



Influence of soliton distributions on the spin-dependent electronic transport through polyacetylene molecule

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Abstract. In this paper, a detailed numerical study of the role of selected soliton distributions on the spin-dependent transport through *trans*-polyacetylene (PA) molecule is presented. The molecule is attached symmetrically to magnetic semi-infinite three-dimensional electrodes. Based on Su–Schrieffer–Heeger (SSH) Hamiltonian and using a generalized Green’s function formalism, we calculate the spin-dependent currents, the electronic transmission and tunnelling magnetoresistance (TMR). We found that the presence of a uniform distribution of the soliton centres along the molecular chain reduced the size of the band gap of *trans*-PA molecule. Moreover, a sublattice of the correlated solitons as binary clusters, which are randomly distributed along the chain, can induce extended electronic states in the band gap of the molecule. In this case, the band gap of the molecule is suppressed and at lower voltages, the TMR bandwidth is narrowed. The current–voltage characteristic then shows an ohmic-like behaviour.

Keywords. Polyacetylene; soliton; spin-dependent current; tunnelling magnetoresistance.

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1. Introduction

In a typical spin-valve geometry, a non-magnetic spacer, which controls the total resistance of the device and hence the spin polarization and transport, is sandwiched between two magnetic contacts. Among many suggestions for possible non-magnetic spacers, organic materials with low fabrication costs and high manufacturability have attracted investigations [1–5]. In general, organic materials have relatively weak spin-orbit and hyperfine interactions, so that spin memory can only be as long as a few seconds [6]. Therefore, spin-flip process during transport through the typical organic molecules can be neglected [3,7]. Such features make them ideal for the spin-polarized electron injection and transport applications in molecular spintronics. The spin-dependent transport through molecular junctions has attracted theoretical investigation [8–20]. Polyacetylene, an organic molecule, is a linear conducting polymer, based on which several molecular junctions

(magnetic and non-magnetic) are proposed [10,21–26]. In *trans*-PA there are two lowest-energy degenerate states, having two distinct bonding structures. This two-fold degeneracy leads to the existence of nonlinear topological excitations, bond-alternation domain walls or solitons, which appear to be responsible for many of the remarkable properties of *trans*-PA molecule [27]. Such topological excitations are produced during doping [28,29]. Solitons created by doping are spinless and carry a charge $\pm e$. It has been found that in the presence of a soliton, some electronic states are created in the middle of the molecular gap [30], and hence it is energetically favourable for the extra doped electrons to create a soliton lattice and occupy the midgap states rather than going into the conduction (valence) band. When *trans*-PA is doped to concentrations in excess of a critical concentration, the system undergoes a transition from the soliton lattice state to a metallic-like state [27]. There are a great number of works concerning the study of physical mechanisms behind the metallic-like transition in *trans*-PA [31–33]. The experimental investigations on the conduction properties of *trans*-PA support the idea that the correlated disorder in soliton arrangements is responsible for the metallic properties of *trans*-PA [34–38]. The occurrence of metallic regime, in the presence of disorder, in *trans*-PA chains is apparently unexpected, because, based on Anderson’s localization criteria, disorder induces electronic localized states in one-dimensional structures [39]. It has been proposed, however, that the existence of the extended electronic states in the structure of the band gap of the molecule occurs when there is a given concentration of the dopants in pairs with an internal structure that is symmetric about some planes [32,40]. In *trans*-PA, solitons do have this symmetry inherently and provide the necessary conditions. However, important factors are still there, whose influence on the electronic transport through *trans*-PA may be studied. In this work, we consider some correlated arrangements of solitons and show how these arrangements affect the spin-dependent currents, tunnelling magnetoresistance (TMR) and other related phenomena in the spin-dependent electronic transport. In our model, *trans*-PA molecule is attached symmetrically to two magnetic semi-infinite three-dimensional electrodes, as schematically depicted in figure 1. The well-known Su–Schrieffer–Heeger (SSH) Hamiltonian is used to describe the molecule and all the calculations are done using a generalized Green’s function formalism. Furthermore, the current–voltage characteristics are computed from the Landauer–Büttiker formalism. The model and description of the computational methods for investigating the spin-dependent transport properties of the model junction are introduced in §2. The results and discussion are presented in §3, followed by conclusion in §4.

