Physica E 84 (2016) 22–26

Contents lists available at ScienceDirect

Physica E

journal homepage: www.elsevier.com/locate/physe

Effect of substitutional impurities on the electronic transport properties of graphene

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HIGHLIGHTS

- Electronic transport in doped graphene ribbon is studied using DFT.
- B, N and Si atoms are used to substitute the center or edge carbon atoms.
- Si-doping results in better electronic transport.
- The transmission spectrum also depends on the location of the dopants.
- The are explained in terms of electron localization near the impurities.

ARTICLE INFO

Article history:
Received 1 February 2016
Received in revised form
18 May 2016
Accepted 19 May 2016
Available online 24 May 2016

Keywords:
Graphene
Transmission
Density functional
Doping

ABSTRACT

Density-functional theory in combination with the nonequilibrium Green's function formalism is used to study the effect of substitutional doping on the electronic transport properties of hydrogen passivated zig-zag graphene nanoribbon devices. B, N and Si atoms are used to substitute carbon atoms located at the center or at the edge of the sample. We found that Si-doping results in better electronic transport as compared to the other substitutions. The transmission spectrum also depends on the location of the substitutional dopants: for single atom doping the largest transmission is obtained for edge substitutions, whereas substitutions in the middle of the sample give larger transmission for double carbon substitutions. The obtained results are explained in terms of electron localization in the system due to the presence of impurities.

1. Introduction

Recent advances in experimental fabrication techniques have opened new possibilities to manufacture new low-dimensional materials and to study their fundamental properties. Among those materials, graphene – a monolayer of hexagonally arranged carbon atoms – has attracted a lot of interest in the past few decades due to its unique electronic structure and transport properties [1,2]. Graphene has the potential to be used for practical applications in the field of electronics and photonics [3,4]. Graphene is also considered as a promising material for sensor applications (see, Ref. [5] for review) due to its exceptionally high surface-to-volume ratio, high charge carrier conductivity, low contact resistance [6], and low thermal noise [7]. In addition, the electronic properties of graphene can further be tuned using external fields, which also increases its potential for practical applications.

Edge and surface modifications with different functional groups are considered as an effective tool in refining structural, thermal, electronic and other measurable properties of pristine graphene [8,9]. Chemical doping of graphene with foreign atoms is considered as one of the grand challenges for the development of graphene-based devices for multiple applications. In this respect, B and N doping is a common method to tune the properties of graphene [10–12]. Such substitutional doping has a profound effect on the charge carrier transport in graphene. For example, for an ordered location of the dopants, the electronic transport can be significantly enhanced [13,14]. Charge carrier rectification [17] and negative differential resistive phenomena [14] are also reported for such hybrid systems. The effect of boron and nitrogen substitution on the transport properties of graphene nanoribbons as a function of the defect distance from the edge of the sample was recently analyzed for both zig-zag edges [15] and armchair edges [16].

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http://dx.doi.org/10.1016/j.physe.2016.05.024
1386-9477/

In this work, we use density-functional theory (DFT) in combination with the nonequilibrium Green's function formalism to study the electronic transport properties of zig-zag graphene nanoribbons with substitutional doping with B, N and Si atoms. As an example, we consider single and double substitutions either at the edges of the sample or in the middle of the nanoribbon. We found that Si substitution results in better transmission for both locations of the dopants as compared to the use of other dopants. Depending on the type of dopant, prominent changes are obtained in the transmission spectrum of the system due to the formation of strongly localized electronic states. The response of the system to an applied potential difference is also studied.

2. Computational details

As an example, we consider a hydrogen-terminated zig-zag graphene nanoribbon of width 11.37 Å. Single and two carbon atoms are substituted respectively with B, N and Si atoms, where the substitutions are done either at the edge of the sample or in the middle of the sample. All considered samples are first optimized using DFT calculations within the generalized gradient approximation (GGA) of Perdew–Burke–Ernzerhof (PBE) for the exchange–correlation energy [18]. The Brillouin zone sampling was performed using $1 \times 1 \times 12$ k-point sampling [19]. The electrostatic potentials were determined on a real-space grid with a mesh cutoff energy of 150 Ry and double-zeta-double-polarized basis sets of local numerical orbitals were employed for all atoms. van der Waals interactions were accounted for by using Grimme's DFT-D2 empirical dispersion correction [20] to the PBE. Using the optimized structures, we constructed device geometries (see Fig. 1), which consists of left and right regions and the central (scattering) region (i.e., a two probe configuration). The electrodes are modelled as an electron gas with a fixed chemical potential. The transmission is calculated along the z-direction. Quantum transport properties of all the considered systems were calculated using the nonequilibrium Green's function formalism with the Brillouin zone sampled with (1, 1, 100) points. All simulations were conducted using the first-principles computational package Atomistix toolkit (ATK) [21].

