Electronic and magnetic properties of BNC nanoribbons: a detailed computational study

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Abstract. Using density functional theory (DFT), we perform a systematic study of the electronic structure of zigzag edge BNC nanoribbons, which have an equal number of boron, carbon and nitrogen atoms. We study two nanoribbon structures. One of them is terminated by carbon and nitrogen atoms on opposite edges, whereas the other is terminated by carbon and boron atoms on opposite edges. We explore the effect of passivation of the edge atoms on the electronic and magnetic properties of the nanoribbons. We also evaluate the changes in these effects brought about by varying the width of the nanoribbons. Our results show that, for ribbons of small width, the ones with a boron edge show semiconducting behaviour regardless of the nature of edge passivation, whereas nitrogen-edged nanoribbons display a range of conduction properties including half-metallic, metallic and semiconducting properties depending on the nature of edge passivation. On the other hand, ribbons of larger width show metallic behaviour. We also study the effect of external electric fields on the band structure of both boron-edged and nitrogen-edged nanoribbons and the trends in these effects with varying width. We find that both boron- and nitrogen-edged nanoribbons retain their zero-field conduction properties even in the presence of an electric field directed from the boron/nitrogen edge to the carbon edge.
Our transport study of hydrogen-passivated carbon- and nitrogen-edged zigzag BNC nanoribbons reveals strong spin-filter properties.

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1. Introduction

Graphene is a two-dimensional (2D) lattice of sp\(^2\) bonded carbon atoms on a honeycomb lattice [1]. The experimental discovery of a strictly 2D lattice has led to the observation of several striking properties, which have also been predicted by several theoretical studies [2]. The possibility of engineering the band structure properties makes graphene a potential candidate for the fabrication of next-generation electronic devices.

It is well known that low dimensionality leads to interesting electronic properties that are a result of the size and geometry of the material [3]–[7]. Graphene, which is 2D, can be truncated in one of the dimensions to obtain a quasi-1D material known as graphene nanoribbons (GNRs). In the laboratory, these can be prepared by cutting and lithographic patterning of mechanically exfoliated graphene sheets [8, 9]. They can also be prepared by chemical methods [10]. Depending on the direction in which the truncation is performed, GNRs with two main types of edge terminations are possible: zigzag and armchair. Armchair graphene nanoribbons (AGNRs) are usually nonmagnetic semiconductors, whereas zigzag graphene nanoribbons (ZGNRs) show spin polarization along the two edges that are coupled antiferromagnetically [11]. The magnetism in ZGNRs was attributed to peculiar localized states along the zigzag edges [12]. DFT studies suggest that ZGNRs show half-metallicity in the presence of a finite external electric field across the ribbon width. This is observed within both local density approximation (LDA) [13] and generalized gradient approximation (GGA) [14]. Thus ZGNRs have received much more attention than AGNRs. The electronic structure and possible applications of ZGNRs have been the subject of several theoretical studies [15]–[24].

Recently, mono-layer boron nitride (BN) sheets have been fabricated in experiments [25]–[27]. Unlike graphene, BN sheets are wide gap insulators. Similarly to AGNRs, armchair BNNRs (ABNNRs) also display nonmagnetic semiconducting behaviour independent of their width [28]. Unlike ZGNRs, however, zigzag BNNRs (ZBNNRs) can be either magnetic or nonmagnetic depending on their edge passivation [29, 30]. In the case of ZBNNRs, the energy bandgap decreases monotonically with increasing ribbon width, whereas gap oscillation is found in the case of ABNNRs. The electronic properties of BN nanoribbons (BNNRs)
are easily tuned by an external transverse electric field. BNNRs with bare zigzag edges show metallic ↔ semiconducting ↔ half-metallic transition under an external electric field [29]. In the absence of an electric field, BNNRs with one bare nitrogen edge and one hydrogen-passivated boron edge are predicted to be half-metals theoretically [30, 31].