2. Model and the computational scheme

We start by describing our model as shown in figure 1. The *trans*-PA molecule by which we are interested to explore several features of the spin-dependent transport phenomena in the presence of solitons, is attached to two ferromagnetic (FM) semi-infinite three-dimensional electrodes with simple cubic structure and square cross-section (x – y plane). This structure is shown schematically in figure 1. The middle panels in figures 1a and 1b illustrate the spin-dependent density of states (DoS) for *trans*-PA molecule in parallel (P) and antiparallel (AP) configurations, respectively. The surface DoS of the isolated FM

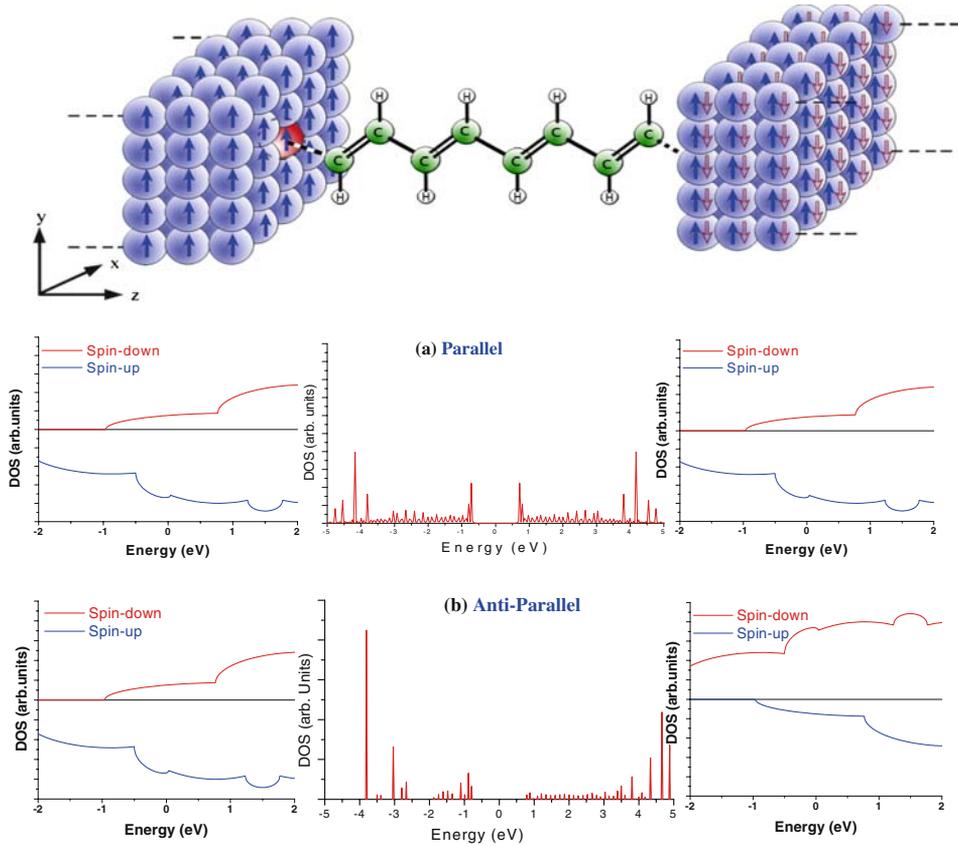


Figure 1. The plots showing a schematic representation of FM/*trans*-PA/FM model junction. As explained in the text, the left (right) contact is considered as a three-dimensional semi-infinite magnetic electrode, described by an effective self-energy Σ . The middle panels in (a) and in (b) illustrate the spin-dependent density of states (DoS) for *trans*-PA molecule with 100 carbon atoms in parallel (P) and antiparallel (AP) configurations, respectively. The surface DoS of the isolated FM electrodes is shown in the left and right panels in (a) for P and in (b) for AP configurations.

electrodes is shown in the left and right panels in figure 1a for P and in figure 1b for AP configurations.

As the electron conduction is mainly determined by the central part of the junction, the electronic structure of this part should be resolved in details. It is therefore reasonable to decompose the total Hamiltonian of the system as

$$H = H_L + H_m + H_c + H_R. \quad (1)$$

The Hamiltonian of the left (L) and right (R) electrodes are described within the single-band tight-binding approximation and are written as

$$H_\beta = \sum_{i_\beta, \sigma} (\varepsilon_0 - \vec{\sigma} \cdot \vec{h}_\beta) \hat{c}_{i_\beta, \sigma}^+ \hat{c}_{i_\beta, \sigma} - \sum_{\langle i_\beta, j_\beta \rangle, \sigma} t_{i_\beta, j_\beta} \hat{c}_{i_\beta, \sigma}^+ \hat{c}_{j_\beta, \sigma}, \quad (2)$$

where $\hat{c}_{i\beta,\sigma}^+$ ($\hat{c}_{i\beta,\sigma}$) creates (destroys) an electron with spin σ at site i in electrode β (L or R) and the hopping integrals $t_{i\beta,j\beta}$ are equal to t for the nearest neighbours and zero otherwise. Here, ε_0 is the spin-independent on-site energy and shall be set to $3t$ as a shift in energy. In addition, the term $-\vec{\sigma} \cdot \vec{h}_\beta$ is the internal exchange energy with h_β and σ denoting the molecular field at site i_β and the conventional Pauli spin operator, respectively. According to the well-known SSH model [29], the Hamiltonian of *trans*-PA molecule in the absence of FM electrodes is expressed as

