Modification of the band offset in boronitrene

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Using density functional methods within the generalized gradient approximation implemented in the Quantum Espresso codes, we modify the band offset in a single layer of boronitrene by substituting a double line of carbon atoms. This effectively introduces a line of dipoles at the interface. We considered various junctions of this system within the zigzag and armchair orientations. Our results show that the "zigzag-short" structure is energetically most stable with a formation energy of 0.502 eV, and with a band offset of 1.51 eV. The "zigzag-long" structure has a band offset of 1.99 eV. The armchair structures are non-polar while the zigzag-single structures show a charge accumulation for the C-substituted B and charge depletion for the C-substituted N at the junction. Consequently there is no shifting of the bands.

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I. INTRODUCTION

Boron nitride (BN) is a versatile material and is one of the most promising semiconductors. This can be attributed to it having the widest bandgap ($\sim$ 6 eV) amongst the group III-V nitrides. It is not surprising that BN exists in the hexagonal (*h*-BN) and cubic (*c*-BN) forms, similar to graphite and diamond, since it is iso-structural to carbon. BN exists in four other known crystalline structures which are metastable, namely, rhombohedral (*r*-BN), wurtizite (*w*-BN), simple cubic, and turbostratic (*t*-BN). This accounts for the wide array of properties of BN. BN also exists in amorphous (*a*-BN) form.[1] The most common phase of BN is *h*-(BN), which has good electrical insulation properties, and is stable with high thermal conductivity. It can be used in electronics, nuclear technology, vacuum technology, lubrication, x-ray lithography masks, ultra-hard ceramics applications etc. In cubic form, it is a hard material, with a bulk modulus rivaling that of diamond.[2]

With the discovery and synthesis of graphene, other two dimensional structures have attracted a great deal of scientific and technological interest.[3] There has been a tremendous interest in the recently discovered two dimensional *h*-BN also referred to as boronitrene,[4,5] due to its distinct properties and potential for a wide range of applications. The predicted wide bandgap of 4.64 eV for boronitrene[6] will be of particular interest for future applications. BN monolayer can be produced by the micromechanical peeling method[7] or by the CVD technique,[8] similar to the methods used for the production of graphene. Boronitrene and graphene have huge technological and engineering importance. Both these materials have an advantage in the manufacture of ultra thin, single layer devices since there is an absence of long range interactions between layers. Boronitrene and graphene are posed to be future materials in advanced solid state devices.[9,10]

Semiconductor heterojunctions was a topic of enormous research activity in the 1980's both experimentally[11] and theoretically,[12–15] for example, the GaAs/AlAs[14,16,17] and Si/Ge[18,19] interfaces have been very extensively studied. Effects of strain are considered to be important for systems that are lattice mis-matched, as is the case with Si/Ge, that result in substantial atomic relaxations at the interface. The valence-band offset ΔE_v and the conduction-band offset ΔE_c at the interface of solid state devices are key design parameters that determine the electronic and optical properties of heterostructured materials. The band offsets of semiconductors can be modified by either doping the interface dipoles or by the deposition of ultra thin interlayers between semiconductors. This modifies the charge distribution creating an interface dipole[11] that results in a relative shifting of the bands.

Muñoz et.al[12] proposed that double layer of Ge along the (111) and (100) geometries of bulk GaAs modifies the band offsets. These structures have being synthesized using molecular beam epitaxy (MBE) for the least and most energetically stable geometry.[20,21] B/C/N materials with graphitic network similar to those of interest in this study has being investigated experimentally[22] using CVD or solid-phase pyrolysis of precursors. And theoretically by Liu et.al,[23] they investigated the electronic structure of various models of BC_2N monolayer using *ab initio* techniques. Recently, Y. Fan et.al[24] reported on BN/C heterostructured zigzag nanotubes predicting enhanced field-emission properties of the heterostructures . However, to date no study has been done on modifying the band offset of the BN/C heterostructured mono-layer. In the present paper, we theoretically modify the band offset in boronitrene. This is motivated by the possibility of creating a nano-sized electrical diode. In this work a *h*-BN mono-layer is used as the base 2D system, and we create an interface using lines of C atoms. This enables us to engineer the band offset in this mono-layer semiconductor. The control of band discontinuities are mainly due to two effects: (i) the effect of strain at the interface, and (ii) the electrostatic interface potential.[12] We probe the atomistic control of the interface composition and the accompanying changes in the electronic properties, using the electrostatic interface potential. Boronitrene and graphene have the same crystal structure with a negligible lattice mismatch. Therefore we consider effects of composition and geometry, with minimal effects due to strain.

