The effect of vacancy-induced magnetism on electronic transport in armchair carbon nanotubes

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(Dated: October 4, 2018)

The influence of local magnetic moment formation around three kinds of vacancies on the electron conduction through metallic single-wall carbon nanotubes is studied by use of the Landauer formalism within the coherent regime. The method is based on the single-band tight-binding Hamiltonian, a surface Green's function calculation, and the mean-field Hubbard model. The numerical results show that the electronic transport is spin-polarized due to the localized magnetic moments and it is strongly dependent on the geometry of the vacancies. For all kinds of vacancies, by including the effects of local magnetic moments, the electron scattering increases with respect to the nonmagnetic vacancies case and hence, the current-voltage characteristic of the system changes. In addition, a high value for the electron-spin polarization can be obtained by applying a suitable gate voltage.

PACS numbers: 72.10.-d, 72.10.Fk

INTRODUCTION

The electrical transport properties of single-wall carbon nanotubes (CNTs) and other carbon-based materials have attracted much attention due to their unusual properties and great potential for technological applications [1–4]. Among these features, the ballistic electron conduction and the long range spin coherent transport for perfect and defective single-wall CNTs have been investigated theoretically and experimentally [5–7]. These important properties of spin polarized electrons in single-wall CNTs has motivated their use in the emerging field of spin electronics [8] which aims to effectively control and manipulate the spin degrees of freedom in the electronic devices [9].

In order to achieve spintronic devices based on single-wall CNTs, it is important to understand the magnetic effect of vacancies and impurities on the electron conduction [8, 10, 11]. because, the electronic properties of carbon-based materials strongly depend on their topological structure [12]. Therefore the electronic structure of the CNTs can differ due to the topological defects or the addition of different compounds. On the other hand, in the transport processes, the ballistic conductance depends on the number of conducting channels at the Fermi energy [13]. Consequently, the appearance of the vacancy defects in a structure can change the electronic and transport properties of the system [5]. Also, the conductance of an imperfect system is lowered due to the reflection of electron waves from the defects [14]. In addition, the localized states near the vacancy are magnetic and change the net magnetic moments in the carbon-based nanostructures. The honeycomb lattice of graphene sheet is formed by two sublattices A and B (bipartite lattice). For a bipartite lattice with different numbers N_A and N_B of sites and the Hubbard repulsive parameter, the total spin, S, of the ground state of the system, which is mainly localized near the vacancy, is $2S = N_A - N_B$ [15]. This important feature can block and change the spin transport especially near the Fermi energy.

In this regard, the electronic and magnetic properties of vacancies in single-wall CNTs [16] and graphene nanoribbons [17] have been investigated. In addition, the electron-spin polarization has been observed in the CNTs when doped with magnetic adatoms or molecules [18]. Moreover, the localized states of the impurity can change the spin-polarized conduction in the presence of a gate voltage or applied bias [8, 19]. Recently, the effect of vacancy on the conductance of single-wall CNTs [20, 21] and the spin-dependent transport properties in ferromagnetically contacted single-wall CNTs have been investigated [19, 22, 23], but the magnetic behavior of vacancy defect as regards the transmission of single-wall CNTs has not been considered.

The purpose of this work is to study the effect of magnetic vacancies on the spin-polarized transport through armchair CNT junctions and manipulate this polarization by means of gate voltages. We simulate ideal vacancies which are made by removing carbon atoms from lattice sites without including the deformation of the tube wall around the vacancies. We consider three typical vacancy types. For the first type, a single carbon site (A or B) is removed. For the second one, two same sites (two A or B sites), and in the last type, four A sites in one carbon ring are removed, as shown in Figs. 1(a) and 1(b), respectively.

Using the single-band tight-binding approximation and the mean-field Hubbard model [24], the electronic structure and the localized magnetic moments around the above-mentioned vacancies are calculated. Also, using the non-equilibrium Green's function technique and the Landauer-Büttiker theory [25], the spin-polarized transport in defective single-wall CNTs is investigated.