments calculated from HF orbitals. Chain length

might play a role in the appearance of several minima and maxima of the absorption which are not present in

the experimental spectra. These different effects are currently under further study.