Regular Article

PHYSICAL CHEMISTRY RESEARCH
Published by the
Iranian Chemical Society
www.physchemres.org
info@physchemres.org

***Phys. Chem. Res.**, Vol. 2, No. 2, 146-150, December 2014.*
DOI: 10.22036/pcr.2014.4722

Spin-Polarized Transport Through a Zigzag-Edge Graphene Flake Embedded between Two Armchair Nanoribbon Electrodes

M.K. Maher[a,b,*], N. Shahtahmassebi[a,b] and M.R. Roknabadi[a,b]

[a]*Department of Physics, Ferdowsi University of Mashhad, Iran*
[b]*Nanoresearch Centre of Ferdowsi University of Mashhad, Iran*

(Received 6 November 2013, Accepted 12 February 2014)

We study the coherent spin-polarized transport through a zigzag-edge graphene flake (ZGF), using Hubbard model in the nearest neighbor approximation within the framework of the Green function's technique and Landauer formalism. The system considered consists of electrode/(ZGF)/electrode, in which the electrodes are chosen to be armchair nanoribbons. The study was performed for two types of electrodes *i.e.*, armchair-edge graphene nanoribbons (AGNRs) and armchair-edge boron-nitride nanoribbons (ABNNRs). Our calculations of the electronic and transport properties of these systems show that both systems posses spin filtering properties, while the spin filtering is higher in the full graphene system than the second system with boron nitride nanoribbon electrodes. The spin filtering in these systems is due to the interaction of the spin of the carriers with the local zigzag-edge magnetism in ZGF. However, the reduction of the spin filtering property in the case of the system with boron-nitride nanoribbon electrodes could be due to the decrease in the effective spin interaction of boron atoms in the contact sites and magnetization of the zigzag-edge of the ZGF.

Keywords: Spin transport, Spin filters, Graphene nanoribbons, Graphene nanoflake, Boron-nitride nanoribbons, Hubbard model, Landauer formalism, Green function's technique

INTRODUCTION

The research on 2D nanomaterials with the potential of next-generation electronic device has seen tremendous progress in the past few years [1]. The properties of the graphene-based materials are renowned and clearly indicate that planar graphene must be a very remarkable material for nanotechnological applications. It is expected to be stable at temperatures up to 3000 °C and should be extremely flexible, but at the same time as hard to tear apart as diamond, similar in fact to carbon nanotubes. The electronic properties of planar graphene are extraordinary too, for example, the mobility of the carriers reaches 15000 cm^2/Vs in room-temperature [2]. In addition, the spin relaxation length is measured to be as long as ~1.5 μm in low-mobility devices, which makes graphene very interesting candidate for spintronic applications, as well [3].

*Corresponding author. E-mail: ma65maher1@gmail.com

Considering the novel electronic properties of graphene, there has been enormous number of research on the development of the nanoscale technology of graphene, and its various shapes, such as nanoribbons and nanoflakes. To explore the spin-dependent transport phenomena a number of nanodevices have also been proposed, especially in graphene nanoribbons [4]. Among the various types of graphene nanoribbons, two types have attracted more researchers' attention, the armchair edge and zigzag edge nanoribbons. These two edges have a 30° difference in their orientation within the graphene sheet [5].

Several intriguing transport properties have been theoretically predicted especially for zigzag graphene nanoribbons (ZGNRs). It has been shown that ribbons with zigzag edges (zigzag ribbons) posses localized edge states with energies close to the Fermi level [6]. The unique properties in the electronic transport properties of ZGNRs (and ZGF) can be attributed to the characteristic band structures of ZGNR and the symmetry of wave functions

near the Fermi level [8]. Also, it has been shown that ZGNRs can be utilized for generating of a spin polarized current [6]. The possibility of spontaneous magnetic ordering which is peculiar to nanometer-scale zigzag edge graphene has also been found [9]. The ground state of ZGNRs has an antiferromagnetic spin configuration where the total spin (S) is zero. However, when the system has different number of A- and B-sublattice sites, the total spin of the ground state is $2S = N_A - N_B$ and by appropriate designing, one can form a ferromagnetic spin configuration at the zigzag edges [6]. This would enable the ribbon to have different conductance channels for the spin up and down electrons and thus show spin filtering property.

