Physica E 74 (2015) 156–159

Contents lists available at ScienceDirect

Physica E

journal homepage: www.elsevier.com/locate/physe

Spin polarization and spin separation realized in the double-helical molecules

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HIGHLIGHTS

- Transport in one four-terminal double-helical molecule is studied.
- Spin polarizations occur in intra-chain electron tunneling and inter-chain reflection.
- In the two processes, spin polarizations show similar strengths and opposite directions.
- Spin polarization and spin separation can be co-realized in this system.

ARTICLE INFO

Article history:
Received 18 May 2015
Received in revised form
6 July 2015
Accepted 7 July 2015
Available online 9 July 2015

Keywords:
Double-helical molecules
Electron transport
Spin polarization
Spin separation

ABSTRACT

We investigate the electron transport through one double-helical molecule with four terminals, by considering one terminal to be the source and others to be the drains. It is found that notable spin polarizations simultaneously occur during the processes of intra-chain electron tunneling and inter-chain electron reflection. More importantly, in these two processes, the spin polarizations always show similar strengths and opposite directions. Based on these results, we consider that the spin polarization and spin separation can be co-realized in this system.

1. Introduction

Spintronis, a multidisciplinary field which aims at manipulating the electron spin to store and process information, has received extensive attention during the last two decades [1]. In order to manipulate an electron spin, high-efficiency spin polarization should be realized first. Researchers from physics, chemistry and biology communities have dedicated themselves to the enhancement of spin polarization by considering various systems under appropriate fields [2,3]. With respect to mesoscopic systems, organic molecules have attracted much interest from the experimental and theoretical aspects, due to their superior performances like flexibility, inexpensive material and production methods, and compatibility with biological systems [4]. However, during the past long time, little progress has been made in the field of organic-based spin polarization, and the realization of spin polarization usually depends on the magnetic properties of the inorganic electrodes [5–7]. Recently, it has been reported that electron transport through double-stranded DNA (dsDNA) oligomers has a chance to be spin selective. Besides, the selectivity of spin exceeds that of any known system at room temperature [8]. It is known that high-efficiency spin polarization in the electron transport process assists the achievement of spin filtering effect. And then, such a system has been considered to be a true organic spin filter. Since the spin effects are only dominated by the intrinsic property of dsDNA, this result arouses researchers' interest to pay more attention to the organic spintronics based on the helical molecules [9,10].

Encouraged by the experimental progress, theoretical researchers dedicated themselves to the investigation on the spin-dependent electron transport through organic molecules. Double-helical (DH) molecules have been one main concern in this field. Guo et al. [11–13] and Gutierrez et al. [14,15] made leading contributions to the underlying physics responsible for the spin polarization in the DH-molecule systems. They demonstrated that in the DH molecules, a helical electric field, mirroring the helical symmetry of the molecular systems, induces finite spin–orbit coupling (SOC), which leads to the spin propagation. Next, some other groups further considered the influence of additional physics

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http://dx.doi.org/10.1016/j.physe.2015.07.005
1386-9477/

mechanisms on the spin transport. Consequently, the underlying physics has been clarified [16–20]. Meanwhile, in order to enhance the efficiency of spin polarization, various mesoscopic circuits with embedded helical molecules have been proposed [21].

Following the clarification about the physics mechanisms, it is necessary to explore new devices based on helical molecules in spintronics for their promising application [20,21]. In this work, we would like to investigate the electron transport through one DH molecule with four terminals, by considering one terminal as the source and others as drains. It is found that notable spin polarizations simultaneously occur during the processes of intrachain electron tunneling and inter-chain electron reflection, whose directions can be reversed by tuning the gate voltage. Moreover, in these two processes, the spin polarization directions are always opposite accompanied by their similar strengths. Therefore, the spin polarization and spin separation can be anticipated to co-realize in this system.

2. Model

The device of a DH molecule with four terminals is illustrated in Fig. 1. Its Hamiltonian can be written as $H = H_m + H_c + H_T$. H_m describes the DH molecule which is depicted as a two-leg ladder model. According to the previous works, H_m takes a form as [21]

$$H_m = \sum_{j=1}^{2}\left\{\sum_{n=1}^{N}\varepsilon_j d_{jn}^{\dagger}d_{jn} + \sum_{n=1}^{N-1}[i\gamma_j d_{jn}^{\dagger}(\sigma_n^{(j)} + \sigma_{n+1}^{(j)}) d_{jn+1} + t_j d_{jn}^{\dagger}d_{jn+1}]\right\} + \sum_{n=1}^{N}\lambda d_{1n}^{\dagger}d_{2n} + h.c. \quad (1)$$

$d_{jn}^{\dagger} = (d_{jn\uparrow}^{\dagger}, d_{jn\downarrow}^{\dagger})$ and $d_{jn} = (d_{jn\uparrow}, d_{jn\downarrow})^T$ are respectively the creation and annihilation operators at site-(j, n) of the DH molecule whose length is N. j labels the helical chain and n is the site index within a single chain. ε_j is the on-site energy, γ_j is the SOC strength, and $t_j(\lambda)$ is the intrachain (interchain) hopping integral. Finally, the term $\sigma_{n+1}^{(j)} = \sigma_z\cos\theta - (-1)^j\sin\theta[\sigma_x\sin(n\Delta\varphi) - \sigma_y\cos(n\Delta\varphi)]$ with $\sigma_{x,y,z}$ the Pauli matrices, θ the helix angle, and $\Delta\varphi$ the twist angle between successive base pairs [11].

