



Size dependence rectification performances induced by boron and nitrogen co-doping in rhombic graphene nanoribbons



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ABSTRACT

Rectification performances of rhombic graphene nanoribbons coupled to gold electrodes through thiolate bonds with left and right vertical carbon atoms substituted by one nitrogen or boron atom are analyzed by performing theoretical calculations using a self-consistent *ab initio* approach that combines the density functional theory with the non-equilibrium Green's function formalism. Increasing the size of graphene nanoribbon markedly improves the rectification effect because of the asymmetric potential profile distribution in rhombic graphene for polarization near the boron and nitrogen atoms.

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1. Introduction

Using individual molecules as possible units in nanotechnology has been a major goal for electronic devices with continuous miniaturization of silicon-based electronic devices and rapid development of microelectronics. Developing high-performance and thermally stable ingredients are important global issues in molecular electronics. Molecular devices have received considerable interdisciplinary interest. Experimental and theoretical analyses indicate that using a single molecule to construct an electronic device is capable of realizing basic electronic functions, such as negative differential resistance (NDR) [1], current rectification [2,3] and current switching [4,5]. The molecular rectifier proposed by Aviram and Ratner in 1974 [6] has a key function in developing molecular electronic devices because this rectifier is the simplest functional element in constricting electronic circuits [7]. Several studies have been performed on molecular rectifiers [8–10] and possible mechanisms have been posited, such as the unequal Schottky barriers under positive and negative biases [11], asymmetric coupling of a molecule to electrodes [12], localization of frontier molecular orbitals [13], asymmetric shift of molecular levels under biases of different polarities [14] and modification of molecular conformation under an external field [15].

Graphene has been beneficial for nanoelectronic analyses since its first preparation in 2004 [16]. However, 2D graphene is a semimetal material that significantly limits its applications in microelectronics. Boron or nitrogen atoms are representative substitutes among foreign atoms and are adopted frequently in graphene because of the stronger and more covalent bonds between B, N, and C compared with that of the host CC [17]. Doped graphene has been synthesized successfully in experiment [18]. Chemical doping with boron or nitrogen atoms on graphene has gained interest and has yielded interesting transport properties because of this synthesis. For instance, Deng et al. studied the electron transport properties of a heterostructure comprising N- and B-doped trigonal graphene nanoribbons, which has manifested rectifying behavior in this molecular device. Zhao et al. found that N-doping density and position could modulate the rectification properties and induce NDR behavior in graphene nanoribbons [19]. Zigzag-edged rhombic graphene nanoribbons (ZRGNRs) are nano-sized graphene flakes produced by geometric cutting of graphene. Fan et al. studied the site effects of B/N doping on the current–voltage (*I*–*V*) characteristics of ZRGNRs, in which significant NDR behavior has been observed in B-doped ZRGNRs [17]. To the best of our knowledge, the rectifying properties induced by B/N doping in ZRGNRs have not been reported. In this Letter, we report the results of theoretical analyses on molecular rectification achieved by B and N co-doping in ZRGNRs. Rectification effect is markedly improved by increasing the size of central ZRGNRs.

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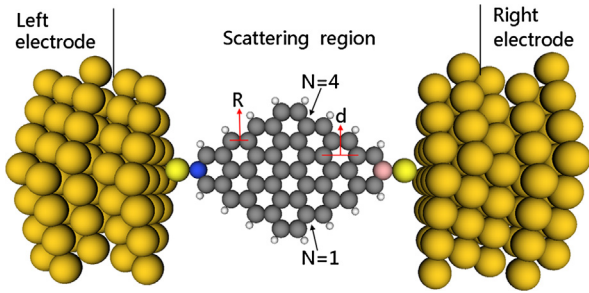


Fig. 1. Schematic of a molecular device in the simulations. ZRGNRs are coupled to both flat (4×4) Au (111) electrodes through the thiol groups, in which the vertical carbon atoms are substituted by one nitrogen or boron atom.

2. Simulation model and computational details

Fig. 1 shows the studied molecular devices. Each comprises the left electrode, the right electrode, and the scattering region. The scattering region or the device area includes two Au layers placed on each side to screen the potential effect of embedded ZRGNRs to Au electrodes and consider molecule–electrode coupling. Central ZRGNRs are saturated with hydrogen atoms. The size parameter N denotes the number of carbon atoms in ZRGNRs. Models M1, M2, and M3 correspond to $N = 2, 3, 4$ in our calculation. R is the bond length of two adjacent carbon atoms, and d is the distance of two next nearest neighbor carbon atoms. We set $R = 1.42 \text{ \AA}$ and $d = 2.46 \text{ \AA}$ in the initial structures, and the geometry is optimized until all residual forces on each atom are $< 0.05 \text{ eV/\AA}$. Sulfur atoms are chosen to be located at the hollow site of Au triangles with Au–S distance of 2.45 \AA representing a relaxed molecule–electrode separation for specific Au (111) flat electrodes used in our calculation.