On the other hand, we know that hexagonal boron nitride (h-BN) is a one-atom-thick layered material with a flat 2-D structure isoelectronic and isomorphic to the graphene honeycomb lattice. An h-BN consists of an equal number of boron and nitrogen atoms in sp^2 hybridization that is bonded together by strong covalent bonds but with a remarkable ionic character [9]. Similar to graphene, the BN sheet can be truncated in one direction to obtain a quasi-one-dimensional system called BN nanoribbon (BNNR). Depending on the direction of the truncation, there are two main types of BNNRs, namely, zigzag (ZBNNR) and armchair (ABNNR) [10].

Hexagonal boron nitride is a honeycomb lattice with a lattice parameter of 2.52 Å, which is only slightly larger than that of graphene's 2.46 Å. It has already been demonstrated that it is possible to grow graphene directly on h-BN and *vice-versa* by means of chemical vapor deposition. Consequently, h-BN is a suitable companion for graphene [11] and is therefore interesting to study the electronic conduction properties of the h-BN as compared to the graphene for the purpose of device designing.

With this motivation, in the present work, we perform a study on the electronic and spintronic properties of graphene and boron nitride nanoribbons. For this purpose, we consider the effect of the type of electrodes in a system consisting of a zigzag-edge graphene nanoflake (ZGF) connected to two armchair-edge nanoribbons as the left and right electrodes. In the first part of the study, we use armchair-edge graphene nanoribbons as electrodes in system 1 (AGNR/ZGF/AGNR), and in the second study, ZGF is embedded between two armchair-edge boron-nitride nanoribbons electrodes (ABNNR/ZGF/ABNNR). We employ Hubbard model, Green function's technique and Landauer formalism to study the spin filtering properties of these systems. We demonstrate that both of these systems show spin filtering properties due to the magnetization of the zigzag-edge of the nanoflake, however, our results show that presence of ABNNRs electrodes in system 2 reduces spin filtering properties.

MODEL AND FORMALISM

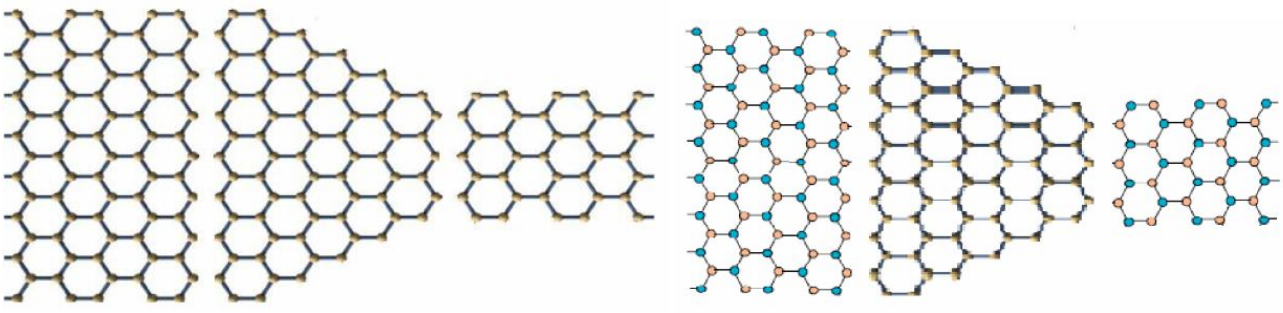
The systems under study, consist of a zigzag-edge graphene nanoflake which is connected to two armchair-edge nanoribbons as the left and right electrodes. In these junctions, the left electrode has a ribbon index n = 15, while the right electrode has a ribbon index n = 7. Furthermore, the central region (ZGF) with a trapezoidal shape consists of N_C = 70 carbon atoms and produces a ferromagnetic spin configuration at its edges. In the first system (system 1), we use armchair-edge graphene nanoribbons as electrodes (Fig. 1a), and in the second system, ZGF is embedded between two armchair-edge boron-nitride nanoribbon electrodes (Fig. 1b). We consider the coherent spin-polarized transport through a zigzag-edge graphene flake (ZGF) in both systems and will make comparison of the spin transport in both systems.

