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Anderson Localization Enhanced Spin Selective Transport of Electrons in DNA*

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Abstract *Recent experiments revealed the unusual strong spin effects with high spin selective transmission of electrons in double-stranded DNA. We propose a new mechanism that the strong spin effects could be understood in terms of the combination of the chiral structure, spin-orbit coupling, and especially spin-dependent Anderson localization. The presence of chiral structure and spin-orbit coupling of DNA induce weak Fermi energy splitting between two spin polarization states. The intrinsic Anderson localization in generic DNA molecules may result in remarkable enhancement of the spin selective transport. In particular, these two spin states with energy splitting have different localization lengths. Spin up/down channel may have shorter/longer localization length so that relatively less/more spin up/down electrons may tunnel through the system. In addition, the strong length dependence of spin selectivity observed in experiments can be naturally understood. Anderson localization enhanced spin selectivity effect may provide a deeper understanding of spin-selective processes in molecular spintronics and biological systems.*

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Key words: spin selective transport, DNA, Anderson localization

Charge transport in DNA has attracted a lot of attention in many areas over the past decades.[1−8] In electron-transfer processes, spin effects are normally seen either in magnetic materials or in systems containing heavy atoms that facilitate spin-orbit coupling. Recently, some experiments revealed the strong spin effects with both high spin selective transmission and its strong length dependence when electrons pass through a double-stranded structure of DNA molecules.[9−11] In particular, a very high spin polarization at room temperature can be achieved by passing free electrons through a gold surface covered with a densely packed layer of doubly-stranded DNA.[9] In experiments, DNA chains standing on the gold surface was grown. Then a linearly polarized laser was shone on to the gold which liberates unpolarized electrons via the photoelectric effect. Some of these electrons travel through the DNA chains and are fed into a device that measures their spin polarization. Amazingly, the electrons are polarized after passing through the DNA strands with high spin polarization. Besides, the polarization was found to be strong length dependent, for 78 base pairs long strands giving 60% polarization while 25 base pairs only yielding about 10%. These findings are quite unusual since carbon-based molecules have typically a small spin-orbit coupling that cannot support significant splitting between two spin states.

The nature of the strong spin effects in such systems are still not quite clear. There are two obvious factors, which may lead to spin polarization. One is associated with DNA double helix structure of handedness or chirality-related. Another one is spin orbit coupling because of the presence of relative heavy atoms as well as the interfacial effect between the substrate and DNA molecules. However, the spin polarization due to these factors is too weak to explain the strong spin effects measured in experiments. Several theoretical studies have been presented for explaining this unusual spin effects.[10−13] Some of them involve the introduction of Rashba type spin-orbit coupling for electron-chiral molecule scattering.[14−16] However, these studies are mostly in qualitative agreement with the experimental observation but most of them do not able to explain them quantitatively.

In this paper, we propose theoretically a new mechanism of the enhanced spin selective transport of electrons in DNA that the strong spin effects could be understood in terms of the combination of the chiral structure, spin-orbit coupling, and Anderson localization. Due to the presence of chiral structure and spin-orbit coupling of DNA, there exists weak energy splitting between the spin up/down states. By employing the transfer matrix method, we show that the splitting spin up/down channels correspond to different localization lengths. In particular, spin up/down channel may have shorter/longer localization length so that relatively less/more spin up/down electrons may tunnel through the system. Figure 1 presents a cartoon picture of such scenario. Moreover, the length dependence of spin selectivity can be naturally understood

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by using spin-dependent Anderson localization effect. Numerical results show the longer the length of the DNA molecule, the greater the rate of spin polarization and in a certain energy range. It is rather clear that intrinsic Anderson localization plays the vital role to strongly enhance the spin selective transport.

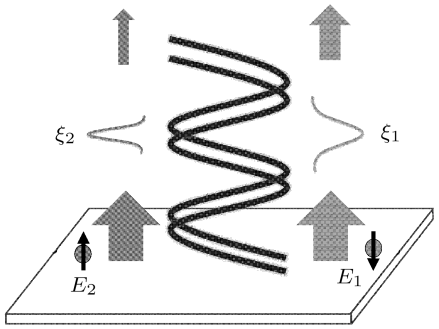

Fig. 1 Schematic configuration of the mechanism of strong spin effects of double-stranded DNA. The chiral structure and spin-orbit coupling of DNA molecules induce a weak energy splitting of two spin states. These two spin states correspond to different Anderson localization lengths (ξ_1 and ξ_2) resulting in the strong enhancement of spin polarization of the transmitted electrons.