Based on our previous work [20], geometric optimization and first-principle electron transport calculations for the two-probe system are performed using density functional theory (DFT) combined with nonequilibrium Green's function (NEGF) technique implemented in the latest version of Atomistix Toolkit [21–24]. The reliability of this method has been demonstrated in some studies in which calculated results are compared with experimental data [25–28]. The generalized gradient approximation scheme of Perdew–Burke–Ernzerhof (GGA,PBE) is employed to describe the exchange–correlation potential in the self-consistent DFT electronic structure. The core electrons are modeled with Troullier–Martins [29,30] norm-conserving pseudopotentials, and the valence electrons are expanded in a SIESTA localized basis set. We used the double- ζ polarized basis set for all atoms of the scattering region and the single- ζ polarized basis set for Au atoms to save computational effort and to improve calculation precision and reliability. The Brillouin zone has been sampled with $1 \times 1 \times 300$ points, and a mesh cutoff energy of 100 Ry is selected to balance the calculation efficiency and the accuracy. The convergence criterion for Hamiltonian and electron density is set to 10^{-5} in total energy. The nonlinear current through the electrode–molecule–electrode sandwich system as a function of the external applied bias can be calculated using the Landauer–Büttiker formula [31], thereby determining the current from the integral area of transmission curves inside the bias window.

3. Results and discussions

The current is of direct interest because it corresponds to an experimentally observable quantity. **Fig. 2(a)** shows the self-consistently calculated currents as a function of the applied bias voltages of three molecular devices (**Fig. 1**) plotted between -1.0 V to 1.0 V with increments of 0.2 V . Several important fea-

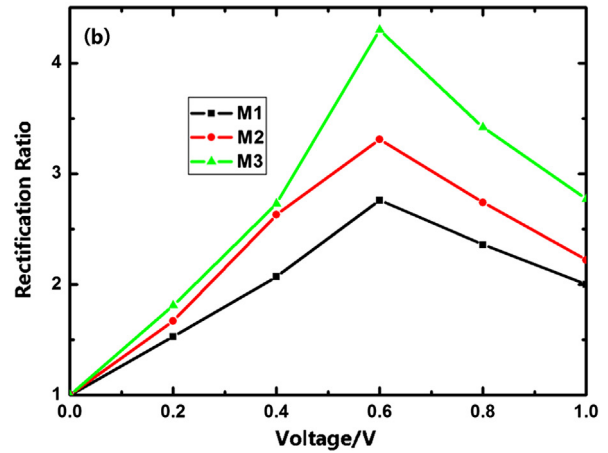
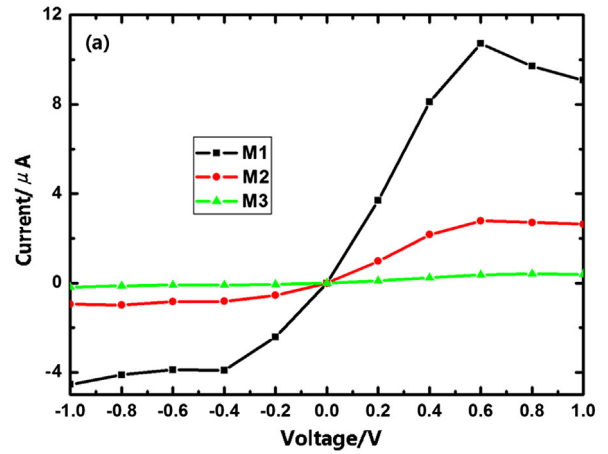


Fig. 2. (a) I – V curves and (b) rectification ratio change with the applied bias voltage for models M1 to M3.

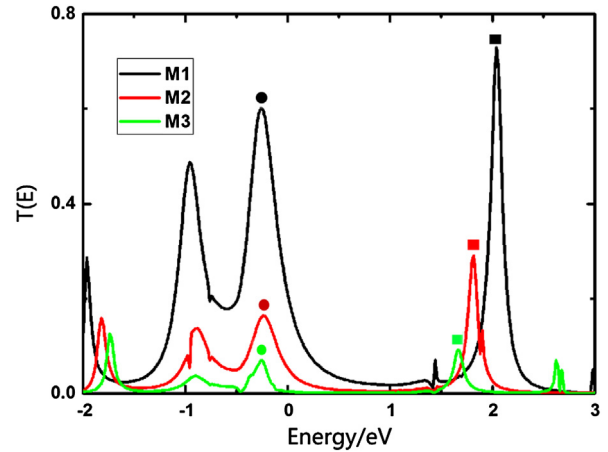


Fig. 3. Transmission spectra of models M1 to M3 at zero voltage. The average Fermi level of the Au electrodes defines the zero energy level.

tures in the evolution of currents are clearly visible. (1) Increasing N of ZRGNRs decrease the current markedly. When $N = 4$, the current reaches its minimum with very small leakage current of $< 0.4 \mu\text{A}$. (2) The I – V curves of these models show asymmetric behavior, which has gained interest because of its necessity for electronic rectifiers. (3) This asymmetric behavior is sensitive to the N of the central graphene. **Fig. 2(b)** shows this asymmetry evaluated by a rectification ratio defined as the ratio of currents under positive and negative biases for the same voltage, and is calculated as $R(V) = I(V)/|I(-V)|$. Model M3 shows stronger

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