In both systems, we examine the effect of the electron-electron interaction using the Hubbard model within the mean field approximation. The Hamiltonian in central part (ZGF) is, therefore written as

$$H_C = \sum_{i,j,\sigma} -t_{i,j} C_{i\sigma}^{+} C_{j\sigma} + U \sum_{i,\sigma} \langle n_{i,-\sigma} \rangle \left[n_{i,\sigma} - \frac{1}{2} \langle n_{i,\sigma} \rangle \right] \qquad (1)$$

Where $C_{i\sigma}^{+}$ and $C_{j\sigma}$ are the electron creation and annihilation operators, respectively, and $n_{i\sigma} = C_{i\sigma}^{+} C_{i\sigma}$ is the number operator for an electron with spin σ at site i. t = 2.66 ev is the transfer integral between all the nearest neighbor sites and U = 1.06 t is the on-site Coulomb interaction [6]. The Fermi energy was also set to zero, *i.e.*, $E_f = 0$.

We solve the mean-field Hamiltonian selfconsistently by iteration method. Therefore, the Green's function and the spin density on each atom of the channel should be calculated iteratively until a convergence of the spin density



(a) (b)

Fig. 1. A schematic representation of ZGF between: (a) two graphene electrodes (AGNR/ZGF/AGNR), (b) two boron-nitride electrodes (ABNNR/ZGF/ABNNR).

is reached. The Green's function of the ZGF is expressed as

$$\hat{G}_C(\omega)=\left[(\omega+i\eta)\hat{I}-\hat{H}_C-\hat{\Sigma}_L-\hat{\Sigma}_R\right]^{-1} \quad (2)$$

Where η is a positive infinitesimal and $\Sigma_{R,L}$ are the selfenergy matrices due to the connection of left and right electrodes to the channel. The effect of different semi-infinite electrodes on the Hamiltonian of system is described using the self-energy terms. The selfenergys are calculated iteratively too, and hopping integrals between different atoms are extracted from Ref. [12].

The spin-dependent density of states and the expectation value for the number operator of electron on each site of the channel (ZGF) are given by

$$g_{i\sigma}(\omega)=-\frac{1}{\pi}\mathrm{Im}\left\langle i\sigma\left|\hat{G}_C(\omega)\right|i\sigma\right\rangle \quad (3)$$

$$\left\langle\hat{n}_{i,\sigma}\right\rangle=\int_{-\infty}^{E_F}g_{i\sigma}(\omega)d\omega \quad (4)$$

In the mean-field approximation, there is not a spin-flip scattering or any other interactions. Therefore, the spin-polarized transport through such a junction can be considered within the coherent regime. In the coherent transport, the spin-dependent conductance at low temperature can be written as

$$G_\sigma=\frac{e^2}{h}Tr\left[\Gamma_L G_C \Gamma_R G_C^+\right] \quad (5)$$

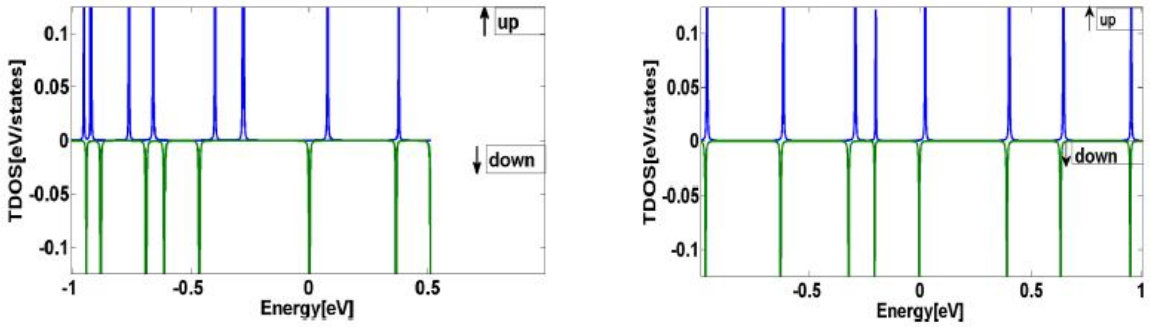
where, $\Gamma_{L,R}$, the coupling matrices can be expressed as $\Gamma_{L,R}=-2*\mathrm{Im}(\Sigma_{L,R})$ for each system [6]. Within the above framework we calculated the electronic density of states and the spin dependence conductance for the two systems of electrodes (graphene and boron-nitride) and we report the results in the next section. In the final section we shall present a discussion accompanied by a comparison of the results for the systems under study.