Using density functional methods within the generalized gradient approximation implemented in the Quantum Espresso codes, we investigate the modification of the band offset in a single layer of boronitrene by substituting a single

or a double line of carbon atoms. This effectively introduces a line of dipoles at the interface. We consider the boronitrene armchair and zigzag structures for our junctions.

In section II, we describe the various interface structures that we considered, and in section III we give a brief description of our theoretical and computational methods. We present our results and discussions in section IV. In section V we summarize our conclusions.

II. BN HETEROJUNCTION STRUCTURES

Each structure that we considered consists of a honeycomb boronitrene mono-layer with C atoms forming the junction interface (henceforth referred to as BN/C). The junction comprising C atoms is created either parallel to the armchair or to the zigzag orientations of the BN honeycomb structure. The armchair-double structure, shown in Fig. 1, contains a double line of C atoms forming the interface with the C atoms placed along an armchair chain with C-C segments parallel to the interface. In the armchair-single structure, shown in Fig. 2, the interface is made up of only a single line of C atoms. For these two armchair configurations, no dipole is expected at the junction by the substitution with the C atoms because of the nonpolar lines comprising both B and N atoms parallel to the junction.

The zigzag-short structure, shown in Fig. 3, contains C atoms along a zigzag chain parallel to the interface which forms a double line of C atoms. This double line is a "short" distance apart. The zigzag-long structure, shown in Fig. 4, has C-C segments oriented perpendicular to the interface. This forms a double line of C atoms a "long" distance apart. For these two zigzag configurations, a line of dipoles is expected at the junction by the double line of C atoms because of the alternating polar lines of B and N atoms parallel to the junction.

The zigzag-single structure with C-substituted B shown in Fig. 5 and the zigzag-single structure with C-substituted N shown in Fig. 6, contains a single line of C atoms parallel to the interface. From a structural point of view, it is not clear *a priori* whether a dipole will form at the interface or not. These systems are also investigated in our studies.

In all cases, the structures are aligned in the *xy*-plane with the junctions parallel to the *y*-axis.

III. THEORY AND METHOD

To study the polarity of a 2D junction, we must look at how the charge density and potential vary across the junction. It is useful to consider the charge density and the potential (represented by f below) averaged along lines parallel to the interface:

$$\bar{f}(x) = \frac{1}{L}\int f(x,y)\,dy\,. \tag{1}$$

Baldereshi et al.[14] suggested that to eliminate bulk effects, the macroscopic average for each line-averaged quantity should be calculated to emphasize the behavior at the junction:

$$\bar{\bar{f}}(x) = \frac{1}{a}\int_{x-a/2}^{x+a/2} \bar{f}(x')\,dx'\,. \tag{2}$$

Here, the macroscopic average is computed over the periodic length a.

Using this method, it can readily be seen whether a dipole is created at the interface as this manifests as an accumulation of electronic charge on the one side of the interface, and a depletion of electronic charge on the opposite side. Also, as will be seen with our results in section IV, the band offset can be readily read off from a graph of the macroscopic average of the potential across the junction.

All calculations were done using density functional theory[25] (DFT) as implemented in the Quantum Espresso PWSCF code.[26] We used the PBE exchange-correlation functional[27] for the generalized gradient approximation (GGA) with ultrasoft pseudopotentials.[28] A kinetic energy cutoff of 38 Ry was chosen to ensure adequately converged total energies.

