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Magnetism and spin transport of carbon chain between armchair graphene nanoribbon electrodes

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HIGHLIGHTS

- Spin-polarized transmission in carbon chain junction without any magnetic field.
- Fully spin polarized current near the Fermi energy in all odd-numbered carbon chain.
- Energy gap and magnetic distribution depend on the position of the carbon chains.
- Spin transport properties depend on the position and the length of the carbon chains.

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ABSTRACT

The magnetic and spin transport properties of a carbon chain between two armchair graphene nanoribbon (AGNR) electrodes were studied using tight-binding Hamiltonian, mean-field Hubbard model and Landauer–Butikker formalism. The results showed that only odd-numbered carbon chains show intrinsic magnetic moments in chain–graphene junctions. It was also found that the electronic, magnetic and spin transport properties of carbon chain–graphene junctions strongly depend on the position and the length of the carbon chains between AGNR electrodes. Interestingly, we found a fully spin-polarized transmission near the Fermi energy in all odd-numbered carbon chain–graphene junctions, regardless of their lengths and without any magnetic field and magnetic electrodes.

1. Introduction

Spintronics is a new field of electronics to use the spin degree of freedom of the electrons [1–3]. This field of research has provided the designing and construction of the faster electronic devices for information processing and storage and other applications. Miniaturization and dimension reduction of these devices are also important issues that have steadily been considered in spin-dependent nanoelectronics. Further, molecular spintronics has recently been investigated theoretically and experimentally [4–7].

Carbon is a unique nonmagnetic element due to its considerable features [4]. Among the carbon allotropes, graphene nanoribbons (GNRs) have attracted more attention than other structures due to their edge state and width [8]. Regarding to the edge states, GNRs can be armchair or zigzag. Unlike the armchair GNRs, zigzag GNRs have magnetic edge states. Also GNRs are metallic and semiconducting according to their width and hence can be used as leads to inject electrons. Therefore, GNR structures can play an important rule to design field effect transistors (FETs). Ponomarenko et al. [9] succeeded to produce graphene FETs experimentally and thus carbon-based electronic device was really made. Moreover, in the presence of the electron–electron interaction, zigzag-edges show magnetic properties [10,11]. Hence, in many researches [12–15], carbon-based systems have been the most acceptable candidates for use as spintronic devices such as spin-filter and spin-valve.

Recently, linear carbon chains (CCs) as one dimensional and *sp* carbon structures have been obtained, which are noteworthy from two aspects. First, CC could be considered as the thinnest carbon nanotube or narrowest GNR, which its features are independent of chirality and edge states. Second, due to the limitation of the current lithography techniques, it is difficult to get sub-10-nm width semiconducting GNRs [9], whereas such problem does not exist in the case of CCs. Therefore, these structures are more appropriate than carbon nanotubes and GNRs not only in terms of their chirality, but also their construction. Furthermore, in order to reduce the size of spin devices, it seems that one-dimensional CCs are good choices as the channel between two quasi-one dimensional GNR electrodes. However, electrodes' structures affect

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transport properties of CCs [16]. Stable CCs have been synthesized experimentally via high energy electron beam by Jin et al. [17]. By this method, carbon atoms are removed row by row from a GNR and finally a CC is remained [17–19]. In this way, experimental and theoretical approaches have been developed to investigate the features of CCs [20,21]. Chuvilin et al. [19] and Jin et al. [17], experimentally and theoretically, respectively, discovered that a CC sandwiched between two GNRs organizes a stable structure and as a result, such system has attracted great attention. Experimental results exhibit that the connection point of CC with graphene nanofragments could migrate along their connection side [19]. Few researches have so far addressed it and its effects on the properties of CCs [22–24].

On the other hand, previous works investigate general magnetic [24,25] and transport [26–29] properties of CCs. Based on previous results, CCs have also shown spintronics effects such as magneto-resistance and spin filter effects [25,30,31]. Furthermore, high magneto-resistance gives rise to the spin-valve effect in such devices. Also, a CC between Au and Al electrodes has also been theoretically studied as a spin-filter and spin-valve, respectively [25,31]. Interestingly, carbon chain–graphene junction shows perfect spin-filtering effect due to zigzag-edge states and magnetic impurities in graphene electrodes [32,33]. Recently, Zhou et al. predicted when two zigzag graphene nanoribbons connected to each other by a double carbon atomic wire, conductance superposition and spin filtering effects can be observed [34].

In this paper, we studied the electronic, magnetic, and spin transport properties of a carbon atoms' chain that is connected on different positions along the zigzag side of AGNR electrodes. Our calculations were based on a tight-binding model combined with the mean-field Hubbard theory. In order to decrease the contact resistance in channel-leads' junction [3], here we considered a spin-filter device including two AGNR electrodes and a CC as a channel. The induced magnetic moments are only localized on the carbon chain (channel) without any magnetic elements in AGNR electrodes so there is no contact resistance (interfacial scattering) and magnetic scattering. Electron–electron interaction may only induce localized magnetic moments in odd-numbered carbon chain with nonmagnetic armchair electrodes. The results showed that these magnetic moments induce fully spin-polarized transmission near the Fermi energy. Moreover, we study the energy gap and magnetic properties by changing the position and the length of the carbon chains between AGNR electrodes.

