

# Dynamics of charge transfer in molecular switches

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## Abstract

With impurity molecules working as switches, the charge transfer on a single conducting polymer chain is studied. The chain is modeled by a modified tight-binding Hamiltonian extended to include the effects of an external field and the parameters of the switching molecules. The charge transfer through the sites that work like a switch is analyzed by the numerical integration of the equations of motion. Two basic types of molecular switches are studied: single and pairs of donor–acceptor molecules bonded to the chain. The main differences between these two models of switches are determined. We have found that the single radical switch has an anisotropic character and only works for solitons with the same parity of bonding site. For the donor–acceptor pair we have encountered that the chain offers a wider range of devices, from simple switches to perfect molecular rectifiers. The influence of the parameters of the molecules on the charge transfer and the changes they must undergo to characterize the molecular switch are obtained. The role of the length of separation between the sites where the donor and acceptor molecules bond is clarified. The optimum switch configuration is determined.

*Keywords:* Switches; Charge transfer

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## 1. Introduction

Molecular electronics is emerging as a promising field of research and a powerful source of technology [1–6]. The manipulation of single molecules opens the possibility of creation of a wide range of functional devices that mimic the solid-state ones, and may also have other new and important characteristics and functions. The fabrication of molecular electronic devices is not so far in the future and we can already foresee and even design various special molecules [7,8].

Conducting polymers are a fundamental part of molecular devices. They can work as molecular level wires linking and carrying charge through the molecular circuit [9]. In this sense, polyacetylene has appeared early as a good candidate to integrate molecular switches. One of its particular ways of conducting charges, through bond order solitons [10,11], seemed an interesting quality that could be used to create molecular switches. Impurities and doping radicals can work as pinning centers and barriers to the solitons. Bistable impurities can also work as switches allowing or denying the passage of moving charged solitons through a certain region of the chain [12].

These molecular devices have been studied with several methods. From tight-binding to *ab initio* methods, many

authors have revealed important characteristics and features of such devices [12,13]. Nevertheless, there has been a relative lack of dynamical simulations [14–17], even though there is a very strong link between the electronic part and the moving bond order configurations of polyacetylene.

The main purpose of the present work is to establish the basic character of radicals that must be bonded to a polyacetylene chain to create molecular switches. Doping molecules are introduced as a means of altering the polymer conduction properties, controlling the charge transfer throughout the chain. The determination of an optimum molecular switch, by varying the parameters of the doping molecules, is accomplished. The dynamics of charged solitons propagating on the polyacetylene chain is studied through numerical solution of the equations of motion for the electronic and lattice degrees of freedom of the system. The model Hamiltonian of Su, Schrieffer and Heeger (SSH) is modified to include an external electric field and short-ranged site-type impurity potentials to represent the radicals bonded to the main chain. We have found the ideal distance between pairs of donor–acceptor radicals bonded to the chain and the relative strength of the parameters of the radicals. Actually, we determine the possibility of a charged moving soliton to cross the region where the radicals are added. We verified that the solitons can pass, be trapped or reflect on this region, depending on the configuration of the radicals.

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This paper is organized as follows. In Section 2 we present the model and a brief description of the simulation method. Section 3 contains the results of the calculations. The last section, Section 4, is devoted to a summary and concluding remarks.

## 2. Model and formalism

We write the Hamiltonian describing the chain with impurities as

$$\mathcal{H} = - \sum_{n,s} (t_{n,n+1} C_{n+1,s}^\dagger C_{n,s} + \text{h.c.}) + \sum_n \frac{K}{2} (u_{n+1} - u_n)^2 + \sum_n \frac{M}{2} \dot{u}_n^2 + \sum_{p,s} V_p (C_{p,s}^\dagger C_{p,s}) \quad (1)$$

with

$$t_{n,n+1} = \exp(-i\gamma A) [t_0 - \alpha(u_{n+1} - u_n)] \quad (2)$$

Here,  $\mathcal{H}$  is an SSH-type Hamiltonian [11], modified to include the electric field and the impurities parameters.  $C_{n,s}$  is the annihilation operator of a  $\pi$  electron with spin  $s$  at the  $n$ th lattice site,  $u_n$  is the displacement coordinate of the  $n$ th CH group,  $t_0$  is the transfer integral between the nearest neighbor sites in the undimerized chains,  $\alpha$  is the electron–phonon coupling,  $M$  is the mass of a CH group,  $K$  is the spring constant of a  $\sigma$ -bond, and  $V_p$  is the strength of an impurity which is located in the  $p$ th site.  $\gamma = ea/(\hbar c)$ ,  $e$  being the absolute value of the electronic charge,  $a$  the lattice constant, and  $c$  the light velocity. The relation between the time-dependent vector potential  $A$  and the uniform electric field  $E$  is given by  $E = (-1/c)\dot{A}$ .