Since DNA molecule is a double helix structure with complex composition, we adopt a simplified two-leg ladder tight-binding model to study the charge transport properties through the DNA. The electronic Hamiltonian can be expressed as

$$\begin{aligned}\mathcal{H} = &\sum_n [\varepsilon_{1,n} c_{1,n}^\dagger c_{1,n} - t(c_{1,n}^\dagger c_{1,n+1} + \text{h.c.})] \\ &+ \sum_n [\varepsilon_{2,n} c_{2,n}^\dagger c_{2,n} - t(c_{2,n}^\dagger c_{2,n+1} + \text{h.c.})] \\ &- V \sum_n (c_{1,n}^\dagger c_{2,n} + \text{h.c.}) \,, \end{aligned} \tag{1}$$

where $c_{i,n}^\dagger (c_{i,n})$ denotes the creation (annihilation) operator of electron on site n along the i-th chain. t and V correspond to the intra-chain coupling and the inter-chain coupling, respectively. The onsite energies for different bases are chosen according to their ionization potentials, where the onsite energy $\varepsilon_A = 8.25$, $\varepsilon_T = 9.13$, $\varepsilon_C = 8.87$, $\varepsilon_G = 7.77$ eV.[17] We choose the hopping parameter t for intrachain adjacent nucleotides and the interchain coupling V to be 1.0 eV and 0.96 eV, respectively.[18] The generic DNA molecules have random sequence of G-C or A-T base pairs. The random sequence of DNA is a nature and logical reason of biological complexity. So the electron states for such a DNA become localized due to Anderson localization effect. During the electron transfer process, we treat the system as a coherent system by neglecting the inelastic scattering effect via the electron-phonon scattering and other inelastic relaxation processes. Here we consider the right-handed double helix structure.

The electronic transport properties are evaluated by a quantitative nonperturbative calculation, the transfer matrix method. From the Schrödinger equation, the eigenstates can be found by solving the following equations:

$$\varepsilon_{1,n}\psi_{1,n} + t(\psi_{1,n+1} + \psi_{1,n-1}) + V\psi_{2,n} = E\psi_{1,n} \,,$$
$$\varepsilon_{2,n}\psi_{2,n} + t(\psi_{2,n+1} + \psi_{2,n-1}) + V\psi_{1,n} = E\psi_{2,n} \,,$$

where $\psi_{i,n}$ $(i = 1, 2)$ is the probability amplitude for an electron on site n along the i-th chain. The above secular equations can be written in matrix form

$$\begin{pmatrix} \Psi_{n+1} \\ \Psi_n \end{pmatrix} = T_n \begin{pmatrix} \Psi_n \\ \Psi_{n-1} \end{pmatrix}, \tag{2}$$

where $\Psi_n = (\psi_{1,n}, \psi_{2,n})^{\mathrm{T}}$ and

$$T_n = \begin{pmatrix} \dfrac{E-\varepsilon_1}{t} & -\dfrac{V}{t} & -1 & 0 \\ -\dfrac{V}{t} & \dfrac{E-\varepsilon_2}{t} & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix},$$

where T denotes the matrix transpose operation. Then the coefficients at two ends of the system are related by

$$\begin{pmatrix} \Psi_{N+1} \\ \Psi_N \end{pmatrix} = T_N \begin{pmatrix} \Psi_1 \\ \Psi_0 \end{pmatrix}, \tag{3}$$

where T_N is the product of all the transfer matrices from 1 to N. The localization length ξ at energy E is the inverse of the Lyapunov exponent γ ($\gamma > 0$), which is the smallest positive eigenvalue of the limiting matrix $\lim_{N\to 0} \ln(T_N T_N^\dagger)^{1/2N}$.[19–21] The localization length λ is used in the following to describe the degree of localization. In the calculations, we have used the reorthogonalization method to obtain reliable values of γ. Comparing to the single-stranded DNA, the localization length of double-stranded DNA is much longer because of the additional transmission channel and the interchain correlations.

