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The study of charge injection and spin polarization in ferromagnetic metal–polymer–ferromagnetic metal structure

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ABSTRACT

By using extended SSH Hamiltonian plus long-range electron correlation Hamiltonian model, we calculated charge injection and spin polarization in a ferromagnetic metal/polymer/ferromagnetic metal structure. We adjust relative chemical potential between the ferromagnetic materials and the polymer to control charge transfer. It is found that when spin orientations of two ferromagnetic materials are parallel to each other, spin-polarized single polaron can be formed in the polymer, but when the spin orientations of two ferromagnetic materials are antiparallel to each other, bipolaron is formed and that spin polarization is found to be zero inside the polymer. The influence of the long-range electronic correlation on these polarons in the polymer is discussed.

1. Introduction

The micro-electronics based on the charge of electron has achieved giant success in the twentieth century. In traditional devices of micro-electronics, the electron is only treated as a carrier of charge. But electron has charge but also has spin. The information carried by the electron spin was omitted in the traditional micro-electronics. Discoveries of giant magnetoresistance (GMR) effect [1,2] and tunneling magnetoresistance (TMR) effect [3,4] have induced a revolution in the field of magnetic store and magnetic recording and thus result in a complete new subject about injection, transport, and control of electron spin–spintronics. The injection of electron spin includes from ferromagnetic metal into superconductor [5], into non-ferromagnetic metal [6], into ordinary metal [7] and from magnetic semiconductor into non-ferromagnetic semiconductor [8].

In recent years, injection of electron spin into organic functional materials that possess productive properties of electricity, magnetism, and optics has attracted more and more attention from the researchers in the spintronics field and that have made many progresses. In 2002, Dediu's research group reported firstly spin polarization and spin transport in organic semiconductor [9]. In their experimental setup, they used colossal magnetoresistance (CMR) material $\mathrm{Re}_{1-x}\mathrm{Sr}x\ \mathrm{MnO}_3$ as an electrode which is a polarized electron donor and used T6sexitxienylas organic layers and found negative magnetoresistance (NMR), which shows the existence of spin polarization injection into the organic medium. Xiong et al. used a small organic semiconductor Alq3 as a middle layer to form an organic spin valve and they found that the negative magnetoresistance was up to 40% at low temperature [10]. Mermer and Wohlgenannt et al. reported organic magnetoresistance (OMAR) [11,12]. They used non-magnetic materials as electrodes and middle molecules and found that there still exists magnetoresistance of 10% under an applied magnetic field. Recent discovery and study of organic spin electronic devices at room temperature [13–15] provide a possibility for the application of the organic spin devices in the future. Theoretically, Zwolak et al. studied spin transport and calculated magnetoresistance through a sandwich structure of ferromagnet/DNA/ferromagnet in terms of Green's function method [16]. Xie et al. studied spin polarization through a CMR/polymer chain system using a one-dimensional tight-bound model [17], where the CMR material is $\mathrm{Re}_{1-x}\mathrm{Sr}x$ MnO_3 that has strong magnetism and has a good applicable range of temperature [18] and the concentration of impurity is controlled by adjusting x.

Generally there are two categories concerning studies for spintronic devices. One is the ferromagnet/organic molecules/ferromagnet sandwich structure, where the organic molecule is treated as a spin passage and spin injection into the organic materials and its transport in the organic materials are studied. Other is to use organic magnetic molecules in the device system where electrodes are ordinary metal and the spin effect of the organic magnetic molecule is utilized. However, organic materials have their special characters in turn. First of all, most of the organic molecule materials experimentally used have low-dimensionality and strong electron–lattice interaction, thus any kind of changes in charge

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densities may induce re-construction of the system's inner structure [19,20]. Second, injected electrons or injected holes do not exist in the form of extended states whereas they may exist in the form of localized element excitations, such as soliton, polaron or bipolaron [21]. Only neutral soliton and single polaron carry spins and bipolaron carries no spin. There does exist some disputes about the stabilization of single polaron and bipolaron.

The present work studied a sandwiched system of ferromagnet/organic polymer chain/ferromagnet in terms of the one-dimensional tight-bound model with electron–electron interactions and long-range electronic correlation [22] effect. The effect of the long-range electronic correlation on polarons in the organic polymer chain is discussed. The spin injection and polarization problems in the organic polymer chain in spin parallel and spin anti-parallel situations in two magnetic materials are compared with each other.