To ensure isolated junction images, 12 and 16 atoms per supercell were used for the BN/C-zigzag and BN/C-armchair structures respectively with atomic composition as shown in Table. I. A vacuum distance of 15 Å was placed between each mono-layer to ensure negligible interaction between the periodic images. A Monkhorst-Pack[29] grid of 4×4×1 was used to sample the Brillouin zone and Methfessel-Paxton smearing[30] with a width of 0.005 Ry was used to integrate the bands at the Fermi level.

All ions were relaxed until the atomic forces were less than 0.0001 Ryd Å^{-1}. The sum of the Hartree, local ionic and exchange-correlation potentials was used to calculate the macroscopic potential across each junction. Planar averaging of the charge density and potential was done over the *yz* planes as a function of x, as this is equivalent to line averaging in the plane of the single layer material.

The heat of formation for each structure was calculated by taking the difference between the total energy of the junction structure and the energies of its constituents in their corresponding bulk forms:

$$\Delta H_{f(BN/C)} = E^{tot}_{(BN/C)} - N_{BN}\,E^{bulk}_{(BN)} - N_C\,E^{bulk}_{(C)}\,, \tag{3}$$

where N_{BN} and N_C are the number of BN units and C atoms in the BN/C supercell, $E^{bulk}_{(BN)}$ is the bulk energy per pair of BN atoms in boronitrene, and $E^{bulk}_{(C)}$ is the energy per C atom in the graphite structure. The calculations were performed using fixed number of **k** points and kinetic energy cutoff for each supercell, thereby minimizing errors.

IV. RESULTS AND DISCUSSION

The similarity of the bond lengths for B-N in *h-BN* and C-C in graphene means that these two structures are reasonably well lattice matched. The nearest neighbor distances are d_{B-N}=1.446 Å in *h*-BN and d_{C-C}=1.425 Å in graphene, i.e. there is a lattice mis-match of $\sim$ 1.5%. The C-N and C-B

bonding around the interface creates slight distortions in the trigonal bonding which determines the polarity of the junction.

A. Armchair double and single structures

The armchair-double and the armchair-single structures comprise non-polar lines of atoms. That is, each line parallel to the interface contains an equal number of B and N atoms. Therefore, substituting a single or a double line of B and N atoms with C atoms does not change the polarity of each line. We expect the junction to be non-polar.

In Fig. 7 and Fig. 8 we plot the line averaged charge density and the macroscopic averaged charge density for the armchair-double and armchair-single structures respectively. We notice that there is an accumulation of charge density at the interface with a depletion of charge density symmetrically on either side of the interface. The dipoles are oppositely directed and therefore cancel each other, resulting in no net dipole at the interface. This results in no shifting of the electronic bands across the interface. The armchair orientations are not candidate systems for modifying the band offset in boronitrene.

B. Zigzag short and long structures

In the zigzag-short structure, the interface is made up of a zigzag chain of C atoms with fully relaxed internal angles of 122.59° and C-C bond lengths of d_{C-C}=1.431 Å indicating an elongated chain as compared to a similar chain in graphene. The C atoms are alternatively bonded to N atoms on one side of the interface and B atoms on the other side. The N atoms form part of a B-N zigzag chain with internal angles of 119.73° and d_{B-N}=1.451 Å. On the opposite side of the interface, the B atoms also form part of a B-N zigzag chain with very similar internal angles of 119.66° and bond lengths of d_{B-N}= 1.452 Å. Both these chains are very similar to those found in the bulk. At the interface, the N-C bond length is d_{N-C}=1.401 Å while that for the C-B bond is d_{C-B}=1.533 Å.

In Fig. 9 we plot the line averaged charge density and the macroscopic averaged charge density for the zigzag-short structure. We note an accumulation of electronic charge on the C-substituted B side of the interface, and a depletion of electronic charge on the C-substituted N side of the interface. The macroscopic average of the charge density converges to the bulk value of 48 electrons per supercell within two atomic lines from the interface. This indicates that our supercell is sufficiently large to enable us to model the single isolated interface. The macroscopic average of the charge density peaks at a value of about 5 electrons per supercell on the C-substituted B side of the interface, and dips to minus this value on the C-substituted N side of the interface. This separation of charge at the interface results in a net dipole at the interface.