In our understanding, there are two obvious factors, which may lead to the energy splitting between spin up/down states. One factor is the helical structure of DNA, which is equivalent to a solenoid. A magnetic field will be produced when electrons moving in such a system, the electrons with spin may gain different Zeeman energy. Another factor is from spin-orbit coupling due to the presence of relative heavy atoms as well as the interfacial effect between the gold substrate and DNA molecules. These combined factors may induce a weak energy splitting between spin up and spin down electrons. This energy splitting may lead to slightly different populations for two spin states but it is too weak to explain the high spin selectivity. Here we highlight the importance of intrinsic Anderson localization effect in generic DNA, which plays a vital role to strongly enhance the spin selective transport.

We have calculated the localization length ξ for system size $N = 10^6$. In Fig. 2 we plot the energy dependence of localization length for double-stranded DNA. E_1 and E_2 correspond to the Fermi energy of spin down and spin up electrons, respectively. The fermi energy of incoming electrons is estimated to be about 0.5 eV (average of E_1 and E_2) according to the experimental measurements.[22] Here we estimate that the energy splitting E_2–E_1 due to

the combined effect of chirality structure and spin-orbit coupling of DNA is around 0.2 eV. This energy splitting itself may lead to slightly different populations for two spin states but it is too weak to explain the high spin selectivity. From Fig. 2, we find that ξ decreases with the increasing of energy for E greater than 0.2 and the curve is rather steep. The localization length of spin down and spin up electrons correspond to $\xi_1 \sim 27$ and $\xi_2 \sim 17$, respectively. Spin up channel has shorter localization length so that relatively less spin up electrons may tunnel through the system. In comparison, spin down channel has longer localization length and relatively more spin down electrons are transmitted. As a result, the number of spin down electrons will be more than that of spin up electrons at the end of the DNA molecules as shown in Fig. 1. The intrinsic Anderson localization in generic DNA molecules magnifies greatly the weak imbalance between two spin states due to energy splitting. It is the key factor to realize such a strong spin polarization in double-stranded DNA.

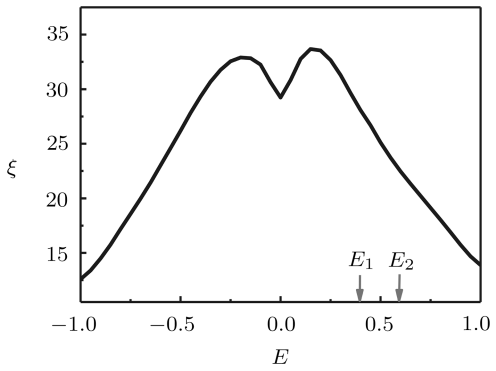

Fig. 2 Energy dependence of localization length ξ for the double-stranded DNA with $N = 10^6$ and the intra-coupling $t = 1.0$ eV, inter-coupling $V = 0.96$ eV. The energy E is in the unit of eV. E_1 and E_2 correspond to the Fermi energy of spin down and spin up electrons, respectively.

We then focus on the length dependence of conductance as well as spin polarization. The spin polarization observed in experiments for electrons transmitted through a monolayer of 25 base pairs DNA is about 10%, while the polarization is about 60% for 78 base pairs long strands.[9] This strong length dependence indicates that the system remains coherent and Anderson localization effect may play an essential role. Figures 3(a) and 3(b) illustrate the length dependence of conductance and spin polarization, respectively. The conductance of both spin down and spin up electrons decreases monotonically with the increasing of number of base pairs $N_{\rm bp}$. It is a characteristic feature of Anderson localization. The amplitude of spin polarization shows a strong length dependence and it increases with increasing $N_{\rm bp}$. Our numerical results show a quantitative agreement with experimental measurements.