Because of the marked difference between graphene and BN ribbons, hybrid structures composed of both graphene and BN ribbon sections have attracted the attention of many theoreticians and experimentalists in recent years. A combination of BN nanoribbons and graphene nanoribbons forms C_{0.5}(BN)_{0.5} nanotubes, which have tunable electronic properties [32]. Very recently, BNC materials with the formula BC_{4}N have been explored in both experimental and theoretical studies [33, 34]. Some interesting electronic properties were also achieved in BNC-hybrid nanostructures, where boron, carbon and nitrogen atoms are mixed in various proportions [35]–[44]. BNC-hybrid nanoribbons, which can be equivalently viewed as either BN nanostructures doped into graphene nanoribbons or GNRs embedded in a BN nanoribbon, exhibit various electronic properties [15, 37, 45]. Most earlier works have focused on tuning the electronic properties of BNC ribbons by varying their width and chemical composition. However, to the best of our knowledge, BNC nanoribbons with an equal number of boron, carbon and nitrogen atoms have not been explored theoretically. This, along with the recent experimental success in producing BNC sheets with essentially equal numbers of boron, carbon and nitrogen atoms [46], has motivated us to pursue a theoretical study of such materials.

As zigzag edge GNRs and BNNRs show interesting and promising properties unlike those of their armchair analogues, in this paper we present a detailed study of hybrid zigzag BNC nanoribbons (ZBNCNRs) with an equal number of boron, carbon and nitrogen atoms. A preliminary study of 2D BNC sheets having an equal number of boron, carbon and nitrogen atoms was performed to determine the most stable configuration of bonds between the three species. The results obtained were used to choose the nanoribbons that would be of interest. We consider two different sets of ZBNCNR structures with equal numbers of boron, carbon and nitrogen atoms: (i) nanoribbon structures with carbon atoms at one edge and nitrogen atoms at the other edge (n-CN) and (ii) nanoribbon structures with carbon atoms at one edge and boron atoms at the other edge (n-CB). Both of the nanoribbon systems are studied considering four different kinds of edge terminations: (i) ZBNCNR with both edges passivated, (ii) ZBNCNR with a bare boron (or nitrogen) edge and a hydrogen-terminated carbon edge, (iii) ZBNCNR with a carbon bare edge and a hydrogen-terminated boron (or nitrogen) edge and (iv) fully bare ZBNCNR. For each of the above systems, we repeat the calculations for various nanoribbon widths, n-ZBNCNR (n is the number of zigzag chains; n = 6, 12, 18, 24). We also study these systems under different electric fields and calculate zero-bias transmission to evaluate their possible applications in nanodevices. Considering the variability in properties seen in n-CN nanoribbons, the present study focuses on n-CN nanoribbons, whereas we only briefly discuss the results for n-CB nanoribbons.

2. Methods and systems

All first principles calculations were performed using the ab initio density functional theory (DFT) software package SIESTA [47]. A double-ζ polarized (DZP) basis set is used. The real space mesh cutoff is set to 300 Ry. Exchange correlation within the DFT calculations is calculated using the Perdew–Burke–Ernzerhof [48] functional within the GGA. The Monkhorst–Pack K sampling grid is set to 50 points in the periodic direction. The conjugate
gradient method was used in geometry optimization. Large vacuum separations are used to suppress spurious interactions in the non-periodic directions. Our spin transport calculations are based on the non-equilibrium Green’s function formalism (NEGF) as implemented in the TRANSIESTA package [49], extended to spin-polarized systems. However, here, we only consider the zero-bias limit and focus on electron transmission close to the Fermi energy. The transmission is obtained from

$$ T(E) = \text{Tr}[\Gamma_L(E)G'(E)\Gamma_R(E)G'(E)] $$

where the retarded Green’s function, $G'(E)$, is calculated from the Hamiltonian and self-energies of the central region. $\Gamma_\alpha(E)$ is the imaginary part of the self-energies (times two) of the left and right electrodes ($\alpha = L, R$).

The first step in the present study was to determine the most stable configuration of bonds between boron, carbon and nitrogen in the nanoribbon structures. In order to determine this, we considered 2D BNC sheets, which are periodic in two dimensions (figure 1). Four primitive unit cells were chosen, each with different numbers of C–C, C–B, C–N and B–N bonds. We did not consider systems with B–B or N–N bonds, which lead to instability.