We prepare initially a stationary state, which is fully self-consistent with respect to both degrees of freedom, of the electrons and phonons, as the initial conditions of the calculations [18]. Then, under the action of the electric field, the electronic and the lattice equations of motion are numerically integrated. Namely, this is the time-dependent Schrödinger equation:

$$i\hbar \dot{\Psi}_{k,s}(n,t) = -t_{n,n+1} \Psi_{k,s}(n+1,t) - t_{n-1,n}^* \Psi_{k,s}(n-1,t) + V\delta_{n,p} \Psi_{k,s}(p,t) \quad (3)$$

and the lattice equation of motion:

$$M\ddot{u}_n = F_n(t) \quad (4)$$

where

$$F_n(t) = -K[2u_n(t) - u_{n+1}(t) - u_{n-1}(t)] + \alpha[\exp(-i\gamma A(t))(B_{n,n+1} - B_{n-1,n}) + \exp(+i\gamma A(t))(B_{n+1,n} - B_{n,n-1})] \quad (5)$$

Here  $B_{n,n'} \equiv \sum'_{k,s} \Psi_{k,s}^*(n,t) \Psi_{k,s}(n',t)$ . The prime on the summation means that the sum is taken over the occupied states in the initial stationary state. These equations of motion are

solved by discretizing the time variable with a step  $\Delta t$ . The time step  $\Delta t$  is chosen so that the change of  $u_n(t)$  and  $A(t)$  during this interval is always very small in the electronic scale. The time-dependent Schrödinger equation is analytically integrated by introducing single-electron eigenstates at each moment.

The solution of the time-dependent Schrödinger equation can then be put in the form:

$$\Psi_{k,s}(n,t_{j+1}) = \sum_l \left[ \sum_m \phi_{l,s}^*(m,t_j) \Psi_{k,s}(m,t_j) \right] \times \exp\left(-i\frac{\epsilon_l \Delta t}{\hbar}\right) \phi_{l,s}(n,t_j) \quad (6)$$

where  $\{\phi_l\}$  and  $\{\epsilon_l\}$  are the eigenfunctions and the eigenvalues of the electronic part of the Hamiltonian  $\mathcal{H}(t)$  at a given time  $t_j$ .

The lattice equations are written as

$$u_n(t_{j+1}) = u_n(t_j) + \dot{u}_n(t_j) \Delta t \quad (7)$$

$$\dot{u}_n(t_{j+1}) = \dot{u}_n(t_j) + \frac{F(t_j)}{M} \Delta t \quad (8)$$

Therefore, using Eqs. (6)–(8), the electronic wave functions and the displacement coordinates at the  $(j+1)$ th time step are obtained from the  $j$ th time step.

We use as parameters the commonly accepted values for polyacetylene:  $t_0 = 2.5$  eV,  $K = 21$  eV  $\text{\AA}^{-2}$ ,  $\alpha = 4.1$  eV  $\text{\AA}^{-1}$ , and  $a = 1.22$   $\text{\AA}$ , and for the impurity potentials we take  $V_p$  ranging from  $10^{-3}$  to  $1t_0$ . Periodic boundary conditions are assumed for the electronic wave functions,  $\Psi_{k,s}$ , and the lattice displacements,  $u_n$ .

In this study, the total number of lattice points on the chain is  $N = 101$ , thus allowing the presence of a soliton on the chain. The total number of electrons on the chain ( $Ne$ ) is  $Ne = 100$  in all cases, which means that in the initial condition we have a positively charged soliton on the chain.

The soliton charge is given by the expression:

$$\rho(n,t) = 1 - \sum_{k,s} \psi_{k,s}^*(n,t) \psi_{k,s}(n,t) \quad (9)$$

To study the position of the soliton as a function of time, we introduce smoothed charge density and bond variable by

$$\bar{\rho}_n = \frac{1}{4}(\rho_{n-1} + 2\rho_n + \rho_{n+1})$$

$$\bar{y}_n = \frac{(-1)^n}{4}(y_{n-1} - 2y_n + y_{n+1})$$

with  $y_n \equiv u_{n+1} - u_n$ . When there is a single soliton,  $\bar{y}_n$  has a tanh-like form. Thus, its difference  $\bar{y}_{n+1} - \bar{y}_n$  has a sech-like form. Since we consider the periodic system in the present simulation, it is convenient to define the soliton position by [16]

$$x(t) = \frac{Na}{2\pi} \arg \left\{ \sum_{n=1}^N \exp \left[ \frac{(2n+1)\pi i}{N} \right] (\bar{y}_{n+1} - \bar{y}_n) \right\} \quad (10)$$

We observe the position at every 100 time steps. A time step of  $\Delta t = 0.04$  fs is used. We follow the dynamics of the systems up to the 5000th time step. Each of these simulations take 2 h of CPU time on a DEC Alpha-400 workstation.

### 3. Simulation results

In all the 220 simulations, we have considered polyacetylene chains with  $N = 101$  CH groups. One single positively charged soliton is initially present around the 20th site. One or two different radical molecules are bonded to different positions on the chain in each case. Fig. 1 shows very schematically the initial configuration of the polymer chain.

