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Potential spin-polarized transport in gold-doped armchair graphene nanoribbons

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ABSTRACT

Based on NEGF-DFT computations, systematic investigation of electronic, magnetic and transport properties of AGNRs are done by employing Au through different doping mechanisms. Remarkable Au–AGNR bonding is observed in case of substitution due to the presence of impurity at the edges. Both substitution and adsorption of Au on AGNR surface induce significant changes in the electronic spin transport of the sp^2 hybridized carbon sheets. AGNRs are semiconducting with lower total energy for the FM configuration, and the I–V characteristics reveal semiconductor to metal transition of Au-doped AGNR. The spin injection is voltage controlled in all the investigated Au-doped AGNRs.

1. Introduction

Graphene, one of the newest materials today, can realize the concept of organic devices in near future. The electronic properties of graphene nanoribbons (GNR) are sensitive to their width, edge geometry, applied stress and the presence of foreign impurities which can be further used to tailor the electronic properties of GNR [1]. Lateral confinement in quasi one-dimensional GNRs leads to a band gap which is highly sensitive to the width and edge shape of the GNR thus opening possibilities to tailor the electronic properties of a device. Modification with various types of elements and functional groups exhibits variety of exotic properties, such as semiconductor with tunable band gap, metallicity and even half-metallicity obtained from the same nanoribbon. Moreover, alteration of the ribbon edges, substitution of host atoms of the nanoribbon with an appropriate guest can result in desired property from the nanoribbon [2]. Several theoretical and experimental investigations have focused on the modulation of physical and chemical properties of metal-doped armchair graphene nanoribbons (AGNRs) specifically [3–8] for various applications.

Studies have shown that graphene properties can be effectively altered by transition metal adsorption and can serve as potential materials in nanoelectronics, spintronics, or electrochemistry [9]. Graphene, a hexagonal arrangement of carbon atoms in a one atom thick layer has properties which could lend themselves to use in a new generation of electronics but devices thus obtained needs metallic contacts. To overcome this, recently, GNRs has been spot-welded to gold (Au) so that it can be used in electronic devices. Combining the microscopy experiments with theoretical modeling, a detailed analysis of the contacted nanoribbon properties was presented by Lit et al. [10]. Interaction between graphene and different configurations of Au adsorbates simulated by first principles calculations as reported in [11] revealed that, different properties of Au–graphene systems are induced by the chemical interactions between graphene and the Au atoms in different configurations.

In this work, we study the spin dependent electronic and transport properties of Au doped AGNRs in different configurations by employing density functional theory (DFT) based first-principles calculations. The ground state of pristine AGNRs is non-magnetic, the presence of Au impurities turn them magnetic in nature. In the present work, we probe the effects of spin polarization on the electronic and transport properties of Au adsorbed/substituted doped AGNRs and compare the findings with spin compensated calculations. Au substitution and adsorption is modeled on the edge-passivated AGNRs. Section 2 discusses the methodology used to obtain the presented results of the Au doped structures. The results and discussion is presented in Section 3 and the conclusions are summarized in Section 4.

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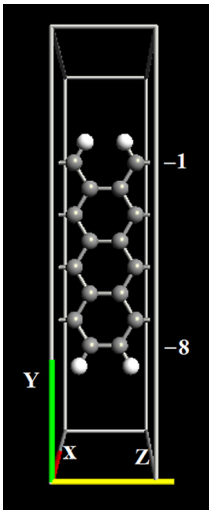

Fig. 1. The schematic representation of super cell of AGNR and the convention of defining the ribbon width ($N = 8$).

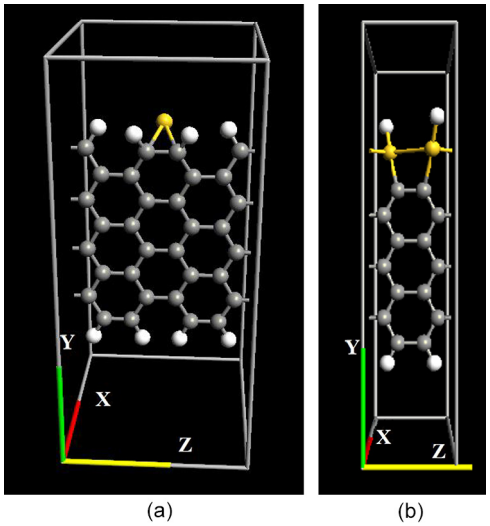

Fig. 2. The optimized geometry of AGNR due to Au (a) adsorbed in hole site (b) substituted at top edge.

