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# Influence of boundary types on rectifying behaviors in hexagonal boron-nitride/graphene nanoribbon heterojunctions

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ABSTRACT

We investigate the effect of boundary types on the rectifying behaviors in heterojunction composed of zigzag graphene and hexagonal boron-nitride (BNC) hybridized nanoribbons by employing nonequilibrium Green's functions in combination with the density-functional theory. The results demonstrate that the rectifying behavior is strongly dependent on the boundary types, while little affected by the width of BNC hybridized nanoribbons. It is noteworthy that the maximum rectifying ratio of the system at finite bias can be high up to orders of $10^7$ in which atoms carbon in graphene nanoribbon are totally connected with atoms nitrogen in boron-nitride nanoribbon. The mechanism is proposed for these phenomena.


## 1. Introduction

Graphene, since its first successful fabrication in 2004, has attracted tremendous attention due to its special two-dimensional honey atomic structure, unique electronic transport properties, and potential applications in the field of nanoelectronics [1–4]. More and more researches have identified that graphene can be a perfect nanomaterial for constructing molecular devices [5–8]. To further broaden its application, many feasible ways have also been adopted to tune its electronic properties, such as hybridization [9–13], surface adsorption [14], chemical modification [15], and external strain [16]. In particular, the atomic layer of hybridized hexagonal boron nitride (h-BN) and graphene, since its successful fabrication experimentally [17,18], has attracted a great deal of attention owing to its unusual physical properties, such as magnetism [19,20], unique thermal transports [21–23], and robust half-metallic behavior [24–27].

However, it is thought that many fundamental issues are still not clear, such as the edge type at the boundary of hybridized h-BN and graphene domains. To clarify it, more recently, Gao etc. al [28] have succeeded in growing nearly seamless BNC hybrids on a substrate of Rh(111) and have achieved atomically resolved structures of the boundaries linking graphene and h-BN, from which it can be inferred that it is of particular importance for its precise structural modulation for high-performance electronic devices. Next, some theoretical researches should be done systematically to keep pace with it about boundary types influencing on the electronic properties. Therefore, in this paper, zigzag graphene and BNC hybridized nanoribbons with four different edge types are constructed to study the corresponding transport properties under the finite bias. Our results show that the hybridization system can present different rectifying effect depending on the boundary type rather than the width of BNC hybridized nanoribbons. It is noteworthy that the maximum rectifying ratio of the system at finite bias can be high up to orders of $10^7$ in which atoms carbon in graphene nanoribbon (GNR) are totally connected with atoms nitrogen in boron-nitride nanoribbon (BNNR), showing that the system possesses the potential value on designing high-performance electronic devices.

## 2. Simulation model and calculation method

The heterojunctions considered are based on n-zigzag BNNR (n-ZBNNR) and n-zigzag GNR (n-ZGNR) structures with various boundaries, as shown in Fig. 1, where the prefix "n" represents width of the nanoribbons. We created a two-probe system that is divided into three regions: the left electrode, the right electrode and the scattering region. The semi-infinite Left (right) electrode is described by a supercell with two repeated B-N (C) unit cells along

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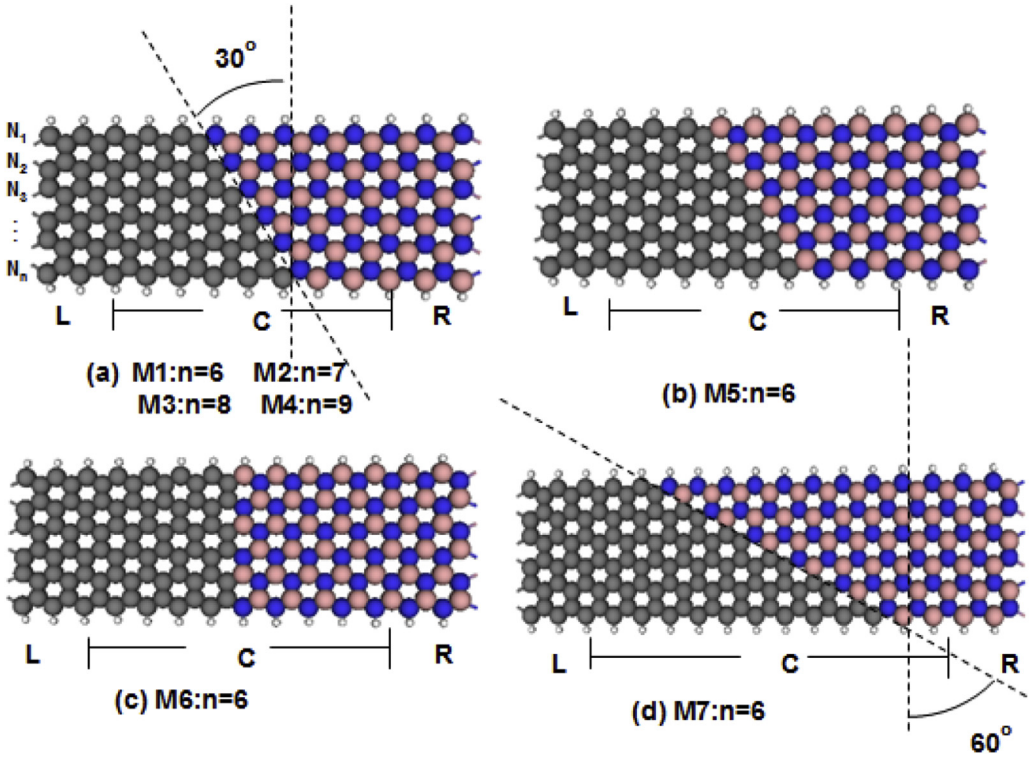