In Fig. 10 we plot the line averaged potential and the macroscopic averaged potential. We note, as expected, a discontinuity of the potential across the interface. We calculate this band offset to be 1.51 eV as listed in Table II. The long-range nature of the local potential results in the shifting of the electronic bands across the junction. Holes in the valence band and electrons in the conduction band experience exactly the same magnitudes for their offsets, namely the valence band offset and the conduction band offset respectively, of 1.51 eV. This is due to the homo-nature of the junction. This, in general, is not true for a heterojunction, for example, in Si/Ge the valence band offset and the conduction band offset differs from each other because of the hetero-nature of the junction.

The saw-tooth potential is an artifact of the supercell construction that imposes an artificial periodicity on the system. We calculate an electric field of $6.081\times10^{9} Vm^{-1}$ across the supercell. In principle, the field can be gotten rid of by creating a large enough supercell with two identical junctions but of opposite orientations resulting in oppositely directed dipoles. However, for the zigzag orientation, this is not possible because the atomic lines are not equidistant from each other.

We turn our attention to the zigzag-long structure. This structure comprises a ladder of C atoms with C-C bond length of d_{C-C}=1.368 Å, which is shorter than that in graphene. One side of the interface consists of C-N bonds with internal angles of 119.27° and d_{N-C}=1.455, while the other side consists of C-B bonds with internal angles of 115.70° and d_{B-C}=1.482 Å.

In Fig. 11 we plot the line averaged charge density and the macroscopic averaged charge density for the zigzag-long structure. We note that the macroscopic average of the charge density peaks at a value of about 7 electrons per supercell on the C-substituted B side of the interface, and dips to minus this value on the C-substituted N side of the interface, which results in a net dipole at the interface. In Fig. 12 we plot the line averaged potential and the macroscopic averaged potential. We note a discontinuity of the potential across the interface. We calculate the band offset to be 1.99eV as listed to Table II.

C. Zigzag-single structures

In Fig. 13 we plot the line averaged charge density and the macroscopic averaged charge density for the zigzag-single C-substituted B structure. In Fig. 14 we do the same for the zigzag-single C-substituted N structure. We note that there is an accumulation of charge for the B-substituted case, and a depletion of charge in the N-substituted case. The macroscopic average of the charge density peaks at a value of about 8 electrons per supercell for the C-substituted B structure and dips to about minus this value for the C-substituted N structure. But there is no separation of charge as is necessary for the creation of a dipole. No dipole is formed and there is no shifting of the bands for both these structures.

D. Heats of formation

The zigzag orientations with double lines of C are the best candidates for engineering the band offset in boronitrene. We

calculated the heat of formation for the zigzag-short structure to be 0.502 eV as listed in Table II. The heat of formation for the zigzag-long structure is 1.764 eV, which is greater than that for the zigzag-short structure, and also greater than the heats of formation for the armchair structures which we calculated to be 1.042 eV for the armchair-double structure and 1.174 eV for the armchair-single structure.

As already referred to in the introduction, Muñoz *et al* considered a double layer of Ge in GaAs oriented along the (111) and (100) directions. For their (111)-near orientation, they computed a heat of formation of 0.12 eV and for the (100) orientation, a heat of formation of 0.48 eV. Both these results suggest that it requires a positive energy input to create these interface structures. Clearly these interfaces do not form spontaneously. The fact that these systems have been synthesized[20] gives an indication of the stability of these systems.

This gives credence to our results and our proposal that the zigzag-short structure of BN/C is the most viable structure for modifying the band offset in boronitrene. The positive heats of formation of our system implies that a positive energy input is required to create this structure. We suggest that controlled heavy ion bombardment in a C-rich environment is one means of exploring the synthesis of our proposed structure.

