Molecular Crystals and Liquid Crystals
Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/gmcl16

# Electron Localization in Polyacetylene

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Version of record first published: 17 Oct 2011.

To cite this article: Bogdan R. Bulka & JÓZef Barnaś (1985): Electron Localization in Polyacetylene, Molecular Crystals and Liquid Crystals, 117:1, 201-204

To link to this article: http://dx.doi.org/10.1080/00268948508074624

*Mol. Cryst. Liq. Cryst.* 1985, Vol. 117, pp. 201-204
0026-8941/85/1174-0201/$10.00/0

Printed in the United States of America

# ELECTRON LOCALIZATION IN POLYACETYLENE

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Abstract Electron localization in the presence of disorder and solitons in a one-dimensional tight-binding model of polyacetylene is analysed.

## INTRODUCTION

Transport properties of such materials as polyacetylene, with a partially ordered quasi-one-dimensional structure and localized electron states, are governed mainly by two parameters: the density of states (DOS) and the localization length, $\lambda$, near the Fermi energy. The aim of this work is to analyse these quantities.

## DESCRIPTION OF THE MODEL

A one-dimensional system described by the Hamiltonian

$$H = \sum_i t_{i,i+1}\, a^+_{i+1}\, a_i + \sum_i V_i\, a^+_i\, a_i$$

is considered. Hopping integrals are $t_{i,i+1} = t_0 + \alpha(u_{i+1}-u_i)$, there $u_i$ is the displacement of the atom from its equilibrium. The second term of the Hamiltonian describes a disorder in the system. DOS and $\lambda$ are determined directly from the Schrödinger equation.

## AMORPHOUS SYSTEM WITHOUT SOLITONS

For a perfectly dimerized chain (i.e. the gap is 1.8 eV and the bandwidth -12 eV) and a rectangular distribution of site energies $|V_i| \leq W/2$, the Schrödinger equation is averaged and the localization length is analytically determined. Fig. 1 shows $\lambda$ and DOS calculated numerically for the $10^5$ atom system.

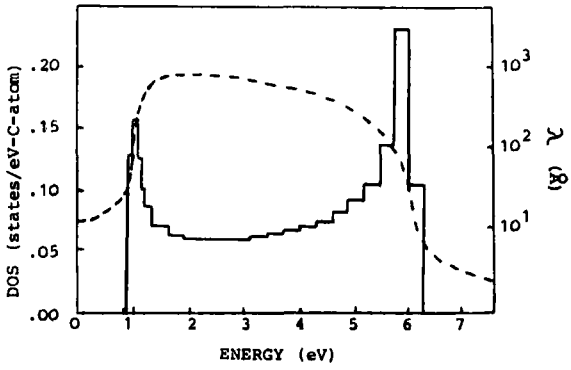


FIGURE 1 DOS and (dashed line) of the dimerized system with the site disorder W = 0.9 eV

## RANDOM DISTRIBUTED SOLITONS WITHOUT INTERACTIONS

In this case, $V_i = 0$ and a random distribution of solitons is assumed. Displacements of atoms arround the soliton center $x_n$ are $u_i = u_0(-1)^i \text{ th } \left(\frac{i-x_n}{l}\right)^1$, where the soliton width is $l = 7$. For a finite concentration of solitons, $y \neq 0$, the state at $E = 0$ is delocalized. The numerically determined $\lambda$ has the following energy dependence

$$\lambda(E) = \lambda_1 + A\, y \ln(1/E)$$

for small y. Here $\lambda_1 = [0.5 \ln(t_2/t_1)]^{-1} = 9.3$ Å is the localization length for a single soliton in the chain, and $A \simeq 43$. Fig. 2 presents DOS and $\lambda$ for the concentration of solitons y = 0.03 and y = 0.01. The soliton bandwidth is rather wide (above 1.4 eV), especially, in comparison with the bandwidth for the lattice of solitons, when it is 0.04 eV at y = 0.03 and $10^{-5}$ eV at y = 0.01.

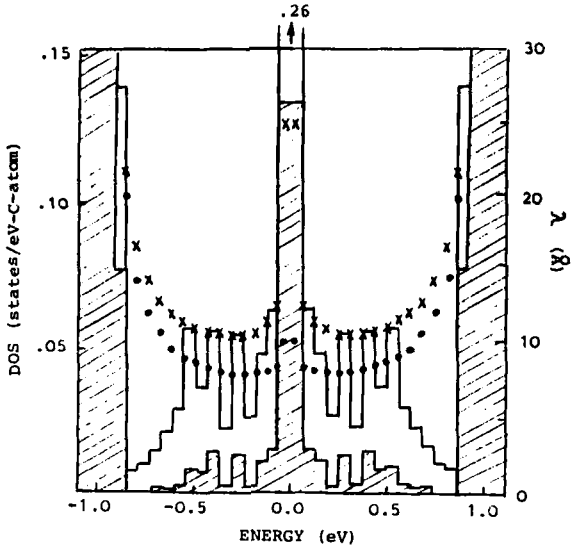


FIGURE 2 DOS and $\lambda$ calculated for the $10^5$ atom system with y=0.01 (shaded area and •) and y=0.03 (unshaded and x)

## SOLITONS INTERACTING WITH DOPANDS

Now, the Coulomb interaction between charges at dopands and in the chain, in the presence of charged solitons is considered. In the Hartree-Fock approximation the site energy is $V_c^{HF} = U_i \langle n_d \rangle$, where $\langle n_d \rangle$ is the average charge transfer and the Coulomb integral is taken $U_i = W \exp(-\gamma r_i)/r_i$. The electronic structure (presented in Fig. 3) is different for acceptor and donor doped system.

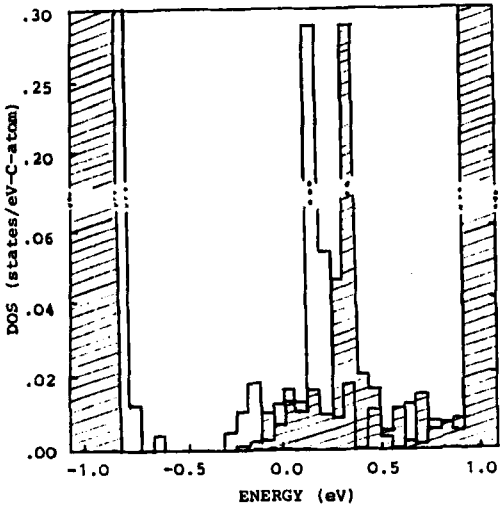


FIGURE 3 DOS of the system with charged solitons interacting with dopands: acceptors (shaded) and donors for y=0.01, W=2 eV, γ=2

## CONCLUSIONS

The system of randomly distributed solitons has very broad bandwidth. The localization length is larger than $\lambda_1 = 9.3$ Å and increases with the concentration. The different shift of the soliton band is predicted for acceptors and donors interacting with solitons.

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