$$H_m = \sum_{n,\sigma} \varepsilon_n b_{n,\sigma}^+ b_{n,\sigma} - \sum_{n,\sigma} (t_0 + \alpha y_n) (b_{n,\sigma}^+ b_{n+1,\sigma} + \text{h.c.}) + \frac{K_0}{2} \sum_n y_n^2, \quad (3)$$

where $\hat{b}_{n,\sigma}^+$ ($\hat{b}_{n,\sigma}$) and $\varepsilon_n = \varepsilon$ are the creation (annihilation) operator of an electron and the on-site energy of the π -electrons at the n th site with spin σ , respectively. Here reference energy is chosen such that the on-site energy is zero. With u_n , the displacement of the n th carbon atom from its equilibrium position, $y_n = (u_n - u_{n+1})$ is the bond alternation. According to SSH model, α is the electron–lattice weak coupling constant so that αy_n modulates the hopping integrals along the molecular symmetry axis. t_0 and K_0 are the hopping integrals of an undimerized molecule and the elastic constant, respectively. For perfectly dimerized molecule and in the weak coupling regime, u_n and the band gap of *trans*-PA molecule are given as $u_n = (-1)^n u_0$ and $2\Delta_0 = 1.4$ eV, respectively. Based on the SSH model hypotheses, we take $\alpha = 4.1$ eV/Å, $t_0 = 2.5$ eV and $K_0 = 21$ eV/Å. These correspond to the equilibrium dimerization amplitude $u_0 \approx 0.04$ Å. However, in the presence of distribution of solitons, the displacement u_n of the carbon atoms is modified with a factor which is a pattern of the soliton shape. Indeed, for a large chain, a soliton corresponds to a phonon field configuration that minimizes the total energy. In the presence of distribution of solitons, the displacement u_n of the carbon atoms in *trans*-PA is determined in such a way as to minimize the total energy of the molecule and to give optimum shape for the soliton. Accordingly, the displacements of the carbon atoms are modelled as [41,42],

$$u_n = (-1)^n u_0 \prod_m \tanh \left[\frac{(n-m)a}{\xi} \right], \quad (4)$$

where $2\xi \cong 14a$, with $a = 1.22$ Å (lattice constant), the width of a soliton, (ma) is the location of the m th soliton centre on the chain. Finally, H_c the molecule–FM electrode coupling Hamiltonian is described by

$$H_c = - \sum_{\substack{i,\sigma \in \beta \\ n,\sigma \in m,j}} t_{i,n,\sigma}^j (c_{i,\sigma,j}^+ b_{n,\sigma,j} + \text{h.c.}) \quad (5)$$

The matrix elements $t_{i,n,\sigma}^j$ represent the coupling strength between the π -orbitals of the molecule and the m th channel in the β (L or R) electrode. Considering the wide-band approximation to treat the FM electrodes, the hopping matrix elements $t_{i,n,\sigma}^j$ are independent of the energy, spin and bias voltage, so that $t_{i,n,\sigma}^j = t_c$. In this study, we assume that the electrons freely propagate and the resistance arises only from the contacts. This means that the transport is ballistic [43]. Therefore, we set $t_c = 0.5t$, because the value

of t_c should be smaller than the order of t . On the other hand, we assume that the spin direction of the electron is conserved in the tunnelling process through the molecule. Therefore, there is no spin-flip scattering and the spin-dependent transport can be decoupled into two spin currents; one for spin-up and the other for spin-down. This assumption is well-justified, because the spin diffusion length in conducting polymers is about 200 nm [3] which is typically greater than the length of polyacetylene molecule.

Because inelastic scatterings are ignored, to calculate the spin currents through FM/*trans*-PA/FM structure, we use Landauer–Büttiker (LB) formalism under an applied bias of V_a . Due to the simplicity and generality of the LB method, it provides a good first-hand understanding of coherent charge transport. The LB method is a semiclassical mechanical formalism with respect to the analysis of quantum mechanical spin degree of freedom; one would ideally have to resort to a full quantum mechanical picture. Thus, the spin-dependent current is written in the form [43,44],

$$I_\sigma(V) = \frac{e}{h} \int_{-\infty}^{+\infty} [f_L(E) - f_R(E)] T_\sigma(E) dE, \quad (6)$$