V. CONCLUSIONS

Our results show that substituting a double line of C atoms in boronitrene in the zigzag-long and zigzag-short orientations gives rise to a net dipole at the interface. This is due to the polar nature of the alternating lines of B and N atoms parallel to the junction. The dipole at the interface results in a shifting of the electronic bands across the junction. This gives rise to a band offset, which we calculate to be 1.51 eV for the zigzag-short orientation, and 1.99 eV for the zigzag-long orientation. The zigzag-short orientation is energetically more favorable with a heat of formation of 0.502 eV compared with the zigzag-long structure which has a heat of formation of 1.764 eV. Because of the minimal lattice mismatch between boronitrene and graphene, we expect that atomic relaxations and strains at the interface play a minor role in altering the electronic properties of this junction .

The armchair orientations contain an equal number of B and N atoms in each line parallel to the interface resulting in non-polar lines of atoms. Substituting lines of C atoms (single or double) does not result in a dipole at the interface, and hence there is no shifting of the bands.

Substituting a single line of C atoms in the zigzag orientation (B-substituted or N-substituted) does not result in a net dipole at the interface despite the polar nature of the alternating lines of B and N atoms parallel to the junction. There is an accumulation of charge for the B-substituted case, and a depletion of charge in the N-substituted case, but no separation of charge as is necessary for the creation of a dipole. Once again, there is no shifting of the bands.

We conclude that the zigzag-short orientation comprising the double line of C atoms is a viable means of modifying the band offset in boronitrene. This can be the basis of creating a nano-sized electrical diode.

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[1] Jianyu Y Huang, Hidehiro Yasuda, and Hirotaro Mori. HRTEM and EELS Studies on the Amorphization of Hexagonal Boron Nitride Induced by Ball Milling. *Journal of American Ceramic Society*, 83(2):403–409, 2000.

[2] M Grimsditch, E S Zouboulis, and A Polian. Elastic constants of boron nitride. *Journal of Applied Physics*, 76(2):832, 1994.

[3] Nelson Y Dzade, Kingsley O Obodo, Sampson K Adjokatse, Akosa C Ashu, Emmanuel Amankwah, Clement D Atiso, Abdulhakeem A Bello, Emmanuel Igumbor, Stany B Nzabarinda, Joshua T Obodo, Anthony O Ogbuu, Olu Emmanuel Femi, Josephine O Udeigwe, and Umesh V Waghmare. Silicene and transition metal based materials : prediction of a two-dimensional piezomagnet. *Journal of Physics: Condensed Matter*, 22(37), 2010.

[4] Jannik C Meyer, Andrey Chuvilin, Gerardo Algara-Siller, Johannes Biskupek, and Ute Kaiser. Selective Sputtering and Atomic Resolution Imaging of Atomically Thin Boron Nitride Membranes 2009. *Nano Letters*, 9(7):2683–2689, 2009.

[5] W Auwarter, T J Kreutz, T Greber, and J Osterwalder. XPD and STM investigation of hexagonal boron nitride on Ni (111). *Surface Science*, 429:229–236, 1999.

[6] M Topsakal, E Aktürk, and S Ciraci. First-principles study of two- and one-dimensional honeycomb structures of boron nitride. *Physical Review B*, 79(11):115442, 2009.

[7] K S Novoselov, D Jiang, F Schedin, T J Booth, V V Khotkevich, S V Morozov, and A K Geim. Two-dimensional atomic crystals. *PNAS*, 102(30):10451–10453, 2005.

[8] Hermann Sachdev, Frank Müller, and Stefan Hüfner. BN analogues of graphene: On the formation mechanism of boronitrene layers-solids with extreme structural anisotropy. *Diamond and Related Materials*, 19(7-9):1027, July 2010.

[9] A K Geim and K S Novoselov. The rise of graphene. *nature materials*, 6:183–191, 2007.

[10] P Widmayer, H G Boyen, P Ziemann, P Reinke, and P Oelhafen. Electron spectroscopy on boron nitride thin films : Comparison of near-surface to bulk electronic properties. *Physical Review B*, 59(7):5233–5241, 1999.