As the initial state in all cases represents a stationary solution, we make the charged solitons start to move through the application of the electric field on the system. The electric field is applied from  $t = 0$  to  $t = t_{\text{off}}$ , a time span necessary for the charged soliton to acquire a velocity close to its maximum possible value [16]. To do that, we put  $A = -cEt$  from  $t = 0$  up to  $t = t_{\text{off}}$ , and then, for times greater than  $t_{\text{off}}$ , we set  $A = -cEt_{\text{off}}$ . We take  $t_{\text{off}} = 60$  fs and  $|E| = 0.025E_0$ , with  $E_0 = \hbar\omega_Q/(ea)$ . Therefore, the soliton is moving at a constant velocity when it reaches the switching sites.

The solitons of polyacetylene have the very interesting property of accumulating charge around the topological defect of the bond order pattern only on even or odd sites (see Fig. 2). This soliton character has important consequences on the switching mechanism. In this work we call solitons that accumulate charge on even (odd) numbered sites as 'even (odd) solitons'.

Besides the parity of the soliton (charge on even or odd sites), the position on the chain where the radicals bond and the consequent alteration of the CH unit site energy play a fundamental role on the switching process. Therefore, we systematically change the bonding sites and the radical parameters. For each configuration we have made the moving charged soliton go through the chain.

Subtle changes on the radical bond positions have proved to lead to very different results. Fig. 3 shows three cases where the same pair of donor–acceptor radicals are bonded to sites close to each other. Fig. 3(a) shows the propagation of a free soliton for comparison. In Fig. 3(b) the donor and acceptor radicals are bonded to sites 53 and 51, respectively. The soliton passes by these sites almost like the free soliton case. Fig. 3(c) shows the same pair of donor–acceptor radicals bonded at sites 52 and 53, respectively. In this case the soliton is trapped by the pair of impurities. In Fig. 3(d) the

donor–acceptor pair is bonded to sites 53 and 52, respectively. A complete reflection of the moving soliton happens for this configuration. Therefore, the order of appearance of the donor and acceptor radicals in the soliton path as well as the parity (even or odd) of the sites where they bond, is fundamental for the charge propagation on the chain. The charged soliton can move forward, be trapped or reflect on the switching sites depending on their arrangement and the parity of the soliton. As will be seen with other cases, the pair of radicals can even work as a rectifier, allowing the passage of the soliton in one direction and blocking it in the opposite one (an inverse behavior is observed changing the parity of the soliton).

We have also performed simulations with one single radical working as a switch. This type of switch has an anisotropic effect on the soliton motion. A single-molecule switch can only be felt by solitons with the same parity as the radical bonding site. Fig. 4 presents the soliton position after it interacts with the switching site. It is verified that the odd moving soliton interacts only with the odd radical sites, being completely indifferent to a radical bonding at an even site. When a reflection occurs, it is found that the positively charged soliton is more reflected on the donor radical than on the acceptor radical. The opposite holds for the negatively charged soliton. This apparently paradoxical behavior takes place because the soliton actually interacts with the charge shielding the radical. The shielding charge concentrates principally on sites with the same parity as the radical site.

Fig. 5 presents the time evolution of odd solitons moving in the direction of a pair radical switches. In Fig. 5(a), we kept fixed the radical intensities  $|V_p| = 7.5 \times 10^{-2}t_0$  and the acceptor bonding site at the 51st site. We varied the donor bonding site from 53 to 61. The soliton behavior changes from passage to reflection as we increase the radical separation. For a given separation, the acceptor radical at the 51st site and the donor radical at the 57th site, we have varied the modulus of the radical parameter,  $|V_p|$ , from  $2.5 \times 10^{-2}$  to  $15 \times 10^{-2}t_0$  (Fig. 5(b)). It is observed that for a low intensity the soliton passes the switching radicals. For a greater intensity it is reflected. For an even greater intensity

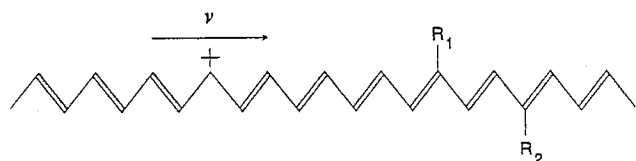


Fig. 1. Schematic representation of a moving charged soliton on polyacetylene and the bonding radicals that could work as a switch.

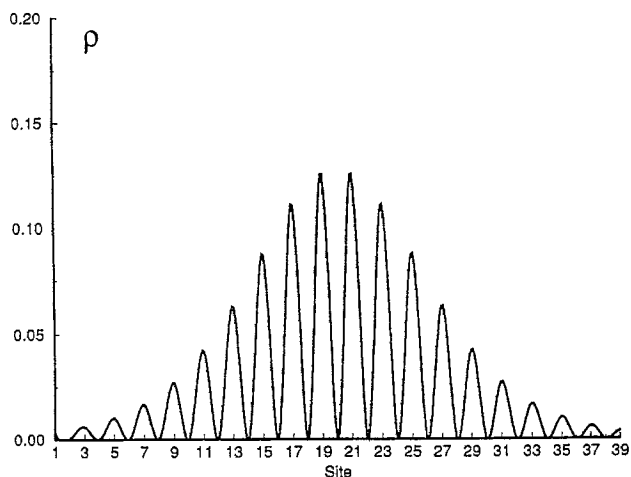


Fig. 2. The charge distribution,  $\rho(n)$ , of an odd soliton.