where $f_{L(R)} = f(E - \mu_{L(R)})$ gives the Fermi distribution function of the two electrodes having chemical potentials $\mu_{L(R)} = E_F \pm eV_a/2$. E_F is the equilibrium Fermi energy. The driving force here is the electric potential bias. Furthermore, $T_\sigma(E) = \text{Tr}\{\hat{\Gamma}_{L,\sigma} G_\sigma \hat{\Gamma}_{R,\sigma} G_\sigma^\dagger\}$ is the energy-dependent transmission function. $\hat{\Gamma}_{L(R),\sigma} = -2\text{Im}\{\hat{\Sigma}_{L(R),\sigma}\}$ is the chemisorption's coupling at the electrode/molecule interface, where $\hat{\Sigma}_{L(R),\sigma}$ represents the contact self-energy introduced to incorporate the effects of semi-infinite FM electrodes coupled to the molecule. However, representing the coupling parameter across the electrode/molecule interface by a spin-dependent contact self-energy may not always give the right physical picture. For example, recent works [45,46] show that the adsorption of the molecule on a magnetic surface can give rise to new interface hybridized states. It can induce a magnetic moment in the molecule and change the surface density of states. Depending on the strength of interaction, the molecular states at the interface can significantly broaden to have states at the Fermi level and hence affect the sign and strength of interface spin polarization (different in the surface density of states of the two spin channels) and hence TMR.

In addition, the spin-dependent Green's function of the polyacetylene molecule coupled to the FM electrodes (as the source and the drain) in the presence of bias voltage is given as

$$G_\sigma(E, V_a) = \left[E\hat{1} - H_m - \hat{\Sigma}_{L,\sigma}\left(E - \frac{eV_a}{2}\right) - \hat{\Sigma}_{R,\sigma}\left(E + \frac{eV_a}{2}\right) \right]^{-1}. \quad (7)$$

The self-energy matrix $\hat{\Sigma}_{\beta,\sigma}$ can be expressed as $\hat{\Sigma}_{\beta,\sigma} = \hat{t}_{c,\beta} \hat{g}_{\beta,\sigma}(E) \hat{t}_{\beta,c}$ where \hat{t} is the hopping matrix that couples the molecule to the electrodes and its elements are t_c . Also, $\hat{g}_{\beta,\sigma}$ is the surface Green's function of the uncoupled electrodes which is given by [47]

$$g_{\beta,\sigma}(i, j; z) = \sum_k \frac{\psi_k(r_i) \psi_k^*(r_j)}{z - \epsilon_0 + \vec{\sigma} \cdot \vec{h}_\beta + E(k)}, \quad (8)$$

where $r_i \equiv (x_i, y_i, z_i)$ and $k \equiv (l_x, l_y, k_z)$. Also $z = E + i\eta$ is considered to be a complex number so that the real part of it, E is the energy at which the transfer occurs. Moreover,

$$\psi_{k(r_i)} = \frac{2\sqrt{2}}{\sqrt{(N_x + 1)(N_y + 1)N_z}} \sin\left(\frac{l_x x_i \pi}{N_x + 1}\right) \sin\left(\frac{l_y y_i \pi}{N_y + 1}\right) \sin(k_z z_i) \quad (9)$$

and

$$E(k) = 2t \left(\cos\left(\frac{l_x \pi}{N_x + 1}\right) + \cos\left(\frac{l_y \pi}{N_y + 1}\right) + \cos(k_z a) \right). \quad (10)$$

N_x and N_y correspond to the number of atoms at the cross-section of the FM electrodes. In the semi-infinite FM electrodes described by the single-band tight-binding model, only the central site at the cross-section is connected to the molecule. However, this approach, as a real-space method, makes it possible to arbitrarily model the number of atoms on the cross-section of the electrodes. However, the core of the problem lies in computing the spin-dependent self-energies $\hat{\Sigma}_{L,\sigma}$ and $\hat{\Sigma}_{R,\sigma}$. In case of coupling through a single carbon atom of the molecule, only one element of the self-energy matrices is non-zero.

The total current through the FM/*trans*-PA/FM junction is given by $I = I_{\uparrow\uparrow} + I_{\downarrow\downarrow}$, based on which we calculate the TMR ratio from the well-known definition, $\text{TMR} \equiv (I_p - I_a)/I_p$, where I_p (I_a) is the total current in the parallel (antiparallel) configurations of magnetization in FM electrodes.

3. Results and discussion

Based on the formalism described in §2, we study the coherent spin-dependent transport and tunnel magnetoresistance of FM/*trans*-PA/FM molecular junction in the absence and in the presence of some selected distributions of solitons. We fixed the direction of magnetization in the left electrode at the $+y$ direction, while the right electrode is free to be flipped to either the $+y$ or $-y$ direction by an external magnetic field. Thus, for the parallel configuration of magnetizations in the electrodes, the spin-up and spin-down electrons encounter a symmetric structure, while for the antiparallel configuration these electrons encounter an asymmetric structure. We set $|\hbar\beta| = 1.5$ eV, $t = 1$ eV, $N_x = N_y = 5$ and a low temperature of $T = 11$ K is taken to avoid the spin-flip in the electron transport process [2].