[11] D W Niles, G Margaritondo, P Perfetti, C Quaresima, and M Capozi. Heterojunction band discontinity control by ultrathin intralayers. *Applied Physics Letters*, 47(10):1092, 1985.

[12] A Munoz, N Chetty, and R M Martin. Modification of heterojunction band offsets by thin layers at interfaces: Role of the interface dipole. *Physical Review B*, 41(5):2976, 1990.

[13] A Mujica, R Perez, F Flores, and A Munoz. Heterojunction band offsets for polar interfaces: From a thin to a thick covalent intralayer. *Physical Review B*, 46(15):9641, 1992.

[14] Alfonso Baldereschi, Stefano Baroni, and Raffaele Resta. Band Offsets in Lattice-Matched Heterojunctions: A Model and First-Principles Calculations for GaAs/AlAs. *Physical Review Letters*, 61(6):734, 1988.

[15] Chris G Van de Walle and Richard M Martin. Theoretical study of band offsets at semiconductor interfaces. *Physical Review B*, 35(15):8154, 1987.

[16] N E Christensen. Dipole effects and band offsets at semiconductor interfaces. *Physical Review B*, 37(9):4528, 1988.

[17] N Chetty and Richard M Martin. GaAs (111) and $(\bar{1}\bar{1}\bar{1})$ surfaces and the GaAs/AlAs (111) heterojunction studied using a local energy density. *Physical Review B*, 45(11):6089, 1992.

[18] L Colombo, R Resta, and S Baroni. Valence-band offsets at strained si/ge interfaces. *Physical Review B*, 44(11):5572, 1991.

[19] Chris G Van de Walle and Richard M Martin. Theoretical calculations of heterojunction discontinuities in the Si/Ge system. *Physical Review B*, 34(8):5621, 1986.

[20] Ruth Klauser, Masaharu Oshima, Hirohiko Sugahara, Yoshitada Murata, and Hiroo Kato. Rbf as reactive and dipole interlayers between the ge/gaas interface. *Phys. Rev. B*, 43(6):4879–4884, Feb 1991.

[21] Shinji Koh, Takashi Kondo, Minoru Ebihara, Tetsuya Ishiwada, Hidetaka Sawada, Hideki Ichinose, Ichiro Shoji, and Ryoichi Ito. Gaas/ge/gaas sublattice reversal epitaxy on gaas (100) and (111) substrates for nonlinear optical devices. *Japanese Journal of Applied Physics*, 38(Part 2, No. 5A):L508–L511, 1999.

[22] M. Kawaguchi. B/c/n materials based on the graphite network. *Advanced Materials*, 9(8):615–625, 1997.

[23] Amy Y. Liu, Renata M. Wentzcovitch, and Marvin L. Cohen. Atomic arrangement and electronic structure of *bc*2n. *Phys. Rev. B*, 39(3):1760–1765, Jan 1989.

[24] Y. Fan, K. Hou, Z. Wang, T. He, X. Zhang, H. Zhang, J. Dong, X. Liu, and M. Zhao. Theoretical insights into the built-in electric field and band offsets of BN/C heterostructured zigzag nanotubes. *Journal of Physics D: Applied Physics*, 44:095405, 2011.

[25] P Hohenberg and W Kohn. Inhomogeneous Electron Gas. *Physical Review*, 136(3B):864, 1964.

[26] Paolo Giannozzi, Stefano Baroni, Nicola Bonini, Matteo Calandra, Roberto Car, Carlo Cavazzoni, Davide Ceresoli, Guido L Chiarotti, Matteo Cococcioni, Ismaila Dabo, Andrea Dal Corso, Stefano de Gironcoli, Stefano Fabris, Guido Fratesi, Ralph Gebauer, Uwe Gerstmann, Christos Gougoussis, Anton Kokalj, Michele Lazzeri, Layla Martin-Samos, Nicola Marzari, Francesco Mauri, Riccardo Mazzarello, Stefano Paolini, Alfredo Pasquarello, Lorenzo Paulatto, Carlo Sbraccia, Sandro Scandolo, Gabriele Sclauzero, Ari P Seitsonen, Alexander Smogunov, Paolo Umari, and Renata M Wentzcovitch. QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials. *Journal of Physics: Condensed Matter*, 21:395502, September 2009.