From the results, as shown in table 1, it is clear that the structure A with the largest number of B–N and C–C bonds is most stable. We therefore choose the unit cells of the nanoribbon such that the numbers of B–N and C–C bonds are maximized.
In figure 2, we present the different structures of BNC nanoribbons in the present study. The dotted line represents the primitive unit cell of the BNC nanoribbon being considered. In the naming convention we follow, the integer prefix specifies the width of the nanoribbon as the number of zigzag chains. The following two letters specify the type of edges: ‘CN’ for a nanoribbon with one of the edges composed of carbon atoms and the other edge composed of nitrogen atoms, and similarly, ‘CB’ for the case of a boron edge in place of the nitrogen edge. The subscripts of these two letters specify the nature of edge passivation, with ‘pass’ indicating passivation with hydrogen and ‘bare’ indicating an unpassivated edge. We consider a supercell consisting of two primitive unit cells in order to determine the ground state spin configurations. This supercell allows us to consider different spin configurations of the edge atoms. The different spin configurations consist of various combinations of ferromagnetically and antiferromagnetically aligned spins along the edges and across the nanoribbon. All further calculations are performed taking into account this supercell consisting of two unit cells for each system.

3. Results and discussion

3.1. Electronic and magnetic properties

In figure 3, we present the spin configurations of optimized geometries for 6-CN nanoribbons in this study. Our spin-polarized calculations show that C and N atoms at the edges align ferromagnetically along the ribbon, whereas the C and N atoms at the two edges interact antiferromagnetically (C(↑, ↑)/N(↓, ↓)) with each other across the nanoribbons in the case of all of the systems. These spin configurations remain the same for 12-, 18- and 24-CN nanoribbons.
Note that whereas the bare edge atoms show large local moment due to dangling bonds, hydrogen passivated N (or C) atoms at the edges show no (or very small) spin polarization in the ground state for all the systems. As expected, the local magnetic moment on each edge atom increases with the width of the nanoribbons (see supplementary table 1 available from stacks.iop.org/NJP/13/053008/mmedia). In figure 4, we present the spin-polarized band structures of 6-CN and 18-CN systems. The band structures show very interesting results. In the case of 6-CN, we find that when the N edge alone is bare, \( C_{\text{pass}}N_{\text{bare}} \) shows metallic behaviour, while when the C edge alone is bare, \( C_{\text{bare}}N_{\text{pass}} \) is semiconducting. However, quite impressively, when both C and N edges are bare (passivated), \( C_{\text{bare}}N_{\text{bare}} \) (\( C_{\text{pass}}N_{\text{pass}} \)) shows neither semiconducting nor metallic behaviour; rather, it shows an intermediate behaviour, known widely as half-metallic (semi-half-metallic) behaviour [50]–[53]. In all systems, we see that as the ribbon width increases, the semiconducting gaps in the spin channels vanish to give rise to metallic behaviour, reflecting the characteristics of both ZGNRs and ZBNNRs.