RESULT AND DISCUSSION

Following the above procedure, we calculate the total density of states (TDOS) per site for each spin subband in the central region (ZGF), $\frac{1}{N_C}\sum_{i=1}^{N_C}g_{i\sigma}(\omega)$, for both systems and the results are presented in Fig. 2. As shown for system 1 (Fig. 2a), the spin dependent electronic states are completely separated into majority and minority electrons around the Fermi energy and thus, one expects a high degree of spin filtering. Despite separation of electronic states into majority and minority spin states, the degree of separation of the states with different spin orientation is reduced in the presence of armchair-edge boron-nitride electrodes, shown in Fig. 2b. This results in the reduction of the spin filtering effect in system 2.

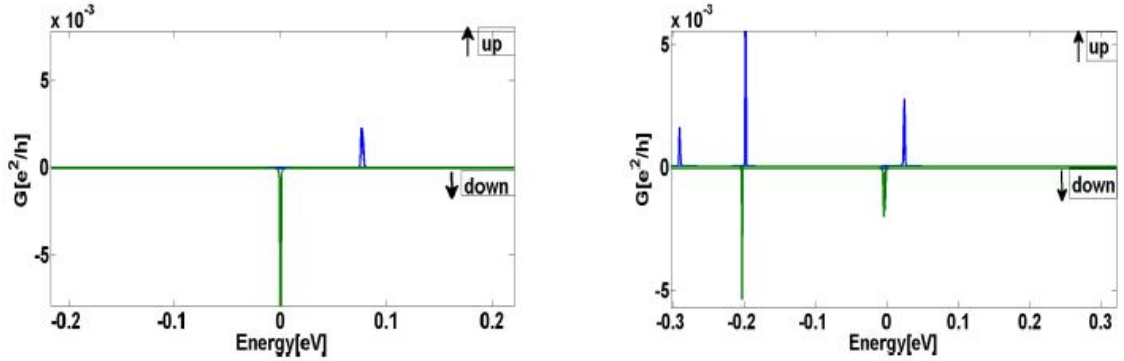
The results could be explained in terms of presence of different electrodes in two systems. System 1 is fully based on graphene while in system 2, we have boron-nitride electrodes *i.e.* boron atoms are located near carbon atoms in junctions (Fig. 1b). We may conclude that, the reduction in spin property is due to the presence of boron atoms in second system.

More explanation may be given in terms of the boron atom's electronic structure, in which outer valence electron



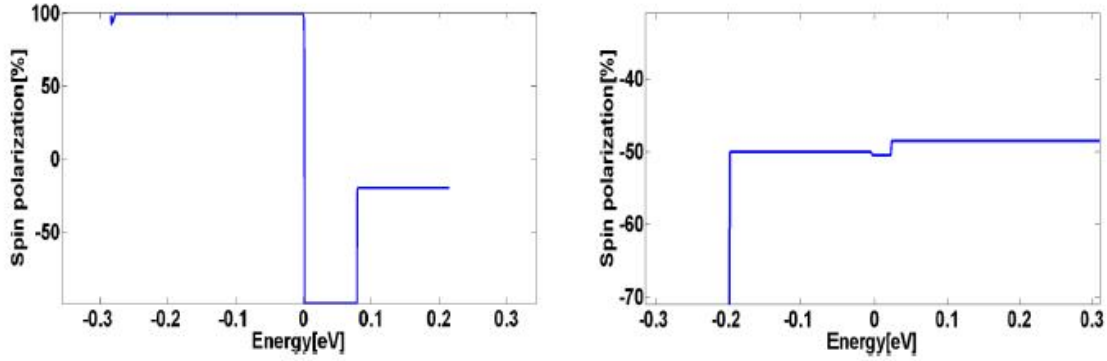
(a) (b)

Fig. 2. The total density of states (TDOS) per site for each spin subband in the central part of system: (a) System 1 (AGNR/ZGF/AGNR) and (b) System 2 (ABNNR/ZGF/ABNNR).



(a) (b)

Fig. 3. Spin-dependent conductance at the central part of the systems: (a) System 1 (AGNR/ZGF/AGNR) and (b) System 2 (ABNNR/ZGF/ABNNR).