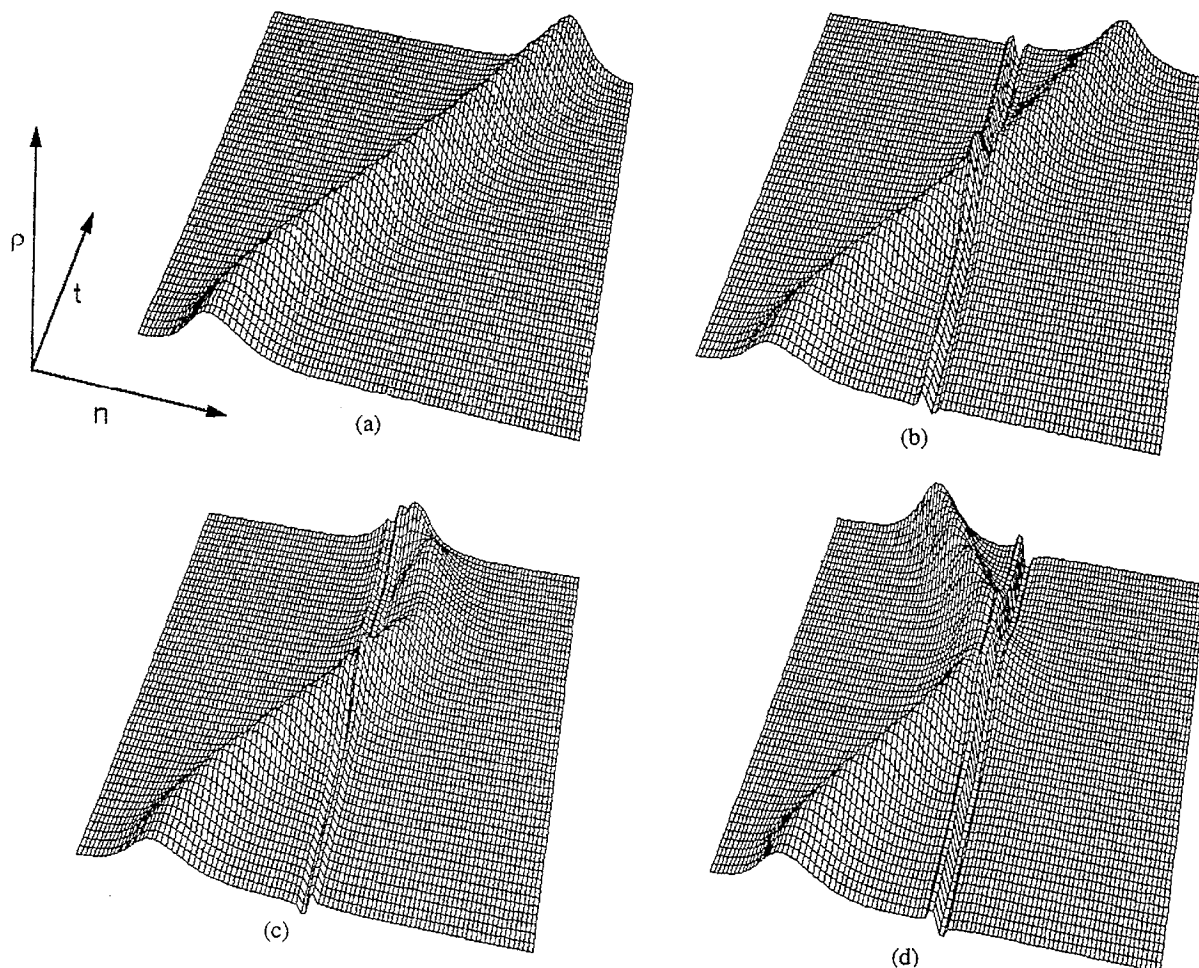


Fig. 3. Time evolution of the smoothed charge density,  $\bar{\rho}(t)$ , in the polyacetylene chain. The three axes represent the site  $n$ , time  $t$ , and smoothed charge density  $\bar{\rho}$ . (a) Free soliton (no radicals bonded to the chain); (b) donor radical on site 53 and acceptor on site 51; (c) donor radical on site 52 and acceptor on site 53; (d) donor radical on site 53 and acceptor on site 52.  $|V_p| = 0.1t_0$ .

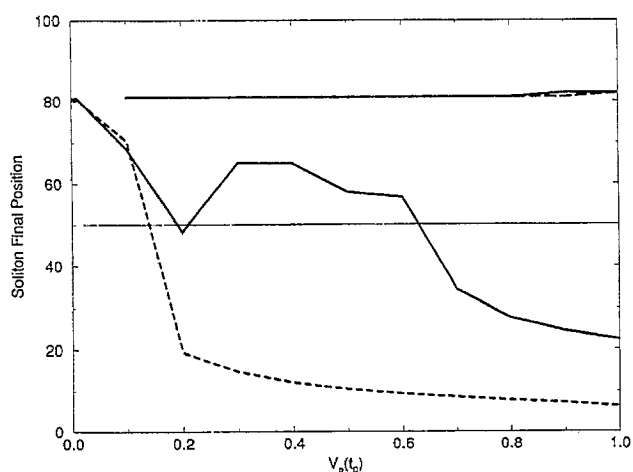


Fig. 4. Positively charged odd soliton propagation in a chain with a single radical (donor or acceptor) bonded to it. Final soliton position as a function of the radical intensity: (—), acceptor radical on odd site; (---), donor radical on odd site; (— — —), acceptor on even site; (·····), donor on even site.