2. Methodology

We perform Density functional theory (DFT) based first principles calculations to explore the spin dependent electronic and transport properties of Au doped AGNR. Atomistix Tool Kit Virtual NanoLab (ATK-VNL) simulation package [12] is used for the present calculations. The schematic diagram of AGNR and the convention of ribbon width have been shown in Fig. 1. The sites chosen for substitution are the top edge, both edges, center, position 2 (from the top edge) and position 3 (from the top edge) as shown in Fig. 1. We considered the plausible Au adsorption sites [13], viz. on atop, bridge and hole positions. To model the ribbons, supercell method is used and the cut off energy of 150 Ryd is selected. All the ribbons are optimized self consistently and all the atoms are fully relaxed so that the maximum force component on all atoms is less than 0.05 eV/Å. Ribbons were allowed to grow along z axis whereas rests of the two directions were confined. We use a k-point grid of $1 \times 1 \times 100$ for the sampling of Brillouin zone. In this work, the exchange correlation functional local density approximation (LDA) is used in all of the present calculations. We consider the two-probe geometry system within the framework of nonequilibrium Green's function (NEGF) formalism where the system is divided into three parts, namely, left and right leads as well as a central scattering region.

After the geometry optimization of considered ribbons, the structural stability, electronic band structure, density of states (DOS) and current–voltage (I–V) characteristics are calculated. The results, thus obtained were compared with that of pristine ribbons. Fig. 2 represents the optimized geometry of Au-adsorbed and Au substituted AGNR. Fig. 3 shows the two probe model of H-passivated AGNR with Au substituted at center.

On optimization, we notice that the atomic structure of the edges of the ribbon is influenced due to Au substitution, whereas on adsorption, it is observed that the Au adatom placed at bridge site migrates to the nearby atop site [13].

We also carried out structural optimization with spin-polarized DFT for all the above mentioned sites of the AGNR, where the same tendency is found with small difference in the total energies. Moreover, the gold atom at equilibrium adsorbs at the vertical of a carbon atom (that is in the direction of the carbon p_z orbital) due to spin and its non-inclusion. Recent DFT studies predict that transition metals generally adsorb at the hole site though Au atoms have been predicted to adsorb preferentially to the atop (A) site [14], we observe no matter where the Au atom is initially placed bridge, hole, or atop site, it always finds its minimum energy state at the hole site after relaxation for both ferromagnetic (FM) and antiferromagnetic (AFM) cases.

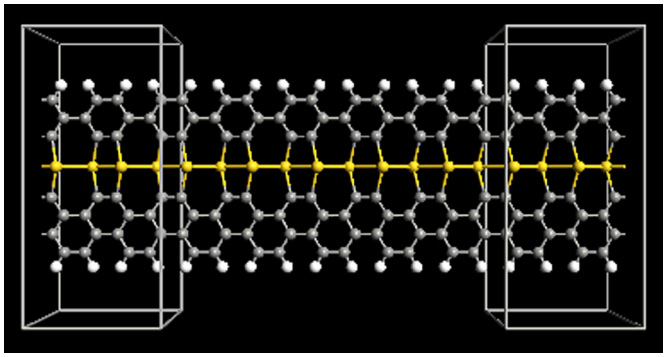

Fig. 3. The two probe model of H-passivated AGNR with Au substituted at center.

To calculate the transport properties, we used two probe models. ATK comprises DFT-based first-principles approach together with NEGF to calculate the transport properties of the central atomic system coupled with left and right semi-infinite electrodes. The calculation of the complete system is obtained from calculations of the two electrode regions, and a central scattering region. The spin-dependent current through the system is obtained from the Landauer–Buttiker formula

$$I_\sigma = \int_{-\infty}^{+\infty} T_\sigma(E, V_b)\big[f_L(E-\mu_L) - f_R(E-\mu_R)\big]dE \quad [5] \qquad (1)$$

where $f_{L/R}\ (E, V_b)$ is the Fermi Dirac distribution function for the left (L)/right (R) electrode, $\mu_{L(R)}$ are electrochemical potentials of the left and right electrodes and the difference of them is given by eV_b with the applied bias voltage V_b and T_σ is the transmission coefficient from left (L) lead to right (R) lead, which can be expressed as

$$T_\sigma = T_r\big(\Gamma_R G_C^R \Gamma_L G_C^A\big) \qquad (2)$$

where G_C^R and G_C^A are the retarded and advanced Green's functions of the conductor, respectively, and $\Gamma_{L(R)}$ is the coupling matrices from the conductor to the left (right) lead.