It is quite clear from the band structure that the nanoribbon with both edges passivated, \( C_{\text{pass}}N_{\text{pass}} \), shows semi-metallic behaviour for the majority spin channel as bands (bands 1 and 2) touch the Fermi level, while a semiconducting gap opens up for the minority spin channel in \( 6-C_{\text{pass}}N_{\text{pass}} \), leading to a semi-half-metal. Replacing 2/3 of the C–C chains of 6-ZGNR by B–N chains, the resulting system, \( 6-C_{\text{pass}}N_{\text{pass}} \), shows half-metallic behaviour, which is unlike the semiconducting behaviour seen in pure 6-ZGNR and 6-ZBNNR. From the projected density of states (PDOS) and wavefunction analysis, we find that the bands near the Fermi level that take part in conduction are mainly derived from both edge and border states (the region where B or N atoms are bonded with C atoms). Owing to their small width, the edge atoms along with border atoms contribute to bands near the Fermi level (see supplementary figure 1, available from stacks.iop.org/NJP/13/053008/mmedia). As the ribbon width increases, the edge atoms and the border atoms decouple and contribute separately to different bands. Consequently, \( 6-C_{\text{pass}}N_{\text{pass}} \) is half-metallic as compared to the wider \( 18-C_{\text{pass}}N_{\text{pass}} \), which is metallic (see figure 4). Moreover, due to their Lewis acid character, boron atoms pull the electrons from adjacent carbon atoms, resulting in a charge transfer from carbon to boron and thereby creating a potential gradient across the ribbon. Due to this strong charge transfer, the hybridized state derived from the border C and B atoms strongly contribute to the metallic band of the ribbon near the Fermi energy. Through Mulliken population analysis, we found that charge transfer is relatively greater in the case where the ribbon has both edges passivated. We also note that this charge transfer becomes stronger with increasing width (see supplementary table 1). This is because, adjacent to the B atoms in the border region, the availability of delocalized \( \pi \) electrons in the carbon region increases with width, which facilitates charge transfer from carbon to boron. It is evident that the wider ribbon \( 18-C_{\text{pass}}N_{\text{pass}} \), unlike \( 6-C_{\text{pass}}N_{\text{pass}} \), has its majority spin conduction band (band 2) and minority spin valence band (band 1) mainly derived from border atoms. Strong hybridization and charge transfer between B and C atoms in the border region tend to make these bands cross the Fermi level (see supplementary figure 1 for pDOS).

Similarly, \( 6-C_{\text{bare}}N_{\text{pass}} \) is semiconducting and \( 6-C_{\text{bare}}N_{\text{bare}} \) is half-metallic, while the wider ribbon \( 18-C_{\text{bare}}N_{\text{pass}} \) is metallic. Also, metallic \( 6-C_{\text{pass}}N_{\text{bare}} \) becomes strongly metallic when the width is increased. This observation unambiguously proves that the narrow ribbon shows a range of conduction properties including semiconducting, half-metallic and metallic properties, mainly decided by the nature of edge passivation. On the other hand, in the case of wider ribbons, it is the border states that play an important role, leading all of the BNC ribbons into a metallic phase (see supplementary figure 1 for pDOS).
Figure 4. Spin-polarized band structures of 6-CN nanoribbons and 18-CN nanoribbons systems. The Fermi level is scaled to zero.
Next, we briefly discuss the results for \( n \)-CB nanoribbons. As can be seen in figure 3, B atoms at the edges are aligned antiferromagnetically (B(↑, ↓)), while the C atoms at the edges interact ferromagnetically (C(↑, ↑)). Note that the local moment on hydrogen-passivated B atoms at the edges is zero. In order to understand the electronic and magnetic structures, we present the band structure and density of states (DOS) plots in supplementary figures 2 and 3 (available from stacks.iop.org/NJP/13/053008/mmedia). We find that, overall, the four structures with boron edges show the semiconducting behaviour of 6-CB nanoribbons. With increasing ribbon width, all of the systems show metallic behaviour for both spin channels. Wavefunction analysis shows that not only the edge states but also the border states contribute to important bands near the Fermi level.