(a) (b)

Fig. 4. Degree of spin polarization as a function of energy at the central part of system: (a) System 1 (AGNR/ZGF/AGNR) and (b) System 2 (ABNNR/ZGF/ABNNR).

occupies the 2p-orbital. Since the spin of this electron is uncoupled, it chooses its orientation in opposite direction to the spin of local edge magnetism to minimize the energy. Thus the ground state of the system is in favor of lowering total magnetization and lowering effective interaction of the spin of carriers with local magnetism. Therefore, there is a reduction in the total magnetism in system 2 and we less subband separation compared to that of the system 1.

The spin dependent conductance G was also calculated as a function of energy for both systems and the results are shown in the Fig. 3. As expected, in system 1 (Fig. 3a), there is a remarkably high conductance for one type of spin (G_{down}) of the carriers at the Fermi energy which is well separated in energy from the other spin orientation (G_{up}). Compared with system1, system 2, shown in Fig. 3b, indicate a reduction in spin filtering property, which is in accordance with the argument presented in above paragraph.

The spin-filtering efficiency for each system P is the degree of spin polarization defined as $P = \frac{G\uparrow - G\downarrow}{G\uparrow + G\downarrow} * 100$ where $G\uparrow$ and $G\downarrow$ are conductances for spin up and down carriers, respectively [6]. The function P was calculated for both systems under study and the results are presented in Fig. 4. Once again, we arrive at the above conclusions. That is, a higher spin polarization for system 1 (~%100) and, a considerable reduction of spin polarization for the system 2 (~%50), in Fermi level.

CONCLUSIONS

In summary, we have studied the spin filtering properties of two electronic devices consisting of a graphene nanoflake as the conducting channel. In first system, armchair-edge graphene nanoribbons are used as electrodes while second system has armchaire-edge boron-nitride nanoribbons electrodes. The study was performed using Hubbard model within the mean-field approximation, Green function technique and Landauer formalism. Total density of states, conductance and the degree of spin polarization were calculated for both systems. It has been expected that, these systems have to show spin filtering property due to the magnetization of the zigzag-edge of the ZGF. This was confirmed by our calculation. In first system, we obtained remarkably high conductance for one kind of spin orientation at the Femi energy which was well separated in energy from the conductance channel for the other spin orientation. However, our results show that presence of boron-nitride electrodes in second system reduces the spin filtering property. This is mainly due to the presence of boron atoms and as a result the interaction of the spin of valance electron of the boron atoms with the magnetization of the zigzag-edge of the ZGF, resulting in the reduction of total magnetization.

ACKNOWLEDGEMENTS

The authors are grateful to Mr M.Modaresi for very useful guidance. Also thank to Dr R. Farghadan and Dr A. Saffarzadeh for helpful discussions.

REFERENCES

[1] Q. Peng, W. Ji, S. De, Comp. Mater. Sci. 56 (2012).

[2] E.W. Hill, A.K. Geim, K. Novoselov, F. Schedin, P. Blake, IEEE 42 (2006) 2694.

[3] K.-H. Ding, Z.-G. Zhu, J. Berakdar, EPL 88 (2009) 58001.

[4] J. Mun´arriz, F. Dom´ınguez-Adame, P.A. Orellana, A.V. Malyshev, Nanotechnology 23 (2012) 205202.

[5] K. Wakabayashi, K. Sasaki, T. Nakanishi, T. Enoki, Sci. Technol. Adv. Mater. 11 (2010) 054504.

[6] A. Saffarzadeh, R. Farghadan, Appl. Phys. Lett. 98 (2011) 023106.

[7] T. Ozaki, K. Nishio, H. Weng, H. Kino, Phys. Rev B 81 (2010) 075422.

[8] M. Fujita, K. Wakabayashi, K. Nakada, K. Kusakabe, J. Phys. Soc. Jpn. 65 (1966) 1920.

[9] A. Lopez-Bezanilla, J. Huang, H. Terrones, B.G. Sumpter, Electronic Structure Calculations on Edge-functionalized Armchair Boron Nitride Nanoribbons.

[10] G.A. Nemnes, J. Nanomate. (2012).

[11] M. Petulante, N. Le, L.M. Woods, Electronic Structure Properties of Graphene/Boron-Nitride Layered Systems, 2011.

[12] M. Modarresi, M.R. Roknabadi, N. Shahtahmasbi, Physica E 43 (2011) 1751.