2. Model and method

Our calculations were based on a tight-binding model and the mean-field Hubbard theory [10,12]. The Hamiltonian of the channel is as follows:

$$H_C = t \sum_{\langle i,j\rangle,\sigma} c^{\dagger}_{i,\sigma} c_{j,\sigma} + U \sum_{i,\sigma} \hat{n}_{i,\sigma} \langle \hat{n}_{i,-\sigma} \rangle \quad (1)$$

where the parameter U=2.82 eV is the on-site Coulomb repulsion. $n_{i\sigma}$ and $c^{\dagger}_{i\sigma}$ ($c_{i\sigma}$) are also the number and creation (annihilation) operators, respectively, at the j-th site with spin σ (for majority- and minority-spin electrons) . In this Hamiltonian, t=2.66 eV corresponds to the hopping between the nearest neighbors. We solve the mean-field Hamiltonian self-consistently by iteration method [10]. Green's function (GF) [35] of the center region is calculated by relation (2) that $\hat{\Sigma}_{S,D,\sigma}(\varepsilon)$ is self-energy [36] and shows the effect of source and drain on the carbon chain:

$$\hat{G}_{C,\sigma}(\varepsilon) = [\varepsilon \hat{I} - \hat{H}_{C,\sigma} - \hat{\Sigma}_{S,\sigma}(\varepsilon) - \hat{\Sigma}_{D,\sigma}(\varepsilon)]^{-1}. \quad (2)$$

The spin-dependent density of states of the carbon chain is given by

$$D_{i\sigma}(\varepsilon) = -1/\pi[\langle i\sigma|\hat{G}_{C,\sigma}(\varepsilon)|i\sigma\rangle] \quad (3)$$

According to the Landauer–Buttiker [35,37] formalism, the spin-dependent currents will be calculated with the following relation:

$$I_{\sigma} = e/h \int T_{\sigma,\varepsilon}(f_S(\varepsilon) - f_D(\varepsilon))\, d\varepsilon. \quad (4)$$

In this relation, $T_{\sigma}(\varepsilon)$ is the transmission function for electrons with spin σ that is obtained by using (4) [3], and $f_{S,D}(\varepsilon)$ shows Fermi distribution function. It should be noted that spin flips and spin scatterings were not considered:

$$T_{\sigma}(\varepsilon) = Tr[\hat{\Gamma}_S \hat{G}_C \hat{\Gamma}_D \hat{G}_C^{\dagger}]_{\sigma}. \quad (5)$$

Using $\hat{\Sigma}_{\alpha,\sigma}$, the coupling matrices $\hat{\Gamma}_{\alpha,\sigma}$ can be expressed as $\hat{\Gamma}_{\alpha,\sigma} = -2\,\mathrm{Im}[\hat{\Sigma}_{\alpha,\sigma}(\varepsilon)]$. Accordingly, the local magnetic moment at site i of the channel can be calculated using $\langle M_i \rangle = \mu_B(\langle \hat{n}_{i,\uparrow} \rangle - \langle \hat{n}_{i,\downarrow} \rangle)/2$.

3. Results and discussion

In order to study the electronic and magnetic properties of free-standing carbon atoms' chains, we solved the mean-field Hubbard Hamiltonian self-consistently, which may induce localized magnetic moments on the carbon chain. We considered two different types of carbon chains as odd-numbered and even-numbered lengths. A chain with an even number of carbon atoms has no a net magnetic moment according to the Lieb's theorem [38]. Further, even-numbered carbon chains have no localized state at the Fermi energy, and hence the degeneracy between spin-up and spin-down electrons preserves in the presence of electron–electron interaction (similar to AGNR). Therefore, in even-numbered chain, the local magnetic moment at each carbon atom is zero. However, the odd-numbered carbon chains have different number of *A*- and *B*-type atoms and therefore, in contrast to even-numbered carbon chain, the net magnetic moment value (intrinsic magnetic moments) of chain reaches 1 μ_B and chain has an anti-ferromagnetic spin configuration.

The magnetic properties of free-standing odd-numbered carbon chains are investigated in Fig. 1. The calculated local magnetic moment at each atomic site for c17 (carbon chain with seventeen atoms) is shown in Fig. 1(a) as a function of the carbon index (shown in Fig. 2). The chain (c17) has different values of magnetic moments in carbon sites. In addition, the maximum value of magnetic moment reaches 0.22 μ_B at the end of the carbon chain. The values of the magnetic moments for the majority (minority) spin electrons are sensibly different and induce a net magnetization in these structures. In order to further clarify the magnetic properties of the carbon chain, we plotted the maximum value of the magnetic moment versus the chain length in Fig. 1(b) in which the chain length varies from 3 to 29 atoms. As the chain length increases, the magnetic ordering of the chain (maximum value) decreases, but the net magnetic moment remains unchanged. The value of the magnetic moment for each atomic site becomes more similar to each other in longer carbon chains. Interestingly, for carbon chain longer than c17, the local magnetic moments' distribution of the carbon chain is approximately independent of the length of the carbon chain. In these cases, the maximum value of the local magnetic moment reaches 0.18 μ_B (see Fig. 1(a)).

In order to see the effects of these localized magnetic moments on the electron conduction, we proposed a carbon chain–graphene junction based on an atomic chain containing n carbon atoms (Cn) as the channel and two semi-infinite 6-AGNRs as electrodes,