In order to investigate the effects of selected distributions of solitons on the spin-dependent transport through the FM/*trans*-PA/FM model junction, first we consider the homogeneous distributions of solitons, which give rise to a soliton band in the band gap of *trans*-PA molecule. In general, in the presence of solitons, the ground state of *trans*-PA is a soliton lattice in which the centres of solitons, are approximately equally spaced along the chain. When the electronic states associated with the solitons overlap, a soliton band is formed in the band gap of polyacetylene. The soliton band is filled or emptied depending on the type of doping (donor or acceptor). Increasing the number of solitons by doping will widen the soliton band, thus reducing the size of the band gap of polyacetylene. Furthermore, we consider a sublattice of the correlated solitons as binary clusters of solitons

which are randomly distributed along the polyacetylene chain. Our investigations suggest that the distribution of the correlated solitons closes the band gap of the molecule. However, the suppression of the band gap is not sufficient for inducing the metallic-like states. The existence of the extended electronic states near the Fermi level is the most significant feature that has to be taken into consideration. This depends on the kind of soliton distributions. We found that the binary clusters of solitons, which are randomly distributed along the chain, may produce conditions for transition to the metallic-like phase. To observe how the electronic structure of the molecule is modified in the presence of selected soliton distributions, we have calculated the corresponding results for the π -electrons density of states for short chains containing 100 carbon atoms. Figure 2a shows an electronic structure for a fully dimerized chain of *trans*-PA. The energy gap of 1.4 eV is quite clear and also the spectrum contains valence (left) and conduction (right) bands, which indicates the semiconducting behaviour of *trans*-PA molecule. In the next plots, the concentration of solitons (10%) is taken into account for two kinds of soliton distributions. Figure 2b shows a soliton band into the band gap of *trans*-PA. In this plot, the solitons are homogeneously distributed corresponding to the formation of an ordered sublattice of solitons in which the soliton centres are equally spaced along the chain. As illustrated, the energy gap of *trans*-PA molecule collapses due to the formation of the soliton band. Thus, by changing the concentration of solitons, one can change and control the width of the soliton band and consequently the size of the band gap within the molecule structure. Figure 2c illustrates the effects of the presence of soliton pairs which are randomly distributed along the chain. We can see that the existence of a disordered sublattice of the binary clusters of

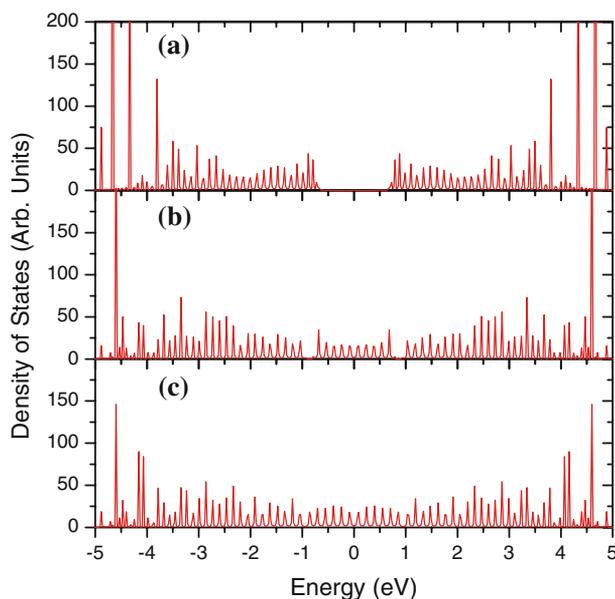


Figure 2. The plots showing the electronic density of states in the absence and in the presence of solitons. (a) The results in the absence of solitons and (b) and (c) the results for a homogeneous distribution of solitons and a disordered distribution of the binary clusters of solitons, respectively.

solitons suppressed the energy gap of *trans*-PA molecule. However, suppression of the band gap is a necessary but not a sufficient condition to ensure the transition to metallic-like state. For this purpose it is necessary that there should be extended electronic states around the Fermi level, which cause an enhancement in the electronic transmission within the energy gap. Moreover, it is expected that the current–voltage characteristic of the molecule at the lower bias voltages shows an ohmic-like behaviour. In figure 3, we illustrate the logarithmic scale of the spin-dependent electronic transmission function $T_{\sigma}(E)$ vs. the energy for the FM/*trans*-PA/FM model junction for parallel (P) and antiparallel (AP) configurations within the FM electrodes. Figure 3a shows $T_{\sigma}(E)$ in the absence of solitons. As shown clearly, there is a conductance band gap corresponding to figure 2a. In the presence of solitons, figures 3a and 3b illustrate $T_{\sigma}(E)$ for a homogeneous distribution of solitons and some binary clusters of solitons which are randomly distributed along the chain, respectively. As can be seen clearly, the band gap has been filled and due to the increase of overlap between the extended electronic states, the electron transmission through the junction has increased. Furthermore, for an electron with energy E , injected from the left side of the junction, the probability of electron transmission has its highest value for the particular energy values. The resonance peaks are related to the eigenenergies of the individual molecule. In the presence of solitons, the resonance peaks reinforced and significantly increased, indicating that there are more accessible extended electronic states. Besides, the difference between P and AP configurations in the transmission spectrums is related to the asymmetry of the surface density of states of FM electrodes for spin-up and spin-down

