



ELSEVIER

Contents lists available at ScienceDirect

## Solid State Communications

journal homepage: [www.elsevier.com/locate/ssc](http://www.elsevier.com/locate/ssc)

# The effects on the electronic properties of BN nanoribbon with C-chain substitution doping



Zhiyong Wang<sup>a,\*</sup>, Yayun Zhao<sup>a</sup>, Mengyao Sun<sup>a</sup>, Jianrong Xiao<sup>a</sup>, Maowang Lu<sup>a</sup>, Liu Wang<sup>a</sup>, Yaping Zeng<sup>a</sup>, Mengqiu Long<sup>b</sup>

<sup>a</sup> College of Science, Guilin University of Technology, Guilin 541008, China

<sup>b</sup> School of Physics and Electronics, Central South University, Changsha 410083, China

## ARTICLE INFO

## Article history:

Received 17 February 2016

Received in revised form

21 April 2016

Accepted 29 April 2016

by L. Brey

Available online 3 May 2016

## Keywords:

A. Boron–Nitrogen nanoribbon

A. Graphene

D. Electronic property

E. Density functional theory

## ABSTRACT

The electronic properties of Boron–Nitrogen (BN) nanoribbon with Carbon (C)-chain substitution doping are investigated by performing first-principle calculations based on density functional theory. For the zigzag BN nanoribbon, the spin-unpolarized calculated results exhibit the insulator–semiconductor–metal transition with the number of substitution C-chain increasing. But for the armchair BN nanoribbon in the spin-unpolarized calculations, it is found that it appears the insulator–metal–semiconductor transition. The band gap of BN nanoribbon can be tuned according to the C-chain doping ratio. Interestingly, spin-polarized calculations exhibiting half-metallic may be tuned by changing the number of C-chain in the zigzag BN nanoribbon, opening a possibility in spintronics device based on BN nanoribbon.

© 2016 Elsevier Ltd. All rights reserved.

## 1. Introduction

One-dimensional (1D) single atomic layer nanoribbons have attracted intensive interest due to their huge potential applications in nanoelectronics and spintronics. Among them, monolayer boron nitride nanoribbons (BNNRs) show tremendous possible applications in nanoscale devices [1–3] due to their unique properties, such as wide band gap et al. Graphene nanoribbons (GNRs) are patterned from graphene, which have been predicted to be a potential candidate for the next-generation electronic devices [4–6]. Because of their novel electronic properties and potential applications in nano devices, the hybrid systems of BNNRs and GNRs attract intense interest among the researchers. Recently, the hybrid Graphene–BN monolayer materials consisting of separate BN and graphene domains have been successfully fabricated, implying a possibility of making hybrid C–BN nanoribbons with a more uniform BN and graphene domains by tailoring the hybrid C–BN monolayer materials with some physical methods [7]. The growth and interface formation of monolayer graphene–BN heterostructures on ruthenium have been investigated [8].

The opening of a variable bandgap of hybrid graphene–BN single monolayer has been predicted by the First-principles calculations [9–11]. Many previous theoretical studies have shown

that the half-metallicity can be found in both GNRs and BNNRs, such as, by applying an in-plane external field [12–13], through chemical functionalizing the edges [14–17], and controlling the edge states by doping [18–19], or by hydrogenation [20–25], thereby enabling spintronic applications. Unlike the previous theoretical studies [9], we report a theoretical study of BNNRs with C-chain substitution along the periodic direction using the Density-Functional-Theory calculations in this paper. It is found that the system undergoes insulator–semiconductor–metal transitions in zigzag edge graphene–BN nanoribbons with the number of C-chains increasing, but it appears insulator–metal–conductor transitions in armchair edge graphene–BN nanoribbons. The spin polarized calculations exhibit half-metallic may be tuned by changing the number of C-chain in the zigzag BN nanoribbons.

