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Analytical study of the ballistic transport of ladder-like graphene nanoribbons within the tight-binding approach

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ABSTRACT

We analytically study the electronic transport properties of ladder-like graphene nanoribbons using Green's function method within the tight-binding approach. We first renormalize the system to have a uniform ladder network with energy dependent tight-binding parameters. Then, we convert the ladder network into two independent uniform simple chains by separating its Hamiltonian modes. Next, we calculate the density of states and transmission coefficient of the considered nanoribbons by employing the corresponding exact analytical formulas related to a uniform chain. Finally, we apply this formalism to some different configurations of brunched and un-brunched nanoribbons and discuss the electron tunneling through such structures. It turns out that in the un-brunched cyclic nanoribbons the electron tunnels easier than the brunched cyclic ones in the center wire gap regions.

1. Introduction

Graphene has attracted a great deal of interest due to the unique electrical, thermal, and mechanical properties after its successful preparation [1–3]. The excellent mechanical properties and easily tunable electron concentration as well as simple production are some advantages that make graphene a greatly favorable material [2–4]. Recently, it is realized that the graphene is a promising material to

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improve the characteristics of electronic devices [5]. Both theoretical [6–9] and experimental [10–12] works exhibit that the band gap of graphene can be created and controlled by edge chirality and width of nanoribbon. Moreover, some chemical groups such as hydrogenated (CH), carbonyl (COH), carboxyl (COOH) and amines (NH_2), could be attached to the edges of the graphene nanoribbons, which are more chemically reactive [3].

The purpose of this paper is analytical treatment of the electronic transport of ladder-like graphene nanoribbons in the presence and absence of hydrogen atoms. Until recently, the molecule in the molecular electronic devices was typically attached between two normal metal (e.g. gold) electrodes [13–18]. However, in this paper, we study the conductance of a finite ladder-like nanoribbon which is connected to two semi-infinite nanoribbons. For this purpose, first we convert the system Hamiltonian into the Hamiltonian of a ladder network. Then, we convert this system to two independent simple chains with renormalized hopping and on-site energies. We then apply the analytical formulas related to a simple chain [19] on these uniform chains and derive exact analytical formulas for calculation of the density of states (DOS) and transmission coefficient (T) based on the nearest neighbor tight-binding approach. Finally, we apply the formalism to study the conductance of some different configurations of hydric and non-hydric ladder-like nanoribbons in the presence/absence of the C–H hopping energies.

The outline of the paper is as follows: in Section 2, we introduce our model which is based on Green's function method at the tight-binding approach. In Section 3, we examine the analytical formalism derived in Section 2 for some configurations of ladder-like nanoribbons. Finally, in Section 4, we summarize the most important results of the paper.

2. Model and formalism

In this section, we analytically describe transport properties of ladder-like graphene nanoribbons depicted in Fig. 1 at tight-binding approach using Green's function technique. Figure 1a and b show two ideal infinite non-hydric (with *uniform* C–C bonds which we call U) and hydric (with *single* and *double* C–C bonds which we call SD) nanoribbons, respectively. In the U nanoribbon there is no C–H bond which hereafter is called *unbranched* nanoribbon. While in the SD case, each benzene includes two C–H bonds which hereafter is called *branched* nanoribbon. Also, Fig. 1c and d, respectively, display two different configurations constructed from U and SD systems namely a finite hydric between two non-hydric semi-infinite hydric (U/SD/U) and a non-hydric between two semi-infinite hydric nanoribbons (SD/U/SD). As it is described in Fig. 2a, at the tight-binding approach, we can reduce such systems to ladders with renormalized energy dependent on-site and hopping terms. Then, we convert each reduced ladder to two independent upper (+) and lower (−) simple uniform chains as shown in Fig. 2b

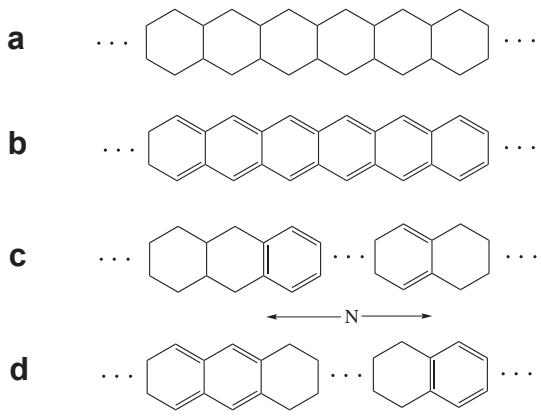

Fig. 1. (a and b) Show the infinite ladder-like *uniform* (U) and *single-double* (SD) bonds graphene nanoribbons, respectively. (c) Shows a finite SD nanoribbon embedded between two semi-infinite U nanoribbons (U/SD/U) and (d) displays the reverse situation of (c) i.e, SD/U/SD.