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Interesting odd-even rules of spin-filtering and magnetoresistance effects in a single-molecule spintronic device

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ABSTRACT

By using nonequilibrium Green's functions in combination with the density functional theory, the spin transport properties of a single-molecule spintronic device are investigated. The computational results show that when the magnetic configuration of the device is set as parallel, the perfect spin-filtering effect can be observed. Especially, this perfect spin-filtering effect is independent of the number of carbon atoms in the carbon chain. However, when the magnetic configuration is set in antiparallel, the spin-filtering effect displays a strong odd-even oscillatory characteristic, namely, the spin-filtering efficiencies of odd-numbered chain systems have a higher values than even-numbered chain systems. Moreover, the magnetoresistance effect can also be observed in this single-molecule spintronic device. In contrast to the odd-even oscillatory characteristic of the spin-filtering effect in the antiparallel magnetic configuration, high magnetoresistance ratios belong to even-numbered chain systems while low magnetoresistance ratios belong to odd-numbered chain systems. The mechanisms are suggested for these interesting phenomena.

1. Introduction

Recently, people are more and more interested in designing single-molecules as the component of molecular devices [1–8]. Especially, single-molecules designed as spintronic devices receive much attention in recent years because they can further improve the integration of molecular circuits in the future [9–16]. So for, many spintronic devices based on single-molecules have been designed, such as spin filters [9–11], spin valves [12,13], spin diode [14], spin switch [15], spin transistor [16], etc. Among them, spin filters and spin valves attract tremendous research interest because of their potential data storage capabilities.

Since it was successfully prepared, the carbon chain has been an interesting topic due to its unique electronic properties [17–22]. As the carbon chain can confine electron to propagate in one-dimensional direction, it can display many particular transport properties in the molecular devices. For example, Fan et al. [17] found that a carbon chains–graphene junction can act as a mechanical switch when the graphene electrode is twisted. Zhou et al. [18] found that when two carbon chains are separated in a certain distance, fine Kirchhoff's superposition law phenomenon can be observed. Zhang et al. [19] observed strong odd-even dependence behaviors of negative differential resistance and rectifying phenomena in a carbon-chain-modified donor-acceptor molecular device. Moreover, earlier studies have also shown that when carbon chains are directly coupled to metal or graphene electrodes, the corresponding conductance varies in an oscillatory manner with the change of the number of carbon atoms [20,21]. However, these studies are mainly focused on the charge transport properties of molecular devices, the spin transport properties are rarely investigated. In the present work, we study a carbon chain-based single-molecule spintronic device. The results show that the magnetic configurations of the device have an important influence on the odd-even oscillatory characteristics of the spin-filtering effect, namely, strong odd-even dependence characteristics of the spin-filtering effects can only be observed in the antiparallel magnetic configuration. Moreover, we also see that magnetoresistance (MR) ratios in this single-molecule spintronic device show a strong odd-even dependence characteristic.

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2. Method and model

The single-molecule spintronic device we study is shown in Fig. 1. The molecular junction is divided into three parts, namely, the left electrode, the central scattering region, and the right electrode. The central scattering region is constructed by Fe-dibenzotetraaza[14]annulene (Fe-DBTAA) molecules connected with the carbon chain C_n (n is the number of carbon atoms), which is boned to Au(111)-(4 × 4) surfaces via S atoms. In this study model, the S atom is placed onto the hollow site of the Au triangle, and the distance between the S atom and the Au surface is set as 1.9 Å [23]. For ease of discussion, the model for two Fe-DBTAA molecules connected with C_n is called as M(C_n). For example, the system in Fig. 1 is called as M(C_5). In the device, the carbon chain acts as the spacer, and thus the two Fe atoms in DBTAA molecules are separated by a long distance. This means that the spin coupling between two Fe atoms can be ignored [24]. By depositing the ferromagnetic stripe on the side of each of Fe-DBTAA, the parallel and antiparallel configurations of M(C_n) can be realized by changing the relative magnetization directions of these two ferromagnetic stripes [25]. In our current work, the spin-transport properties for M(C_3)-M(C_8) in the parallel and antiparallel configurations are investigated by adopting the ATOMISTIX TOOLKIT (ATK) package, which uses first-principles method based on the fully self-consistent ab initio density-functional theory [26,27]. In our transport calculations, the single-zeta plus polarization basis set is used. Previous references have shown that the single-zeta plus polarization basis set can provide sufficient accuracy for all the elements in the spin transport properties of the device [24,28], and thus it is used to achieve a balance between the calculation efficiency and the accuracy in the present work. Moreover, the norm-conserving pseudopotentials, the local-density approximation, a Monkhorst-Pack K-mesh of (3, 3, 100), and 150 Ry for cutoff energy are adopted. The geometrical structures are fully relaxed until all residual forces on each atom are smaller than 0.05 eV · A^{-1}. The spin transmission coefficients are calculated by using the formula:

$$T_\sigma(E,V_b) = Tr\left[\mathrm{Im}\left\{\Sigma^R_{L\sigma}(E,V_b)\right\}G^R_\sigma(E,V_b) \times \mathrm{Im}\left\{\Sigma^R_{R\sigma}(E,V_b)\right\}G^A_\sigma(E,V_b)\right], \quad (1)$$

where σ indicates a spin index (↑ and ↓), $\Sigma^R_{L\sigma}$ and $\Sigma^R_{R\sigma}$ indicate the retarded self-energy matrix which takes into account the left and right electrodes, respectively. G^R_σ and G^A_σ indicate the retarded and advanced Green functions of the central region, respectively. In order to obtain the spin-dependent currents, the Landauer formula is adopted [29]:

$$I_\sigma(V_b) = \frac{e}{h}\int T_\sigma(E,V_b)[f_L(E-\mu_L) - f_R(E-\mu_R)]dE, \quad (2)$$

where f_L and f_R are the Fermi-Dirac distribution function of the left and right electrodes, respectively.

3. Results and discussion

In Fig. 2(a), we plot the total current values (the bias value is set as 0.01 V) as a function of the number of carbon atoms in the parallel and antiparallel magnetic configurations, respectively. It is seen clearly that for the parallel magnetic configuration, high current values belong to odd-n carbon chain systems while low current values belong to even-n carbon chain systems, indicating an oscillatory conductance characteristic in the single-molecule spintronic device. These results are in agreement with the carbon chains connected with the metal or graphene electrodes [20,21]. Furthermore, it is also seen that similar oscillatory characteristic can also be observed in the antiparallel magnetic configuration, which means that this interesting physical phenomenon is independent of the magnetic configurations of the single-molecule spintronic device.

The odd-even oscillatory conductance of carbon chains-based molecular device has been reported extensively in previous references [20,21]. However, some interesting new physical phenomena appear when the spin-transport properties of the single-molecule spintronic device are further investigated. From Fig. 2(b), we can find that when the magnetic configuration of the device is set as parallel, the perfect spin-filtering effect can be observed, which is independent of the number of carbon atoms in the chain. Thus, the single-molecule spintronic device can act as a perfect spin-filter once the two Fe-DBTAA molecules connected with the carbon chain. However, when the magnetic configuration is set in antiparallel, the number of carbon atoms in the chain need to be considered if we want to obtain high spin-filtering efficiencies in the design process of the device. This is based on the fact that the spin-filtering efficiencies in the antiparallel magnetic configuration display a strong odd-even oscillatory characteristic [see Fig. 2(b)]. Clearly, the spin-filtering efficiencies of odd-numbered chain systems have a higher value than that of even-numbered chain systems. Moreover, we also investigate the MR ratios for M(C_3)-M(C_8), as shown in Fig. 2(c). In contrast to the odd-even oscillatory characteristic of spin-filtering efficiencies in the antiparallel magnetic

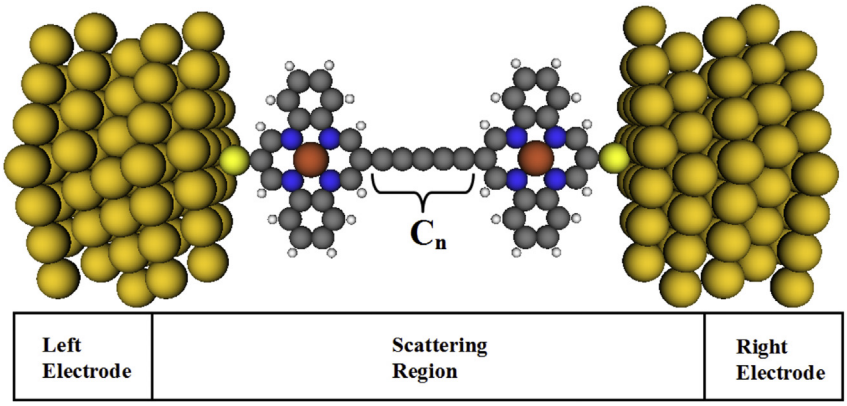

Fig. 1. A schematic of the carbon chain-based single-molecule spintronic device. C_n (n is the number of carbon atoms) indicates the carbon chain. (A color version of this figure can be viewed online.)