## 2. Calculation method

We performed first-principles calculations based on density functional theory (DFT) by utilizing the SIESTA code [26–28], where the exchange–correlation potential is a generalized gradient approximation (GGA) in the form of Perdew, Burke, and Ernzerhof [29]. The atomic orbital basis set was a double- $\xi$  plus polarization function (DZP). The numerical integrals were performed on a real space grid with an equivalent cutoff of 200 Ry. A periodic boundary condition along y direction was applied to the 8Z-BNNRs (8 zigzag BN chains) and 6A-BNNRs (6 armchair BN

\* Corresponding author.

E-mail address: [zhiyongwang520@gmail.com](mailto:zhiyongwang520@gmail.com) (Z. Wang).

chains), and three unit sizes were used for 8A-BNNRs (five unit sizes for 8Z-BNNRs), while a vacuum region larger than 10 Å along the  $x$  and  $z$  direction was set to decouple the interaction between adjacent 8Z-BNNRs (6A-BNNRs) to ensure an isolated single-layer 8Z-BNNRs (6A-BNNRs) being considered. All the atomic positions were relaxed during the geometry optimization until the Hellman–Feynman forces were below  $0.01 \text{ eV \AA}^{-1}$ . The  $k$ -point mesh for zigzag and armchair nanoribbons is  $1 \times 15 \times 1$ . The edges were terminated by hydrogens to form C–H, N–H or B–H bonds for neutralizing valencies of all the edge atoms. The models used here are shown as Fig. 1. They are obtained by substituting zigzag (armchair) BN-chain of 8Z-BNNRs (6A-BNNRs) with zigzag (armchair) C-chain.

### 3. Results and discussion

Using the periodic boundary condition, all the investigated configurations are fully optimized. As shown in Fig. 1, the pink, white and blue balls represent boron, hydrogen and nitrogen atoms, respectively. For the 8Z-BNNRs, 8Z-BN configuration refers to the perfect 8Z-BNNR. 8Z-BN1 configuration refers to the 8Z-BNNR with one armchair C-chain substituting for one armchair BN-chain (Fig. 1a). Similarly, 8Z-BN2, 8Z-BN3, 8Z-BN4, 8Z-BN5 configurations refer to the 8Z-BNNR with two (three, four and five) armchair C-chains substituting for two (three, four and five) armchair BN-chains, respectively. For the 6A-BNNRs, 6A-BN configuration refers to the perfect 6A-BNNR. 6A-BN1 configuration refers to the 6A-BNNR with one zigzag C-chain substituting for one zigzag BN-chain (Fig. 1b). Similarly, 6A-BN2, 6A-BN3, 6A-BN4, 6A-BN5 and 6A-BN6 configurations refer to the 6A-BNNR with two (three, four, five and six) zigzag C-chains substituting for two (three, four, five and six) zigzag BN-chains, respectively. We have calculated the formation energy of these doped configurations, and found that its energy stabilities depend on the number of increasing substitution C-chains. The 8Z-BN5 and 6A-BN6 configurations are the most stable for the 8Z-BNNRs and 6A-BNNRs, respectively.

Fig. 2 shows the band structures of 8Z-BNNRs with or without C-chain substituting for BN-chain. The calculated results show that the band gap of the 8Z-BN configuration is about 4.38 eV at the  $\Gamma$  point, it appears the insulating character (Fig. 2), and the band structures appear the degeneracy at the  $\Gamma$  point, which is nearly in accordance with the previous results [9]. For the 8Z-BN1 configuration, the degeneracy degree disappear near the Fermi level, and the band gap of the 8Z-BN1 configuration decreases to 1.3 eV; it may be attributed to the C-chain substituting for the BN-chain. For the 8Z-BN2 configuration, the band gap decreases to 0.2 eV

compared to the 8Z-BN1 configuration; it may be attributed to increasing the number of the substitution C-chain. For the 8Z-BN3 configuration, the band gap is 0.06 eV, it is attributed to the hybrid effect between BNNRs and GNRs. For the 8Z-BN4 configuration, the band gap is 0.03 eV, the symmetry of band structures appears near the Fermi level owing to the effect of GNRs' symmetry. For the 8Z-BN5 configuration, namely, the 8ZGNRs configuration, the band gap is 0 eV, inducing the metallic character. It can be found that it exhibits the insulator–semiconductor–metal transition with the number of substitution C-chain increasing in the 8Z-BN configurations, which is in accordance with the phenomena of the previous results [9] in spite of hybridizing along different directions. It is found that the band gap of hybrid nanoribbon is mainly determined by the number of the substitution C-chains and less insensitive to the size of BN-chains [30].

