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Structural and electronic properties of $B_xC_yN_z$ nanoribbons: A first principles study

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ABSTRACT

We have performed an extensive *ab initio* study on the energetic stability of hydrogen passivated $B_xC_yN_z$ nanoribbons and at the electronic structure and magnetic properties of BC_2N ribbons with different widths and configurations. In particular, it was investigated that BC_2N ribbons composed of boron–nitride clusters surrounded by carbon atoms are showing armchair and zigzag edges. It was seen that the zigzag and armchair BC_2N ribbons can be small gap semiconductors or metallic according to the ribbons width. Also, magnetic behavior is observed for these structures, for all the considered widths, while the armchair ones do not show any magnetization.

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C. First-principles calculations

D. Electronic structure

D. Structural properties

1. Introduction

Unidimensional materials are thought to be used as parts of electronic devices, and amongst these, the graphene nanoribbons (GNR) occupy a special place. It was shown that the origin of energy gaps for armchair graphene nanoribbons (a-GNR) is due to quantum confinement as well as edge effects, while for zigzag graphene nanoribbons (z-GNR) gaps appear because of a staggered sublattice potential on the hexagonal lattice due to edge magnetization [1]. Also, it is known that z-GNR present a metallic character for widths greater than 10 nm, while for the a-GNR the gap oscillates as a function of the ribbons width [2]. Boron nitride nanoribbons (BNNRs) were also synthesized [3] and it has been shown that zigzag ribbons (z-BNNRs) possess an energy gap that decreases with the increasing of the ribbons width, while the armchair ones (a-BNNRs) present a width-oscillating gap. It is known that the presence of impurities alters the electronic properties of carbon compounds. This leads to a suitable way to control the energy gap of a given ribbon, or any carbon structure, by changing and controlling the dopant concentration. Together with the dopant concentration, its distribution and arrangement affect the doped structures electronic character [2]. It was shown that, when the dopants (at carbon systems) are boron (B) and

nitrogen (N) atoms, they “prefer” to form island in order to maximize the structure stability [3–5]. Finally, contrary to the first thoughts, the conduction in $B_xC_yN_z$ compounds is not only due to carbon atoms concentration, but also by having a strong dependence on the atomic arrangement of the dopants in the structure [3,5,6]. Previous works have shown that some compounds having a higher carbon concentration presented a greater energy gap when compared to others with less carbons and different BN distributions [7].

In this work we have performed a systematic study on $B_xC_yN_z$ nanoribbons taking as starting structures the sheets studied in [6] and generating zigzag and armchair nanoribbons through passivation of the dangling bonds at the edges with hydrogen (H) atoms. Through the energetic point of view, BC_2N nanoribbons are stabler than other stoichiometries and, amongst these the stablest ones are those which maximize the number of BN and CC bonds (i.e. forming BN and CC islands, now called island type structures), both for the zigzag and armchair configurations. Taking this behavior into account we have investigated the structural stability and electronic properties of island type BC_2N nanoribbons as a function of the ribbons width and number of islands in the structure. It was found that the armchair nanoribbons formation energy is inferior when compared with the zigzag ones and that, there is an increase (little decrease) in its value with the increasing of the ribbons width for the armchair (zigzag) systems. The band structure analysis indicates that both types of ribbons present a similar behavior, with the energy gap decreasing as the nanoribbons width increases and that Dirac points are formed

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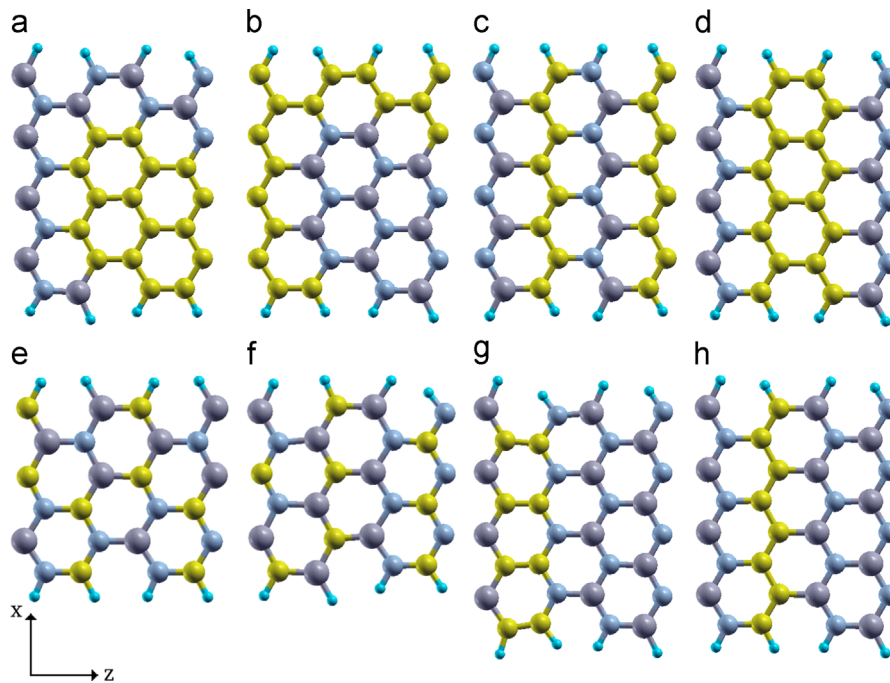