( $|V_p| = 1.5 \times 10^{-1}$ ) the soliton gets trapped by the impurity. That is the overall pattern observed in the extensive studied cases: as the radical intensity gets bigger than a given threshold the soliton becomes trapped by the switch.

We have verified that the parity of the soliton and the parity of the radicals (bonded to even or odd sites) is decisive on the mechanism of charge transport on polyacetylene-based molecular circuits. In Fig. 6 we present the outcome of a positively charged odd soliton colliding with the same pair of donor–acceptor radicals bonded to different site positions. In Fig. 6(a) we fixed the acceptor bond site in the 51st site and kept the radical intensity at  $|V_p| = 0.1t_0$ . The donor bonding site is varied from the 41st to the 61st site. We can distinguish two different patterns. When the donor radical bonds at even sites the soliton passes through the switch. For the donor radical bonding at odd sites, the order of appearance and the distance between the radicals lead to passage or reflection (and trapping for large radical intensities). In Fig. 6(b) the acceptor radical is bonded at the 52nd site, and the donor

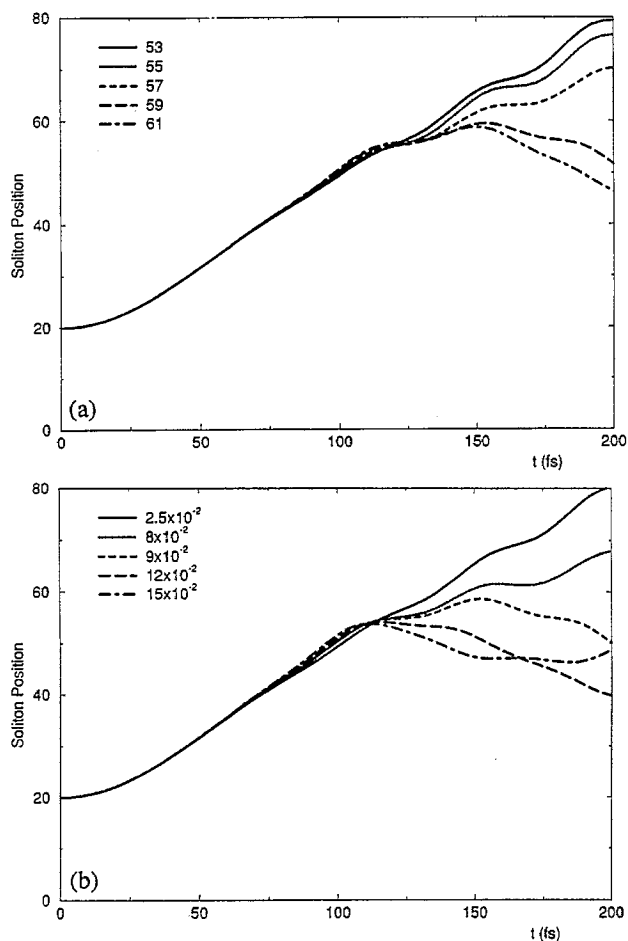


Fig. 5. Time evolution of a positively charged odd soliton moving on a polyacetylene chain with a pair of radicals bonded to it. (a) The intensity of the radicals are fixed ( $|V_p| = 7.5 \times 10^{-2} t_0$ ) and the acceptor bonding site is fixed at the 51st site. The donor bonding site is varied from the 53rd to the 61st site. (b) The position of the acceptor bonding site is kept at the 57th site. The radical strength is varied from  $2.5 \times 10^{-2}$  to  $15 \times 10^{-2} t_0$ .

radical bond site varies from the 42nd to the 62nd site. The donor radical bonding at even sites allows the soliton passage. When it bonds to odd sites the soliton also passes the switch, except in one case: acceptor on site 52 and donor on site 53, in which case the soliton is reflected. Fig. 6(a) and (b) may look redundant, but they are not. The order of appearance, in the soliton path, of donor and acceptor radicals as well as the parity of the radical bonding sites is distinctive. One may have donor–acceptor as well as acceptor–donor pairs. And they may bond at odd–odd, odd–even, even–odd, and even–even numbered sites. This parity distribution is due to the parity of the soliton itself. Tables 1–4 display several examples belonging to all eight parity-order classes.

