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## Electron Localization in Polyacetylene

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## 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.

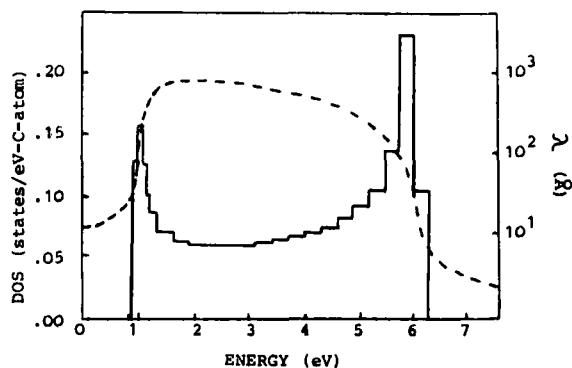


FIGURE 1 DOS and  $\lambda$  (dashed line) of the dimerized system with the site disorder  $W = 0.9$  eV

### RANDOM DISTRIBUTED SOLITONS WITHOUT INTERACTIONS

In this case,  $V_i = 0$  and a random distribution of solitons is assumed. Displacements of atoms around the soliton center  $x_n$  are  $u_i = u_0(-1)^i \text{th} \left( \frac{i-x_n}{l} \right)$ , 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  $\lambda_1 = [0.5 \ln(t_2/t_1)]^{-1} = 9.3 \text{ \AA}$  is the localization length for a single soliton in the chain, and  $A \approx 43$ . 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  $y = 0.01$ .

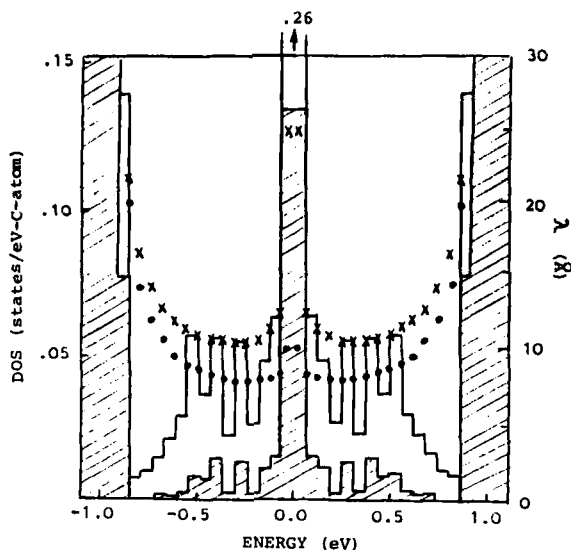


FIGURE 2 DOS and  $\lambda$  calculated for the  $10^5$  atom system with  $y=0.01$  (shaded area and  $\bullet$ ) and  $y=0.03$  (unshaded and  $\times$ )

### 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.

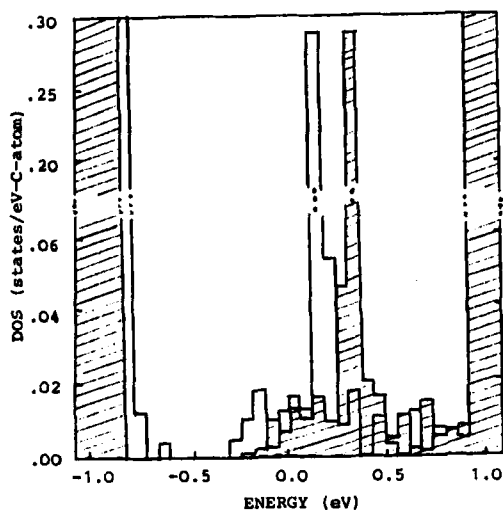


FIGURE 3 DOS of the system with charged solitons interacting with dopands: acceptors (shaded) and donors for  $y=0.01$ ,  $W=2$  eV,  $\gamma=2$

### CONCLUSIONS

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

### REFERENCES

1. W.P. Su, J.R. Schrieffer, and A.J. Heeger, Phys. Rev., **B 22**, 2099 (1980)

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