Fig. 1. (Color online) Ball-and-stick illustration of the studied armchair $B_xC_yN_z$ nanoribbons. From (a)–(d) we have different configurations to the narrowest BC_2N studied ribbon unit cell, composed of 32 atoms (16 C (yellow) + 8 B (light purple) + 8 N (light blue)). At (a) and (b) we have the C and BN island configurations, respectively. At (e) and (f) we have the BCN ribbons, while at (g) and (h) we have two different $B_3N_3C_2$ structures. Hydrogen atoms are represented by the tiny cyan spheres.

within a certain width limit. Finally, it was seen that the zigzag ribbons present spin polarization while the armchair ones do not.

2. Methodology

We have performed a theoretical study of $B_xC_yN_z$ nanoribbons, more specifically, BCN, BC_2N , and $B_3N_3C_2$ with two different orientations, namely zigzag and armchair. In Fig. 1(a), (b), (c), and (d) we can see four different configurations for the armchair BC_2N (a- BC_2N) structures: (a) we have the C-island that is carbon surrounded by B and N atoms; (b) BN-island, where we have B and N forming a cluster with surrounding C atoms; (c) BN and C intercalated lines, perpendicular to the ribbon growth direction; and (d) two consecutive BN and C lines. In Fig. 1(e) and (f) we have two a-BCN ribbons with minimum structural differences concerning the atoms bonding pattern. Finally, in Fig. 1(g) and (h) we have two possible configurations for the a- $B_3N_3C_2$ ribbons. It is valid to point out that the dangling bonds are saturated with H atoms and that this saturation defines the ribbon chirality, for example, in Fig. 1 we have the H bonded to the atoms at the armchair edges and these systems are classified as armchair. The calculations were also realized for the same configurations (shown in Fig. 1) with the change in the chirality, i.e., the H atoms were bonded to the zigzag edges, generating zigzag $B_xC_yN_z$ ribbons (z - $B_xC_yN_z$) as can be seen in Fig. 2.

We have also performed a theoretical study of BC_2N nanoribbons (see Figs. 3 and 4) with a configuration previously shown to be the stabler one amongst the ribbons and monolayers [6]. In Fig. 3 we can see the z - BC_2N ribbons, where the B and N atoms form a small cluster surrounded by C atoms in an island configuration. In Fig. 3(a) we have a narrow ribbon in which unit cell is composed of 16 C plus 16 BN atoms (8 B and 8 N). This cell is replicated along the z -axis generating the ribbon. In Fig. 3(b) and (c) we have the unit cell (Fig. 3(a)) duplicated and triplicated (along the x -axis), respectively. These are then replicated along the z direction to generate the respective ribbons. In Fig. 4(a), (b), and

(c) we have the a- BC_2N ribbons. The structure shown at Fig. 4(a) is pretty much the same as the one in Fig. 3(a), except that it is rotated by 90° in order to change the generated ribbon. The dangling bonds to be saturated with H atoms, at the sides of the structures, define the ribbon as either zigzag or armchair. The ribbons in Fig. 4(b) and (c) are the duplication and triplication of Fig. 4(a) (along the x -axis), respectively. These, in their turn, are replicated along the z -axis to generate the armchair ribbons.

We carried out first-principles density functional theory calculations [8,9] to study several zigzag and armchair BCN nanoribbons with exact BC_2N stoichiometry. Norm-conserving pseudopotential for B, C, and N was generated using the Troullier–Martins scheme [10] within the generalized gradient approximation as parameterized by Perdew–Burke–Ernzerhof [11]. Linear combinations of numerical Gaussian basis sets were used to represent the valence electrons [12]. The double-zeta augmented by a polarization function (DZP) was the employed Gaussian basis set. The charge density was represented in the real space by a mesh cutoff of 150 Ry. The Brillouin zone was sampled by the minimum number of k -points [13] necessary to achieve a total energy convergence within 5 meV. The unit cell size in the direction perpendicular to xz plane was big enough to avoid interactions between nanoribbons images at neighboring cells. The atomic positions and the dimensions of the employed supercell have been optimized using conjugated gradient methods until the forces on the atoms were less than 0.05 eV/Å.

3. Results and discussion

3.1. Energetics

In order to address the relative stability of various $B_xC_yN_z$ structures (ribbons and monolayers), we introduce the theoretically calculated chemical potentials that are μ_N , μ_B , and μ_C for nitrogen, boron and carbon, respectively. For the case of BCN structures, the energy reference is taken to be the completely

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