3. Results and discussions

As a typical example, we study a graphene nanoribbon with zigzag edges. The edge atoms are terminated by hydrogen atoms to obtain better structural and electronic stability and saturates the carbon 2p states dangling bonds at the edges which give rise to localized states in the bare graphene nanoribbon. We consider single and double carbon substitutions by B, N and Si atoms either at the edges of the sample (Figs. 1a and c) or in the middle of the ribbon (Figs. 1b and d). In our device geometries, the size of the active layer was 24.61 Åand the size of the electrodes was 7.38 Å. After optimization, B and N atoms stay in the same plane of graphene, whereas a small vertical displacement is obtained for Si atoms due to their larger atomic radius.

We start by considering the effect of single carbon substitution on the electronic transport in the graphene nanoribbon. Fig. 2 shows the zero-bias transmission spectra (a) and device density of states (DDOS) (b) as a function of the electronic energy for samples with edge doping. Solid-black curves show the results for pristine graphene as a reference. In the latter case, $T(E)$ exhibits a sequence of steps of integer transmission and an enhanced transmission at the Fermi level, which are typical for graphene nanoribbons (see solid-black curve in Fig. 2(a)). This feature in the transmission spectrum originates from the edge-localized electronic states with

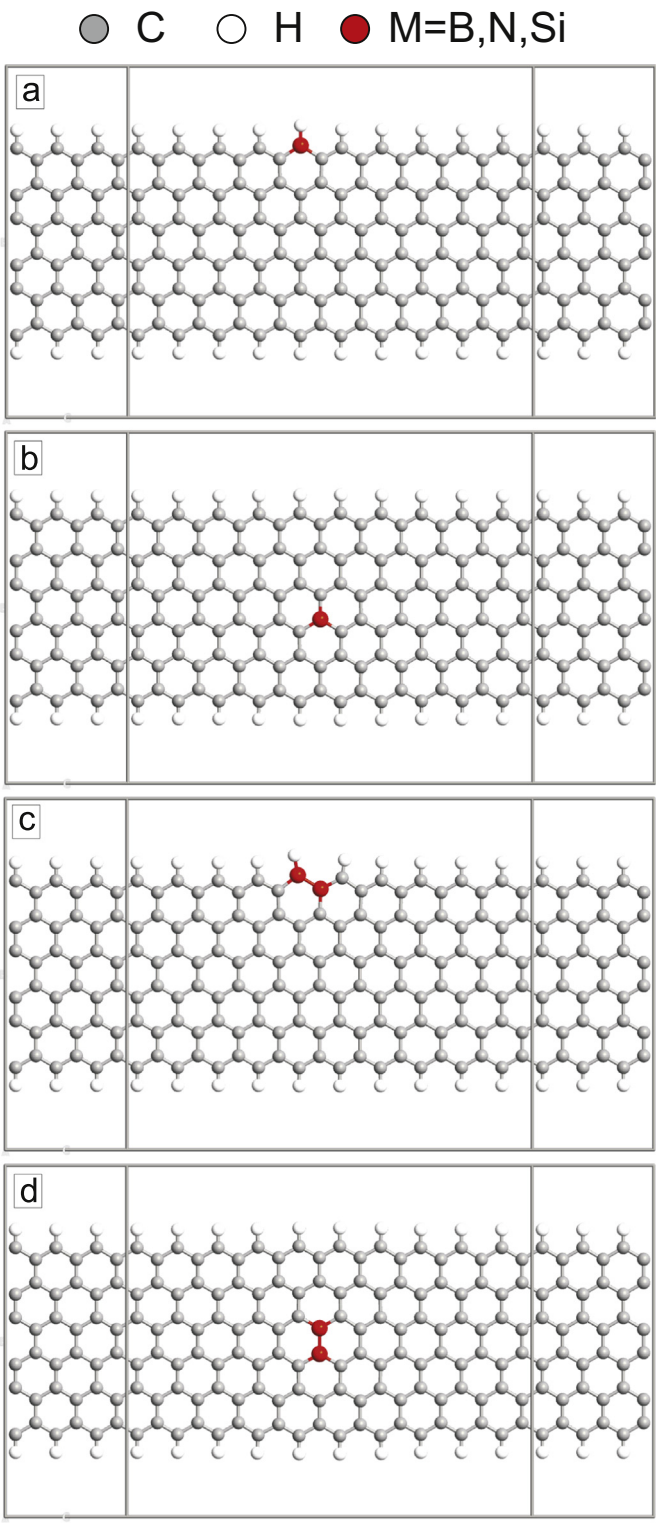

Fig. 1. Device geometries: hydrogen passivated graphene nanoribbons with single (a and b) and double (c and d) substitutional doping at the edge (a and c) and at the center (b and d). Substitutions are performed with B, N and Si.

energies close to the Fermi energy. The transmission spectrum changes drastically when B and N atoms substitute the edge carbon atoms (dashed-red and dotted-green curves). $T(E)$ becomes smaller at the Fermi level and it drops sharply with increasing (decreasing) electron energy away from the Fermi energy for B and N doping. In fact, electrons can be totally reflected at these small energies. Interestingly, the obtained minima in the transmission