[27] John P Perdew, Kieron Burke, and Matthias Ernzerhof. Generalized Gradient Approximation Made Simple. *Physical review letters*, 77(18):3865, October 1996.

[28] David Vanderbilt. Soft self-consistent pseudopotentials in a generalized eigenvalue formalisn. *Physical Review B*, 41(11):7892, 1990.

[29] Hendrik J Monkhorst and James D Pack. Special points for Brillouin-zone integrations. *Physical Review B*, 13(12):5188, 1976.

[30] M Methfessel and A T Paxton. High-precision sampling for Brillouin-zone integration in metals. *Physical Review B*, 40(6):3616, 1989.

TABLE I. Number of B, N and C atoms per unit cell for the armchair and zigzag structures.C_B and C_N refers to C-substituted B and N respectively.

structure	B	N	C	Total
armchair-double	6	6	4	16
armchair-single	7	7	2	16
zigzag-long	5	5	2	12
zigzag-short	5	5	2	12
zigzag-single (C_B)	5	6	1	12
zigzag-single (C_N)	6	5	1	12

TABLE II. The values for the dipole (eV), electric field (10^9 V m^{-1}) and heat of formation ΔH (eV).

structure	ΔV_{gap}	E_{field}	ΔH_f
armchair-double	-	-	1.042
armchair-single	-	-	1.174
zigzag-long	1.99	5.568	1.764
zigzag-short	1.51	6.081	0.502

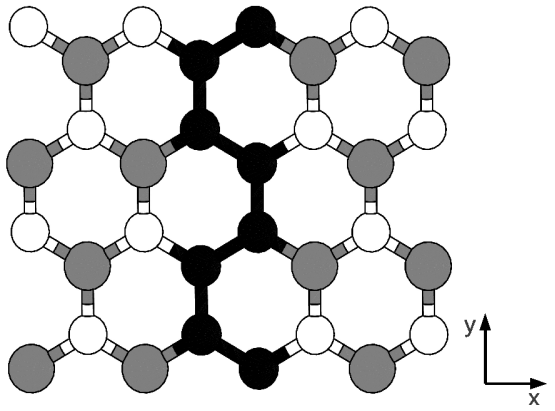

FIG. 1. The BN/C armchair-double structure showing a double line of C atoms. B atoms (●), N atoms (○) and C atoms (●). Because of the nonpolar lines comprising both B and N atoms parallel to the junction, no dipole is created at the junction by the double line of C atoms

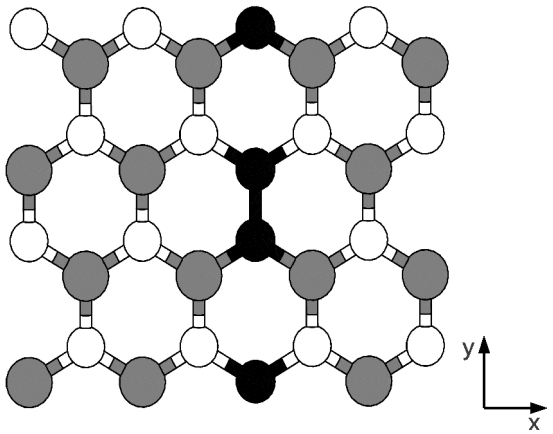

FIG. 2. The BN/C armchair-single structure showing a single line of C atoms. B atoms (●), N atoms (○) and C atoms (●). Because of the nonpolar lines comprising both B and N atoms parallel to the junction, no dipole is created at the junction by the single line of C atoms