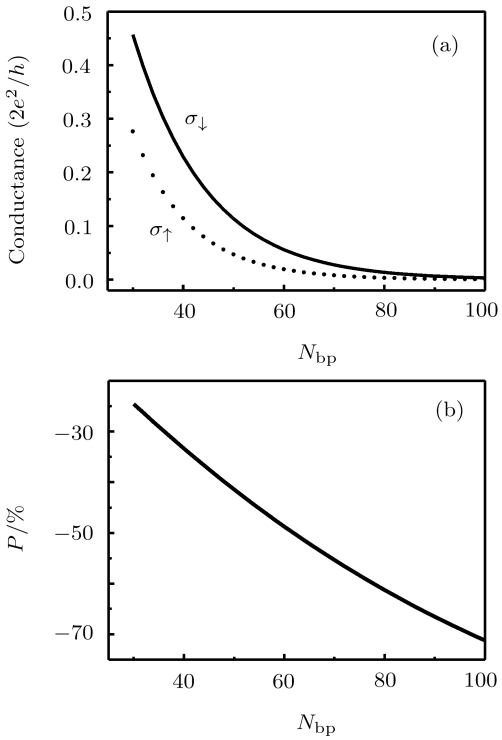

Fig. 3 (a) DNA length dependence of the conductance σ for electrons with spin up and spin down. (b) DNA length dependence of the spin polarization P.

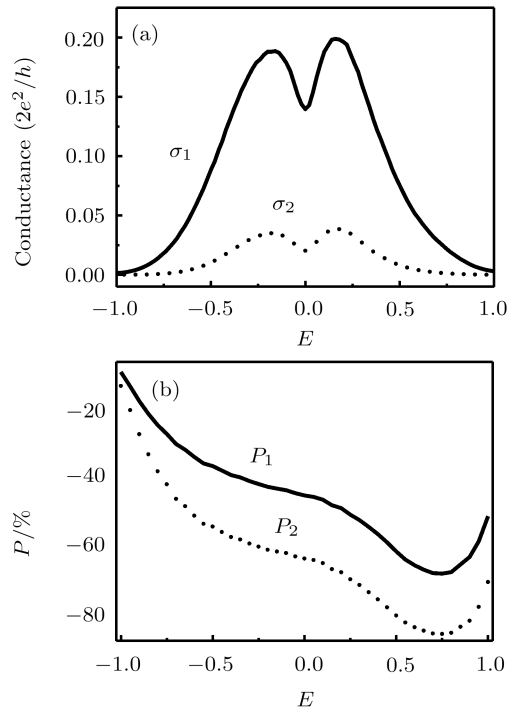

Fig. 4 (a) Energy dependence of the conductivity for electrons transferring in DNA of 50 (solid curve 1) and 78 (dashed curve 2) base pairs long. (b) Energy dependence of the spin polarization P for electrons transferring in DNA of 50 (solid curve 1) and 78 (dashed curve 2) base pairs long.

Let us further investigate the energy dependence of the conductance and spin polarization for different number of base pairs $N_{\rm bp}$. As presented in Fig. 4(a), a double peak structure of conductance shows up as a function of energy around the band center. The physical reason for such peak structure is due to the finite energy splitting of two spin states. We calculate the energy dependence of the spin polarization P for electrons transferring in DNA of 50 and 78 base pairs long, as shown in Fig. 4(b). The spin polarization as a function of energy exhibits a rather flat region in between $E = 0.4$ to 0.6, which is in qualitative agreement with experiments.

Very recently, a clear evidence for spin-dependent electron transmission through the living proteins in its native membrane environment is experimentally observed.[23] This results show the possibility that the spin selective effect may play a role in electron transfer in biological systems. Our studies may provide a deeper understanding of spin-selective processes in biology in terms of high spin selectivity enhanced by Anderson localization effect.

To conclude, we have proposed that the mechanism of strong spin effects observed in recent experiments when electrons pass through a double-stranded structure of DNA molecules could be understood in terms of the combination of the chiral structure, spin-orbit coupling and Anderson localization. Due to the presence of chiral structure and spin-orbit coupling of DNA, there exists weak Fermi energy splitting between two spin states. We find that intrinsic Anderson localization in the simplified two-leg ladder system may play the vital role to strongly enhance the spin selective transport. In particular, the splitting spin up/down channels have different localization lengths. Spin up/down channel may have shorter/longer localization length so that less/more spin up/down electrons may tunnel through the system. Moreover, the length dependence of spin selectivity can be naturally understood by using spin-dependent Anderson localization effect. Numerical results show the spin polarization will be greatly enhanced by increasing the DNA length. Our studies may provide a deeper understanding of spin-selective processes in both molecular spintronics and biological systems in terms of Anderson localization enhanced spin selectivity effect.

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