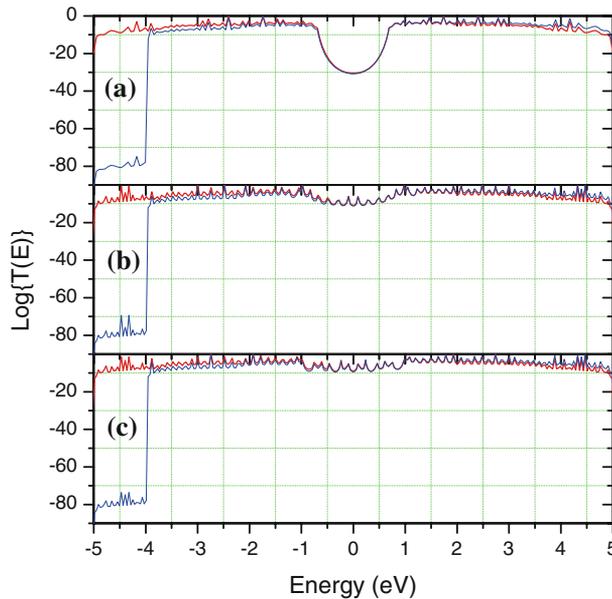


Figure 3. The plots showing the spin-dependent electronic transmission coefficient of FM/*trans*-PA/FM junction for P (red curve) and AP (blue curve) configurations in the absence and in the presence of solitons. (a) The results in the absence of solitons and (b) and (c) the results for a homogeneous distribution of solitons and a disordered distribution of the binary clusters of solitons, respectively.

electrons, as illustrated in figure 1, and also the quantum tunnelling phenomenon through the molecule. Figure 4 shows the low-temperature spin-dependent currents of the junction. Figures 4a–4c illustrate the results in the absence of solitons, in the presence of solitons for a homogeneous distribution and some binary clusters of solitons with random distribution, respectively. Here we present the results of the spin-dependent currents only for P configurations of magnetizations within the FM electrodes. Similar results were found for the AP configurations. However, the parallel configurations produce much higher currents through the molecule than do the AP configurations. The current curve in figure 4a shows clearly a nonlinear dependence and it has a good qualitative agreement with the energy gap of *trans*-PA molecule along the zero current part in the absence of solitons. In other words, the low-voltage part of the current curve in figure 4a arises from the semi-conducting behaviour of *trans*-PA molecule. On the other side, the presence of solitons within the molecular structure crucially modifies this behaviour such that a homogeneous distribution of solitons reduces the size of the band gap (figure 4b) and for a random distribution of the paired solitons the band gap closed (figure 4c) such that the current–voltage characteristic of the junction shows an ohmic-like behaviour. Figure 5 shows the TMR ratio using the results of the P and AP spin currents in the absence (figure 5a) and in the presence of solitons (figures 5b and 5c) as a function of an applied bias voltage. As illustrated, generally, the TMR ratio has its maximum value (about 60%) at the region of lower bias voltages. As the applied voltage increases, the TMR declines which is

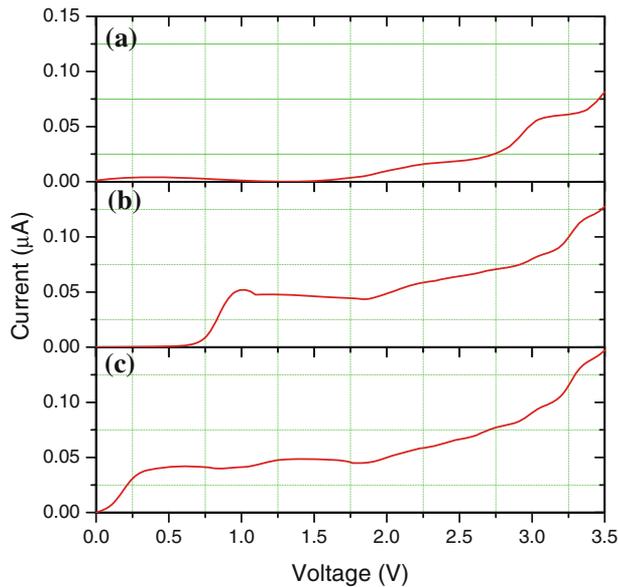


Figure 4. The plots showing the spin-dependent currents in the presence of soliton distributions for P configurations vs. the applied voltage. Role of a uniform distribution (b) and a disordered distribution of binary clusters of solitons (c) are compared with the current obtained in the absence of solitons (a). Similar results are obtained for currents in the AP configuration, which reach lower values compared to the currents for P configurations, as discussed in the text.