4. External electric field and transport properties

In the absence of an electric field, 6-CN systems show a range of electronic behaviour (semiconducting/half-metallic/metallic) depending on edge passivation. Thus, it is also important to study these systems when subjected to an electric field. Across each of the nanoribbon systems, electric fields in the range of \(-0.2 \text{ V Å}^{-1}\) to \(+0.2 \text{ V Å}^{-1}\) are applied. Positive values of the electric field indicate an electric field directed from the boron/nitrogen edge towards the carbon edge, whereas negative values indicate a field directed from the carbon edge towards the boron/nitrogen edge. 6-CN systems show varying behaviour depending on the electric field strength and direction. The semi-half-metallic nanoribbon, 6-\( \text{C}_{\text{pass}} \text{N}_{\text{pass}} \), maintains its zero-field behaviour irrespective of the strength and direction of the electric field. With the application of a positive field, we find that 6-\( \text{C}_{\text{pass}} \text{N}_{\text{bare}} \), which is metallic at zero field, remains metallic, whereas a negative electric field induces a band gap to appear, and this causes the system to become semiconducting at a critical field, \( E_C \sim -0.15 \text{ V Å}^{-1} \). For the semiconducting nanoribbon 6-\( \text{C}_{\text{bare}} \text{N}_{\text{pass}} \), the system maintains its semiconducting character in the presence of an external electric field irrespective of the applied direction. For 6-\( \text{C}_{\text{bare}} \text{N}_{\text{bare}} \), with the application of a positive field, the half-metallicity remains intact. However, when the field is reversed, i.e directed from the carbon to the nitrogen edge, at a threshold value of the field, a gap opens up in the majority spin channel. The gap widens as the field strength increases. We want to stress the fact that the intrinsic behaviour, namely semiconducting/half-metallic/metallic, remains intact when the electric filed is applied in the direction from the nitrogen edge towards the carbon edge across the ribbon. In the case of the wider ribbons 18-CN, all of the systems remain metallic irrespective of strength and direction of the electric field. For both narrow and wide ribbons, \( n \)-CB systems maintain their zero-field conduction behaviour under all conditions of electric field that we have studied. We conclude that \( n \)-CB nanoribbon systems are less sensitive to external electric fields, whereas \( n \)-CN systems (especially ribbons with bare \( \text{N} \) edge) are very sensitive to external transverse fields. This is because the external electric field can greatly influence the degree to which excess electrons (due to the dangling bonds at the \( \text{N} \) edges) float across the ribbon.

We subsequently study the transport properties of ZBNCNR in order to explore possible device applications. We choose a narrow ribbon, 6-\( \text{C}_{\text{pass}} \text{N}_{\text{pass}} \), which is semi-half-metallic and also chemically more stable. The NEGF technique used to study the electronic transport employs a two-probe system: semi-infinite left and right electrode regions are in contact with a confined central scattering region. Both electrodes and the central region are made from 6-\( \text{C}_{\text{pass}} \text{N}_{\text{pass}} \). The central scattering region contains six primitive unit cells (see figure 5) with
Figure 5. Top schematic view of the two-probe $6$-$C_{\text{pass}}N_{\text{pass}}$ system. The central region and the left and right electrodes are indicated. Bottom: spin-polarized transmission function for $6$-$C_{\text{pass}}N_{\text{pass}}$. The Fermi level is scaled to zero.

A total length of 15 Å. In figure 5, we present the spin-polarized zero-bias transmission function for both the spin channels. The transmission function shows a step-like behaviour with a dip in transmission in the vicinity of the Fermi energy for the majority spin channel. It is clear that in a small energy window near the Fermi energy, the majority spin channel shows a strong transmission value ($T = 0.66$), whereas the minority spin channel does not take part in transmission, pointing to its spin-filter property.
5. Conclusions

We have performed a systematic study of the effect of edge passivation on the electronic structure of zigzag edge BNC nanoribbons, which have an equal number of boron, carbon and nitrogen atoms. We study two sets of BNC nanoribbon structures, namely $n$-CB and $n$-CN, and discuss the effect of selective passivation along with trends seen with varying the width of the ribbons. For small widths (six zigzag chains), we find that all nanoribbons with a boron edge show semiconducting behaviour regardless of the nature of edge passivation, whereas nitrogen-edged nanoribbons display a range of conduction types including semiconducting, half-metallic and metallic behaviour depending on the nature of edge passivation. In the case of ribbons of larger width (18 zigzag chains), all of the systems show metallic behaviour. We also study the effect of external electric fields on the band structure of these nanoribbons. In summary, we show that selective edge passivation can be the deciding factor in determining whether a narrow nanoribbon has a metallic, half-metallic or semiconducting property. We conclude that border states play an important role in making the wider ribbons metallic. Additionally, we show that boron-edged nanoribbons as well as nitrogen-edged nanoribbons retain their conduction properties even in the presence of a positive electric field. These results, along with our zero-bias transmission study, predict spin-filter properties for $6$-$C_{\text{pass}}N_{\text{pass}}$, suggesting possible applications in spintronic devices.

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