2. Theoretical formation

We adopt *cis*-polyacetylene of ground state non-degeneracy as the organic polymer part in the sandwiched system. The model Hamiltonian adopted for the organic polymer part is the extended SSH model [17,23] plus long-range electronic correlation Hamiltonian [24]

$$H_P = H_{SSH} + H_{ee}^{HF} + H_c \tag{1}$$

where we adapt the Hartree–Fock approximation Hamiltonian H_{ee}^{HF} of the e–e interaction plus the long-range electronic Hamiltonian H_c to treat the e–e interaction Hamiltonian H_{ee}. H_{SSH} is the extended SSH Hamiltonian that describes electron–lattice interaction, kinetic energy of lattice sites, potential energy of sites, and the elastic energy between carbon atomic sites [17,23]:

$$\begin{aligned} H_{SSH} = & -\sum_{n\sigma} \varepsilon_P a_{n\sigma}^{\dagger} a_{n\sigma} - \sum_{n\sigma} [t_0 - \alpha(u_{n+1} - u_n) - t_1 \cos(n\pi)] \\ & \times (a_{n+1,\sigma}^{\dagger} a_{n\sigma} + h.c.) + \frac{1}{2} K \sum_n (u_{n+1} - u_n)^2 \end{aligned} \tag{2}$$

where ε_p is the on-site energy of π electron, t_0 is the hopping integral before dimerization, α is the electron–lattice coupling constant, t_1 is the degeneracy broken parameter, $a_{n\sigma}^{\dagger}$ and $a_{n\sigma}$ are productive and annihilation operators of electron with spin σ in the site n, u_n is the displacement of the nth carbon atom which deviates from its equilibrium position, K is the elastic constant between two carbon atoms. H_{ee}^{HF} is the Hartree–Fock approximation of electron–electron interaction Hamiltonian H_{ee} [25]:

$$H_{ee} = U \sum_n \left(\hat{\rho}_{n\uparrow} - \frac{1}{2} \right) \left(\hat{\rho}_{n\downarrow} - \frac{1}{2} \right) + V \sum_{n\sigma\sigma'} \left(\hat{\rho}_{n\sigma} - \frac{1}{2} \right) \left(\hat{\rho}_{n+1,\sigma'} - \frac{1}{2} \right) \tag{3}$$

where $\hat{\rho}_{n\sigma} = a_{n\sigma}^{\dagger} a_{n\sigma}$; U is the Hubbard interaction energy between different spin electrons in the same site, V is the long-range electronic interaction that lies at adjacent sites. H_c is the long-range electronic correlation Hamiltonian [26]:

$$H_c = -\frac{\lambda V}{2} \sum_{n\sigma} \hat{\rho}_{nn}^{\sigma} \hat{\rho}_{n+1,n+1}^{\sigma} \tag{4}$$

where λ takes $1/2$ in calculation.

For a simple ferromagnetic metal, it can be described by using the one-dimensional tight-bound model Hamiltonian [17]

$$H_{FM} = H_{Fe} + H_J \tag{5}$$

where

$$H_{Fe} = -\sum_{m\sigma} t_F (b_{m+1,\sigma}^{\dagger} b_{m\sigma} + b_{m\sigma}^{\dagger} b_{m+1,\sigma}) \tag{6}$$

and

$$H_J = -\sum_m J_m (b_{m\uparrow}^{\dagger} b_{m\uparrow} - b_{m\downarrow}^{\dagger} b_{m\downarrow}) \tag{7}$$

Here t_F is the nearest-neighbor electron hopping integral between the metal lattice sites, $b_{m\sigma}^{\dagger}$ ($b_{m\sigma}$) is electron's productive (annihilation) operator with spin σ at the site m. H_J describes the spin split energy of the magnetic atoms and J_m is the strength of the spin split.

In the interface between the magnetic part and the organic polymer part, the hopping integral is described as $t_{F-P} = \frac{1}{2}\beta_{F-P}(t_F + t_P)$, where β_{F-P} is the end atomic coupling factor. In calculation, $\beta_{F-P} = 1$ for simplicity. t_P is the hopping integral for the organic polymer part.