**Fig. 1.** Geometric structures in our simulations, where n denotes the ribbon widths of BNC hybridized systems. Atoms colored gray, pink and blue denote atoms carbon, boron and nitrogen respectively. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

transport direction, and the scattering region is BNC hybridized nanoribbon in the intermediate of which ZBNNR and ZGNR are hybridized with four types edges. We have chosen a supercell with a vacuum of more than 10 Å in the x and y directions, which is large enough to keep the device from any interaction with its mirror images.

The nonlinear current through the central scattering region is calculated using the Landauer formula [29]:

$$I(V_b) = \frac{2e}{h}\int T(E,V_b)[f_l(E-\mu_l) - f_r(E-\mu_r)]\mathrm{d}E, \quad (1)$$

where $\mu_l$ and $\mu_r$ are electrochemical potentials of the left and right electrodes respectively. The difference of them is $\mu_l - \mu_r = eV_b$. In the transmission spectrum, the energy region which contributes to the current has been known as the bias window. The total transmission probability:

$$T(E,V_b) = Tr\left[\Gamma_l G^R \Gamma_r G^A\right] \quad (2)$$

where $G^{R(A)}$ is the retarded (advanced) Green functions of the central region. We perform the geometrical optimization of the model structures and the calculation of electron transport properties by applying an *ab initio* software package, ATOMISTIX TOOLKIT (ATK) [30,31] based on fully self-consistent non-equilibrium Green's function and density functional theory. The local-density approximation (LDA) has been used to describe the exchange-correlation potential and single $\xi$ polarization basis set was used for the geometrical optimization and the electronic transport calculation. The core electrons are described by norm-conserving pseudopotentials. The k-point sampling is 1, 1, and 100 in the *x*, *y*, *z* direction respectively, and the cutoff energy is set to 150 *Ry* to achieve the balance between calculation efficiency and accuracy. All structures were relaxed until atomic forces were below 0.02 eV/Å and the convergence criterions for Hamiltonian and the electron density were $10^{-5}$ eV.

## 3. Results and discussions

### 3.1. Influence of width on rectifying behaviors

Firstly we consider the electronic transport properties of the structures which have the same boundary as those shown in Fig. 1(a), but with four different widths, namely M1, M2, M3 and M4 (the ribbon width is 6, 7, 8 and 9 respectively). The self-consistently calculated current–voltage ($I$–$V$) characteristics for the above models in a bias range from −2.0–2.0 V are shown in Fig. 2(a). Two important features of the curves can be addressed as follows: (i) for all of M1–M4, the corresponding $I$–$V$ curves are completely asymmetric, which present strong rectifying behaviors. What is more, under negative bias, the current is increasing with the bias, while the current under positive bias is greatly suppressed. (ii) There is no obvious change in the tendency of the $I$–$V$ curves when the ribbon width increasing. Inset in Fig. 2(a) shows the rectification ratio of M1 via bias voltage, which is defined as $R(V) = I(V)/|I(-V)|$ where $I(V)$ and $I(-V)$ are the current at positive and negative voltages with the same voltage magnitude. The rectifying ratio is high up to orders of $10^7$, showing it can be a candidate of high-performance rectifier.

To explore the origin of the obvious rectifying performance above, we plot a series of transmission spectra under several typical biases for M1, M2, M3 and M4 respectively in Fig. 3 and the molecular projected self-consistent Hamiltonian (MPSH) of LUMO (lowest unoccupied molecular orbital) in Table 1. It is well known