For the spin-polarized calculations, Fig. 3 shows the spin density of states (DOS) of the 8Z-BNNRs with or without C-chain substituting for BN-chain along the period direction. The calculated results show that the band gap of both of the spins is 4.16 eV, which makes the 8Z-BN configuration insulating. Replacement of one BN-chain by one C-chain along the period direction, the band gap of both of the spins is 1.73 eV for the 8Z-BN1 configuration. For the 8Z-BN2 configuration, it is noted that the band gap of one of the spins is decreasing to 1.16 eV and that of the other spin is decreasing to 1.39 eV compared to the 8Z-BN1 configuration. Interestingly, for the 8Z-BN3 configuration, the band gap of one of

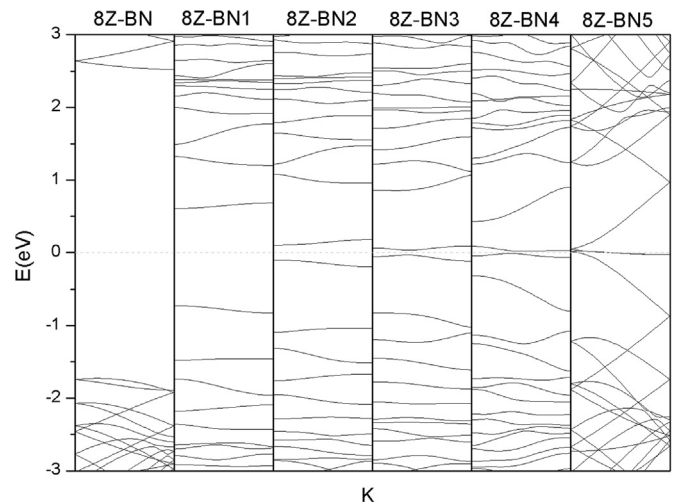


Fig. 2. (Color online) Band structures of the 8Z-BNNRs without or with C-chain substituting for BN-chain. The wave vector  $K$  is from  $\Gamma$  to  $X$ . The energy at Fermi level is set to zero and shown as the green dashed line.

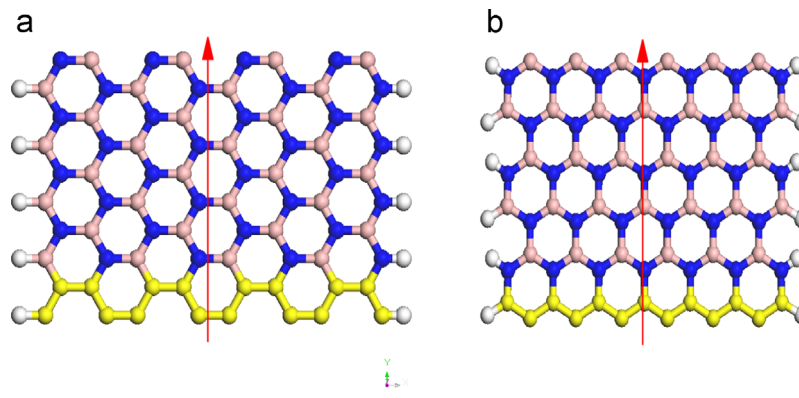


Fig. 1. (Color online) The schematic description for C-chain in substitution for BN chain in the 8Z-BNNRs (Fig. 1a) and 6A-BNNRs (Fig. 1b). The yellow armchair (zigzag) chain refers to the substitution chain. The pink, white and blue balls represent boron, hydrogen and nitrogen atom, respectively. The arrow shows the periodic direction.

Download English Version:

<https://daneshyari.com/en/article/1591130>

Download Persian Version:

<https://daneshyari.com/article/1591130>

[Daneshyari.com](https://daneshyari.com)