From Tables 1–4 one can devise a phase diagram as depicted in Fig. 7. In this impurity separation versus impurity intensity graphic one can distinguish two lines separating three different charge conducting phases. Each line separates radical configurations allowing or blocking (reflecting or trapping) the soliton passage. The descent line is characteristic of solitons that reach the first radical site with the same

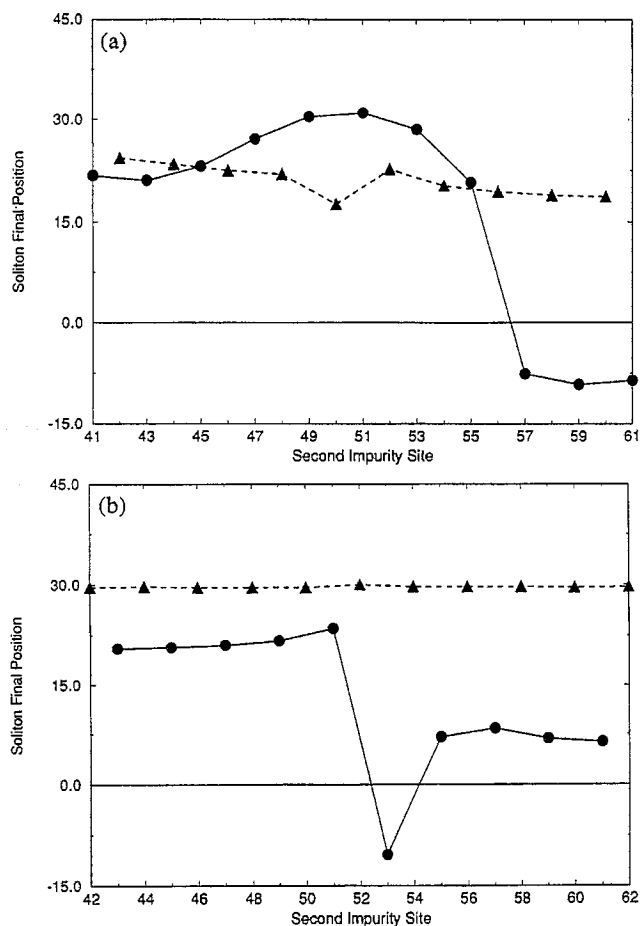


Fig. 6. Final soliton (odd and positively charged) position, relative to the bonding sites of the radicals. (a) Acceptor radical on the 51st site and donor radical varying from the 41st to the 61st site. (b) Acceptor radical on the 52nd site and donor radical varying from the 42nd to the 62nd site.  $|V_p| = 0.1 t_0$ .

Table 1

Final soliton position as a function of the sites of the two impurities ( $n_1$  and  $n_2$ ). The first impurity is negative and it is bonded at an even site. The second impurity is positive. The two impurities have the same intensity modulus (Int)

$n_2$	Int		
	0.1	0.12	0.2
Even–even (first on 52th site and second on even site)			
54	81		81
56	81		81
58	81		81
60	81		81
62	81		81
Even–odd (first on 52th site and second on odd site)			
53	68	56	48
55	71	63	49
57	73	66	51
59	73	68	54
61	74	70	56

Table 2

Final soliton position as a function of the sites of the two impurities ( $n_1$  and  $n_2$ ). The first impurity is negative and it is bonded at an odd site. The second impurity is positive. The two impurities have the same intensity modulus (Int)

$n_2$	Int					
	0.1	0.12	0.15	0.17	0.2	1
Odd-even (first on 51st site and second on even site)						
52	74	<b>67</b>	<b><u>26</u></b>		<b><u>21</u></b>	
54	72	<b>39</b>	<b><u>25</u></b>		<b><u>20</u></b>	
56	71	<b>36</b>	<b><u>25</u></b>		<b><u>20</u></b>	
58	71	<b>35</b>	<b><u>24</u></b>		<b><u>20</u></b>	
60	71	<b>34</b>	<b><u>24</u></b>		<b><u>19</u></b>	
Odd-odd (first on 51st site and second on odd site)						
53	80		80	79	78	<b><u>49</u></b>
55	77		72	69	63	<b><u>57</u></b>
57	73		64	59	55	
59	71		63	62	65	
61	72		69	<b>34</b>	<b>24</b>	

parity as the soliton parity. The rising line represents the cases where the soliton meets the first radical bonded at a site with different parity from its own. Therefore, there exist three different phases: Phase I contains configurations allowing the soliton passage isotropically (solitons can propagate to the left or to the right on the chain). Phase II represents anisotropic configurations where the solitons can pass in one direction but not in the opposite one. In Phase III all the solitons reaching the switch are blocked. Actually, the two lines appearing in Fig. 7 each represent four lines. For each parity-order configuration the phase diagram lines present different slopes (not shown in the figure).

The total energy, i.e. the sum of the electronic, lattice kinetic and lattice potential energy, increases rapidly during the application of the electric field, as should be expected. After the field is switched off, the total energy becomes constant. A small variation of the total energy is observed over the time; it is thought to come from the discretization of the time variable. Since this variation is small enough (smaller than 0.0001%), it is verified that the mesh adopted for the time variable is quite good.