The total Hamiltonian of a ferromagnet/polymer structure is

$$H = H_{FM} + H_P + H_{F-P} = H_e + H_{ela} \tag{8}$$

where H_e is the electronic part of the total Hamiltonian, including the coupling Hamiltonian H_{F-P} at the interface. Here $H_{F-P} = -t_{F-P}(a_{P\sigma}^{\dagger} b_{F\sigma} + b_{F\sigma}^{\dagger} a_{P\sigma})$, where $a_{P\sigma}^{\dagger}$ ($a_{P\sigma}$) represents electron's productive (annihilation) operator in the end of the polymer and $b_{F\sigma}^{\dagger}$ ($b_{F\sigma}$) represents electron's productive (annihilation) operator in the end of the ferromagnetic materials which is connected to the polymer. H_{ela} is the elastic energy in the polymer part, that is, $\frac{1}{2}K\sum_n (u_n - u_{n+1})^2$.

The eigen equation of electrons in the system is as follows:

$$H_e \sum_n Z_{\mu,n}^{\sigma} |n> = \epsilon_{\mu}^{\sigma} \sum_n Z_{\mu,n}^{\sigma} |n> \tag{9}$$

For the magnetic part of the system, the corresponding eigen equation of electrons is

$$-t_F Z_{\mu,n-1}^{\sigma} - t_F Z_{\mu,n}^{\sigma} - J_n \sigma Z_{\mu,n}^{\sigma} = \epsilon_{\mu}^{\sigma} Z_{\mu,n}^{\sigma} \tag{10}$$

Here $\sigma = 1$ and $\sigma = -1$ correspond to two cases for spin up and spin down respectively.

For an organic polymer part, the eigen equation of electrons is

$$\begin{aligned} & \left[2U \left(\rho_{nn}^{-\sigma} - \frac{1}{2} \right) + V \left(\sum_{\sigma'} (\rho_{n-1,n-1}^{\sigma'} + \rho_{n+1,n+1}^{\sigma'}) - 2 \right) \right. \\ & \quad \left. - \frac{V}{4} (\rho_{n-1,n-1}^{\sigma} + \rho_{n+1,n+1}^{\sigma}) - \varepsilon_p \right] Z_{\mu,n}^{\sigma} \\ & \quad - \left[\frac{3}{4} V \rho_{n-1,n}^{\sigma} + t_0 - \alpha(u_n - u_{n-1}) - t_1 \cos((n-1)\pi) \right] Z_{\mu,n-1}^{\sigma} \\ & \quad - \left[\frac{3}{4} V \rho_{n+1,n}^{\sigma} + t_0 - \alpha(u_{n+1} - u_n) - t_1 \cos(n\pi) \right] Z_{\mu,n+1}^{\sigma} = \epsilon_{\mu}^{\sigma} Z_{\mu,n}^{\sigma} \end{aligned} \tag{11}$$

where $\rho_{nn}^{\sigma} = \sum_{\mu}^{occ} |Z_{\mu,n}^{\sigma}|^2$ and $\rho_{n,n+1}^{\sigma} = \sum_{\mu}^{occ} Z_{\mu,n}^{\sigma} Z_{\mu,n+1}^{\sigma}$ are site charge density and the bond charge density of the adjacent sites in the organic polymer, respectively. According to the equilibrium condition when the energy of the system is minimum, it yields

$$u_n = \frac{1}{2} \left[u_{n+1} + u_{n-1} + (-1)^n \frac{2\alpha}{K} \sum_{\mu}^{occ} (Z_{\mu,n+1}^{\sigma} Z_{\mu,n}^{\sigma} - Z_{\mu,n}^{\sigma} Z_{\mu,n-1}^{\sigma}) \right] \tag{12}$$

Through self-consistent iterative solution of Eqs. (9) and (12), stable site configurations of the whole system and charge density distribution, spin density distribution can be obtained.

3. Results and discussion

We discuss two kinds of layout of the sandwich structure. One is that the direction of spins of two ferromagnetic materials is parallel to each other and other is that the direction is anti-parallel to each other.

The present calculation was made in ideal conditions: there is no disturbance from outside and the system is always in its minimum state of energy. The parameters used in this study are