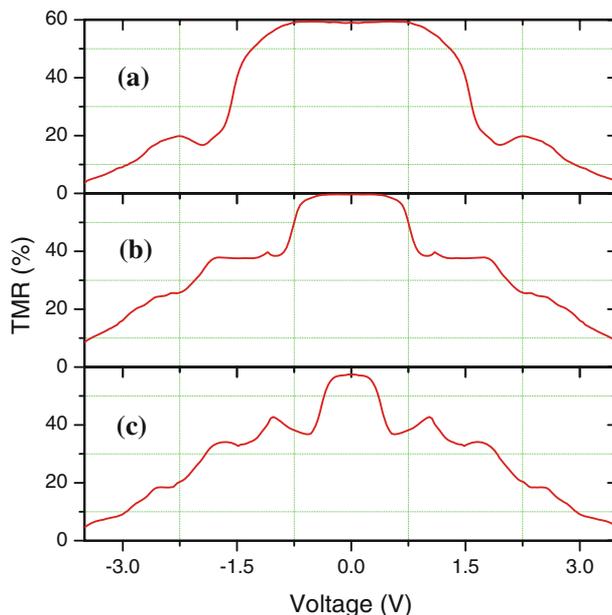


Figure 5. The plots showing the influence of soliton distributions on TMR ratio through the molecular junction. Panels (b) and (c) illustrate the results for a homogeneous distribution of solitons and a disordered distribution of binary clusters of solitons, respectively compared with (a) in the absence of solitons.

sharper in the case of a random distribution of the soliton pairs and we then observe a slow varying part. In fact, in the region of maximum value of TMR and at lower bias voltages, there are no accessible molecular levels within the gap region of the molecule for electron tunnelling between the chemical potential of the left and right FM electrodes. Therefore, at the low voltage regime, the spin-dependent currents are small and thus the TMR ratio is large. When the bias voltage increases, the electrochemical potentials in the electrodes are shifted gradually, and some of the energy states are pushed up between the chemical potentials of the right and left electrodes and thus the tunnelling current through the junction increases remarkably. Moreover, as clearly seen from figures 5b and 5c, the presence of solitons in the structure of the molecule, narrowed the TMR bandwidth of the junction at the middle of the spectrum, in which the random distributions of the paired solitons are the most effective, in agreement with the current curve in figure 4c.

4. Conclusion

In conclusion, based on the methodology presented in §2, we have investigated the role of soliton distributions on the spin-dependent currents, TMR and some other significant features in FM/*trans*-PA/FM model junction. The SSH Hamiltonian is used to describe the polyacetylene molecule and the spin currents are computed from the Landauer–Büttiker formalism. Our results suggest that the semiconducting behaviour of *trans*-PA molecule can be modified by the presence of solitons, which are induced via doping process. Moreover, we found a large tunnel magnetoresistance of 60% with a TMR bandwidth of about

1.5 eV that can be narrowed to 0.5 eV or less in the presence of random soliton distributions. Our calculations indicate the existence of a sublattice of the binary clusters of solitons which are randomly distributed along the molecular chain. The band gap of the semiconductor structure of *trans*-PA molecule is suppressed and the low temperature current–voltage characterization of the molecule shows an ohmic-like behaviour.