#### 4. Discussion and summary

The propagation of a moving charged soliton on a single polyacetylene chain, where radical molecules bonded to the chain work as a switch, has been investigated. This study was carried out through numerical calculations using an improved version of the SSH model to accomplish the characteristics of the actual system. We have used an electric field to put a charged soliton in motion. The electric field is introduced in the model Hamiltonian as a time-dependent vector potential in the phase of the transfer integral. The time-dependent

Table 3

Final soliton position as a function of the sites of the two impurities ( $n_1$  and  $n_2$ ). The first impurity is positive and it is bonded at an even site. The second impurity is negative. The two impurities have the same intensity modulus (Int)

$n_2$	Int		
	0.1	0.12	0.2
Even-even (first on 52nd site and second on even site)			
54	81		81
56	81		81
58	81		81
60	81		81
62	81		81
Even-odd (first on 52nd site and second on odd site)			
53	<b>41</b>	<b>33</b>	<b>30</b>
55	58	<b>39</b>	<b><u>35</u></b>
57	59	<b>43</b>	<b><u>39</u></b>
59	58	<b>46</b>	<b><u>43</u></b>
61	57	<b>50</b>	<b><u>46</u></b>

Schrödinger equation and the equation of motion for the time-dependent lattice displacements form a coupled set that was numerically integrated over the time in a self-consistent way.

The switching molecules are modeled by the change they cause in the energy of the polyacetylene site where they bond.

The soliton passage, reflection or trapping on the switch is investigated for a large amount of configurations of the bonding molecules. Changes in the bonding site positions and site energies are carried out and the characteristics of the various switches are analyzed. An initially static charged soliton is accelerated through the application of an electric field until it reaches a velocity close to its maximum possible velocity. Then the electric field is switched off and the soliton continues to move until it reaches the switching region.

We have verified that the molecular switches on polyacetylene are very sensitive to the parity of the charged soliton and consequently to the parity of the radical bonding sites. The same pair of donor-acceptor bonding radicals can be transparent or an insurmountable obstacle to a given soliton. The passage depends on the parity of the sites where the radicals bond, the order of appearance, the parity of the soliton and its charge sign.

As a consequence of the parity-charge sign dependence, we have found very anisotropic switches. They allow the passage of a given soliton in one direction and block it in the opposite one. There have been switches that allow the passage of solitons of odd parity and block even parity solitons, and vice versa. All these switch types are illustrated in Tables 1–4. Anisotropic switches are in bold face. Switches that block the soliton passage in both directions are in bold face and underlined. Therefore, optimum molecular switches can be devised using the convenient radical configurations.

We have been using solitons moving close to their maximum velocity. If one allows the solitons to move with smaller

Table 4  
Final soliton position as a function of the sites of the two impurities ( $n_1$  and  $n_2$ ). The first impurity is positive and it is bonded at an odd site. The second impurity is negative. The two impurities have the same intensity modulus (Int)

$n_2$	Int ( $10^{-2}$ )													
	2.5	5	6	7	7.5	8	9	10	11	12	14	15	20	100
Odd-even (first on 51st site and second on even site)														
52								73		67	59	54	<u>50</u>	
54								70		63	<b>51</b>	<b>48</b>	<u>48</u>	
56								69		60	<b>49</b>	<b>47</b>	<u>48</u>	
58								69		59	<b>48</b>	<b>47</b>	<u>48</u>	
60								69		59	<b>49</b>	<b>47</b>	<u>48</u>	
Odd-odd (first on 51st site and second on odd site)														
53	80	80	80	80	79	79	79	79	78	77		75	67	<u>55</u>
55	80	79	79	77	77	76	74	71	68	56		<b>38</b>	<b>50</b>	<u>58</u>
57	80	78	75	72	70	68	<b>50</b>	<b>42</b>	<b>40</b>	<b>40</b>		<b>49</b>	<b>49</b>	
59	80	75	71	64	<b>52</b>	<b>46</b>	<b>42</b>	<b>41</b>	<b>41</b>	<b>43</b>		<b>51</b>		
61	79	73	67	<b>50</b>	<b>46</b>	<b>45</b>	<b>43</b>	<b>41</b>	<b>41</b>	<b>43</b>		<b>51</b>		

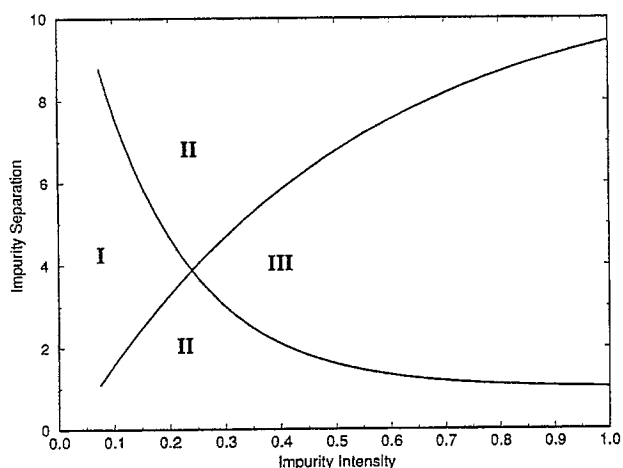


Fig. 7. Charge conduction phase diagrams for a polyacetylene chain with a pair (donor-acceptor) of radicals. Phase I, configurations that allow the passage of a soliton. Phase II, configurations that block the soliton in one direction but allow its passage in the opposite direction. Phase III, configurations that block (reflect or trap) the soliton moving in either direction.

velocities, it can obviously change the passage, reflection and trapping patterns. As the soliton velocity slows down, the passage through a switch becomes increasingly difficult.