With respect to H_c and H_T, they represent the Hamiltonians of the leads and the molecule-lead couplings. To be concrete, the expressions of them can be given by

$$H_c = \sum_{\alpha k\sigma}\varepsilon_{\alpha k\sigma}c_{\alpha k\sigma}^{\dagger}c_{\alpha k\sigma},\ H_T = \sum_{k\sigma}V_{1\sigma}c_{1k\sigma}^{\dagger}d_{11,\sigma} + \sum_{k\sigma}V_{2\sigma}c_{2k\sigma}^{\dagger}d_{21,\sigma} + \sum_{k\sigma}V_{3\sigma}c_{3k\sigma}^{\dagger}d_{1N,\sigma} + \sum_{k\sigma}V_{4\sigma}c_{4k\sigma}^{\dagger}d_{2N,\sigma}. \quad (2)$$

$c_{\alpha k\sigma}^{\dagger}$ and $c_{\alpha k\sigma}$ $(\alpha = 1, 2, 3, 4)$ are the creation and annihilation operators respectively for spin-σ electron at state $|k\sigma\rangle$ in lead-α, and $\varepsilon_{\alpha k\sigma}$ is the energy level. $V_{\alpha\sigma}$ denote the molecule-lead couplings.

Electron transport through this system can be studied by employing the Laudauer–Büttiker formalism [22]. Accordingly, the conductance in the channel between lead-α and lead-α' can be expressed as

$$G_{\alpha\sigma,\alpha'\sigma'} = \frac{e^2}{h}\mathrm{Tr}[\Gamma_{\alpha\sigma}G^r\Gamma_{\alpha'\sigma'}G^a]. \quad (3)$$

Here, $\Gamma_{\alpha\sigma} = 2\pi|V_{\alpha\sigma}|^2\rho_{\sigma}(\omega)$ represents the coupling strength between the molecule and lead-α in which ρ_{σ} is the density of state of the spin-σ electron in the corresponding terminal. Based on the above theory, the spin conductance can be defined, i.e.,

$$G_{\alpha\alpha'}^{S} = G_{\alpha\uparrow,\alpha'\uparrow} - G_{\alpha\downarrow,\alpha'\downarrow}, \quad (4)$$

which reflects the spin polarization efficiency.

3. Numerical results and discussions

Following the theory in the previous section, we proceed to perform the discussion about the spin transport in this multi-terminal structure. Before calculation, we consider the electronic parameters to be uniform along each helical chain of the DH molecule. As for the structural parameters, they are fixed to be $t_2 = 0.1$, $\lambda = -0.08$, and $\Gamma_{\alpha\sigma} = 0.1$ with their units being eV. In order to describe the asymmetry between the two chains of the DH molecule, we suppose $t_1 = -xt_2$ and $\gamma_2 = x\gamma_1$, in which x is the parameter to reflect the asymmetry degree between the two helical chains. In addition, the remaining parameters are chosen as $N = 20$, $\theta = 0.66$ rad, and $\Delta\varphi = \pi/5$ to mimic the double-stranded DNA molecule. This parametrization was demonstrated as the favorable situation to obtain large spin polarization [15,23–25]. After these assumption, we take lead-1 to be the source terminal of this system and other leads to be drain terminals for investigating the spin polarizations in respective channels.

In Fig. 2, we present the electron and spin conductances in respective channels. For calculation, we take $x = 1.5$ and $\gamma_1 = 0.01$. Besides, the onsite levels of the two chains are respectively considered to be $\varepsilon_1 = E_g$ and $\varepsilon_2 = E_g + 0.3$ in which E_g can be changed by introducing a tunable gate voltage proximity to the molecule. First, Fig. 2(a) show the electron conductances. In this figure, we clearly find the asymmetry of the conductance spectra about the energy zero point. The reason is that the asymmetric structure of the molecule causes the highest occupied molecular orbital

Fig. 1. Four-terminal circuit based on the DH molecule coupling to four normal metallic leads.

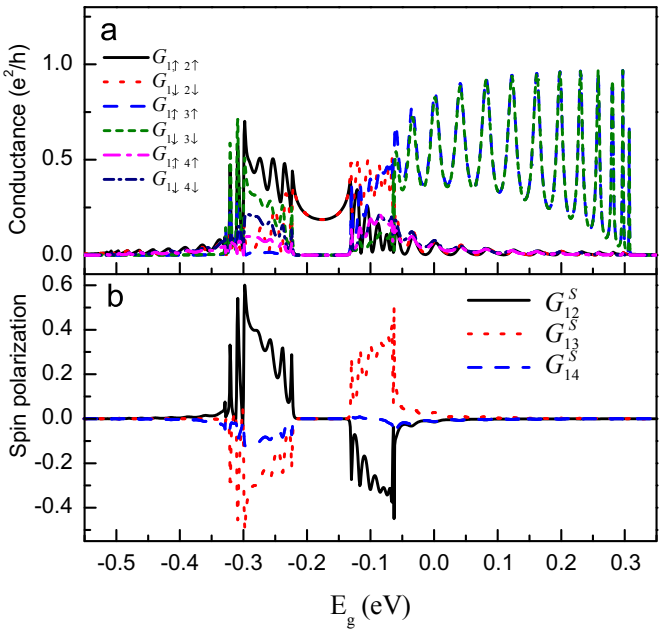

Fig. 2. Conductance and spin polarization in the four-terminal circuit. Lead-1 is considered to be the source and the other leads are assumed to be the drains.