References

- [1] K Tsukagoshi, B W Alphenaar and H Ago, *Nature* **401**, 572 (1999)
- [2] Z H Xiong, D Wu, Z V Vardeny and J Shi, *Nature (London)* **427**, 821 (2004)
- [3] V Dediu, M Murgia, F C Maticcotta, C Taliani and S Barbanera, *Solid State Commun.* **122**, 181 (2002)
- [4] M Ouyang and D D Awschalom, *Science* **301**, 1074 (2003)
- [5] J R Petta, S K Slater and D C Ralph, *Phys. Rev. Lett.* **93**, 136601 (2004)
- [6] S Sanvito, *Nature Nanotechnol.* **2**, 204 (2007)
- [7] S Pramanik, C G Stefanita, S Patibandla, S Bandyopadhyay, K Garre, N Harth and M Cahay, *Nature Nanotechnol.* **2**, 216 (2007)
- [8] R Pati, L Senapati, P M Ajayan and S K Nayak, *Phys. Rev. B* **68**, 100407 (2003)
- [9] L Senapati, R Pati and S C Erwin, *Phys. Rev. B* **76**, 024438 (2007)
- [10] H Dagleish and G Kirczenow, *Phys. Rev. B* **72**, 184407 (2005)
- [11] R Liu, S H Ke, H U Baranger and W Yang, *Nano Lett.* **5**, 1959 (2005)
- [12] A R Rocha, V M García-Suárez, S W Bailey, C J Lambert, J Ferrer and S Sanvito, *Nature Mater.* **4**, 335 (2005)
- [13] D Waldron, P Haney, B Larade, A MacDonald and H Guo, *Phys. Rev. Lett.* **96**, 166804 (2006)
- [14] B Wang, Y Zhu, W Ren, J Wang and H Guo, *Phys. Rev. B* **75**, 235415 (2007)
- [15] H He, R Pandey and R Pati, *Phys. Rev. B* **73**, 195311 (2006)
- [16] Z Ning, Y Zhu, J Wang and H Guo, *Phys. Rev. Lett.* **100**, 056803 (2008)
- [17] R Q Wang, Y Q Zhou, B Wang and D Y Xing, *Phys. Rev. B* **75**, 045318 (2007)
- [18] H Mehrez, J Taylor, H Guo, J Wang and C Roland, *Phys. Rev. Lett.* **84**, 2682 (2000)
- [19] S Krompiewski, R Gutiérrez and G Cuniberti, *Phys. Rev. B* **69**, 155423 (2004)
- [20] E G Emberly and G Kirczenow, *Chem. Phys.* **281**, 311 (2000)
- [21] H Guichao, G Ying, W Jianhua and X Shijie, *Phys. Rev. B* **75**, 165321 (2007)
- [22] H Guichao, H Keliang, X Shijie and A Saxena, *J. Chem. Phys.* **129**, 234708 (2008)
- [23] S A Ketabi and M Ashhadi, *Physica E* **53**, 150 (2013)
- [24] M Ashhadi, S A Ketabi, N Shahtahmasebi, D Vahedi Fakhrabad and M Askari, *Physica E* **43**, 924 (2011)
- [25] S-J Sun, *Eur. Phys. J. B* **72**, 423 (2009)
- [26] S A Ketabi, D Vahedi and H F Khozestani, *Phys. Scr.* **83**, 015802 (2011)
- [27] A J Heeger, S Kivelson, J R Schrieffer and W P Su, *Rev. Mod. Phys.* **60**, 781 (1988)
- [28] W P Su, J R Schrieffer and A J Heeger, *Phys. Rev. Lett.* **42**, 1698 (1979)
- [29] W P Su, J R Schrieffer and A J Heeger, *Phys. Rev. B* **22**, 2099 (1980)
- [30] S Stafström, *Phys. Rev. B* **43**, 9158 (1991)
- [31] F C Lavarda, D S Galvao and B Laks, *Phys. Rev. B* **45**, 3107 (1992)
- [32] P Phillips and H L Wu, *Science* **252**, 1805 (1991)
- [33] T A Skotheim, *Handbook of conducting polymers* (Dekker, New York, 1986)
- [34] Z H Wang, E M Scherr, C Li, A G MacDiarmid and A J Epstein, *Phys. Rev. Lett.* **66**, 1745 (1991)
- [35] T Ishiguro, H Kaneko, Y Nogami, H Ishimoto, H Nishiyama, J Tsukamoto, A Takahashi, M Yamaura, T Hagiwara and K Sato, *Phys. Rev. Lett.* **69**, 660 (1992)

- [36] A K Meikap, A Das, S Chatterjee, M Digar and S N Bhattacharyya, *Phys. Rev. B* **47**, 1340 (1993)
- [37] K Lee, A J Heeger and Y Cao, *Phys. Rev. B* **48**, 14884 (1993)
- [38] N J Pinto, P K Kahol, B J McCormik, N S Dalal and H Wan, *Phys. Rev. B* **49**, 13983 (1994)
- [39] P W Anderson, *Phys. Rev.* **109**, 1492 (1958)
- [40] H L Wu and P Phillips, *Phys. Rev. Lett.* **66**, 1366 (1991)
- [41] V M Agranovich and A A Maradudin, *Solitons* (North-Holland, Amsterdam, 1986)
- [42] S Stafström and K A Chao, *Phys. Rev. B* **30**, 2098 (1984)
- [43] S Datta, *Electronic transport in mesoscopic systems* (Cambridge University Press, Cambridge, 1997)
- [44] S Datta, *Quantum transport: Atom to transistor* (Cambridge University Press, Cambridge, 2005)
- [45] K V Raman, A M Kamerbeek, A Mukherjee, N Atodiresei, T K Sen, P Lazić, V Caciuc, R Michel, D Stalke, S K Mandal, S Blügel, M Münzenberg and J S Moodera, *Nature* **493**, 509 (2013)
- [46] N Atodiresei, J Brede, P Lazić, V Caciuc, G Hoffmann, R Wiesendanger and S Blügel, *Phys. Rev. Lett.* **105**, 066601 (2010)
- [47] A Saffarzadeh, *J. Appl. Phys.* **104**, 123715 (2008)