Our results are certainly dependent on the numerical parameters used for the SSH model. Changes in these parameters do change the physical parameters of solitons, e.g. the soliton length. Solitons of different length have a different interaction with a donor-acceptor pair of a given length of separation. For example, a wide soliton interacting with the donor-acceptor pair at a given distance will correspond to a narrow soliton interacting with the same pair separated by a shorter distance. Thus, we expect a shift of the lines separating the propagating phases in Fig. 7.

A single bonding impurity can work as a switch. Nevertheless, solitons with parity different from the impurity bond-

ing site are very insensitive to it. Moreover, this single-radical switch is anisotropic. The shielding caused by the impurity is asymmetric because of the single-double bond pattern of the polyacetylene chain. Hence, after encountering the switch the soliton has a different velocity depending on the former's original direction.

We have seen that radical molecules bonded to the polyacetylene chain can work as molecular switches. It is not necessary to add impurity molecules to the chain backbone. However, the addition of impurities to the body of the polymer chain could bring interesting new features to the switches.

The present model does not consider any change in the pattern of single-double bonds on the polyacetylene chain prior to the soliton passage. The bonding radicals did not alter this pattern between their bonding sites. Therefore, the structural change in the single-double configuration between the radicals is not indispensable to the switching function.

The inclusion of impurities on the chain backbone and the influence of several switches on the soliton pathway are currently being studied and results concerning molecular circuits will be presented in a forthcoming paper.

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## References

- [1] R.A. English, Z.L. Miskovic, S.G. Davidsson and F.O. Goodman, *Phys. Rev. B*, **54** (1996) 10.
- [2] Z.L. Miskovic, R.A. English, S.G. Davidsson and F.O. Goodman, *Phys. Rev. B*, **54** (1996) 255.

- [3] F.L. Carter (ed.), *Molecular Electronic Devices*, Marcel Dekker, New York, 1982.
- [4] C. Nicolini, M. Adami, F. Antolini, F. Beltran, M. Sartore and S. Vakula, *Phys. World*, 5 (1992) 30.
- [5] M. Pomerantz, in P.C. Pedersen and B. Onaral (eds.), *Proc. Ann. Int. Conf. IEEE Engineering in Medicine and Biology Society*, Vol. 12, Institute of Electrical and Electronics Engineers, Inc., Washington, DC, 1990, p. 1687.
- [6] A. Aviram, in F.A. Spelman and Y. Kim (eds.), *Proc. Ann. Int. Conf. IEEE Engineering in Medicine and Biology Society*, Vol. 11, Institute of Electrical and Electronics Engineers, Inc., Washington, DC, 1989, p. 1385.
- [7] J.S. Foster, J.E. Frommer and P.C. Arnett, *Nature*, 331 (1988) 324.
- [8] S. Hameroff, C. Schneiker, M. Voelker, J. He, E. Dereniak and R. McCuskey, in G. Harris and C. Walker (eds.), *Proc. Ann. Int. Conf. IEEE Engineering in Medicine and Biology Society*, Vol. 10, Institute of Electrical and Electronics Engineers, Inc., Washington, DC, 1980, p. 1009.
- [9] A.G. MacDiarmid and A.J. Epstein, in F.A. Spelman and Y. Kim (eds.), *Proc. Ann. Int. Conf. IEEE Engineering in Medicine and Biology Society*, Vol. 11, Institute of Electrical and Electronics Engineers, Inc., Washington, DC, 1989, p. 1299.
- [10] W.P. Su, J.R. Schrieffer and A.J. Heeger, *Phys. Rev. B*, 22 (1980) 2099; 28 (1983) 1138.
- [11] W.P. Su, J.R. Schrieffer and A.J. Heeger, *Proc. Natl. Acad. Sci. USA*, 77 (1980) 5626; W.P. Su, J.R. Schrieffer and A.J. Heeger, *Phys. Rev. B*, 46 (1981) 738.
- [12] R.A. English and S.G. Davidson, *Phys. Rev. B*, 49 (1994) 8718.
- [13] K. Tanaka, S. Yamanaka, T. Koike and T. Yamabe, *Phys. Rev. B*, 32 (1985) 2731.
- [14] A.R. Bishop, D.K. Campbell, P.S. Lomdahl, B. Horovitz and S.R. Phillpot, *Phys. Rev. Lett.*, 52 (1984) 671; A.R. Bishop, D.K. Campbell, P.S. Lomdahl, B. Horovitz and S.R. Phillpot, *Synth. Met.*, 9 (1984) 223.
- [15] G. Magela e Silva and A. Terai, *Phys. Rev. B*, 47 (1993) 12 568.
- [16] Y. Ono and A. Terai, *J. Phys. Soc. Jpn.*, 59 (1990) 2893.
- [17] A. Terai and Y. Ono, *J. Phys. Soc. Jpn.*, 60 (1991) 196.
- [18] A. Terai and Y. Ono, *J. Phys. Soc. Jpn.*, 55 (1986) 213.