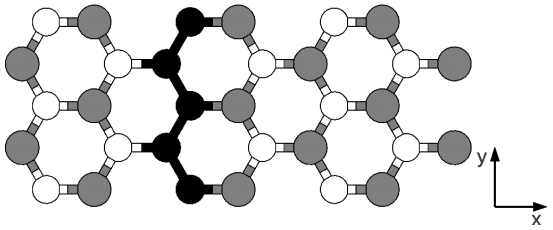

FIG. 3. The BN/C zigzag-short structure showing a double line of C atoms. B atoms (●), N atoms (○) and C atoms (●). Because of the alternating polar lines of B and N atoms parallel to the junction, a line of dipoles is created at the junction by the double line of C atoms

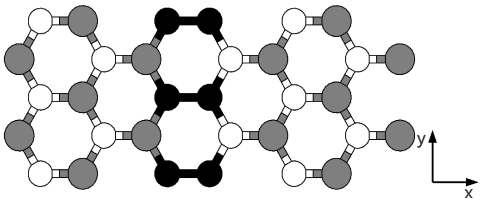

FIG. 4. The BN/C zigzag-long structure showing a double line of C atoms. B atoms (●), N atoms (○) and C atoms (●). Because of the alternating polar lines of B and N atoms parallel to the junction, a line of dipoles is created at the junction by the double line of C atoms

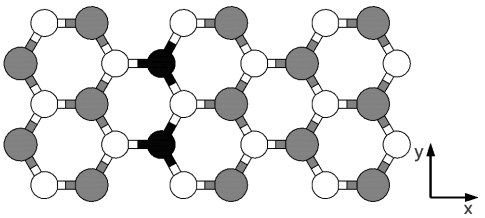

FIG. 5. The BN/C zigzag structure showing a single line of C-substituted B atoms. B atoms (●), N atoms (○) and C atoms (●).

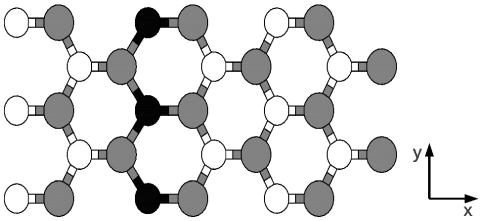

FIG. 6. The BN/C zigzag structure showing a single line of C-substituted N atoms. B atoms (●), N atoms (○) and C atoms (●).

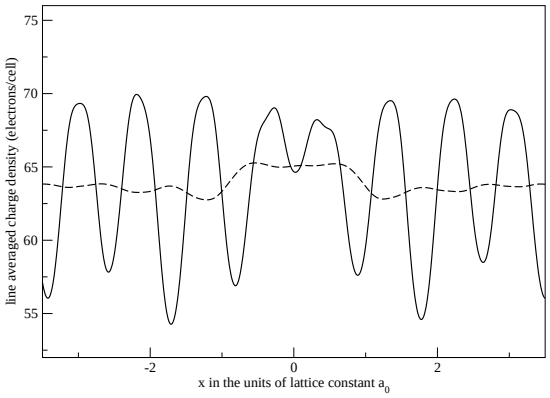

FIG. 7. The BN/C armchair-double structure showing no net dipole across the junction . The line-averaged charge density $\tilde{n}(x)$ as a solid line and the macroscopic average $\tilde{\tilde{n}}(x)$ as a dashed line.

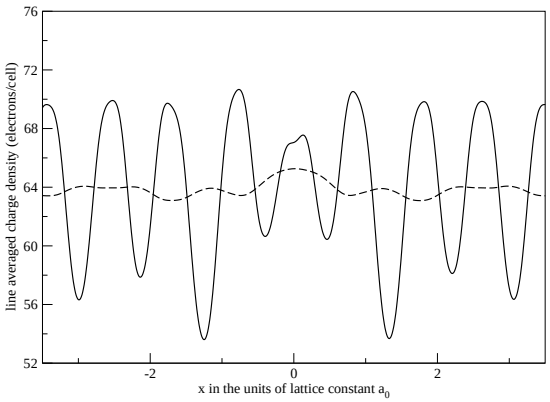

FIG. 8. The BN/C armchair-single structure showing no net dipole across the junction. The line-averaged charge density $\tilde{n}(x)$ as a solid line and the macroscopic average $\tilde{\tilde{n}}(x)$ as a dashed line.

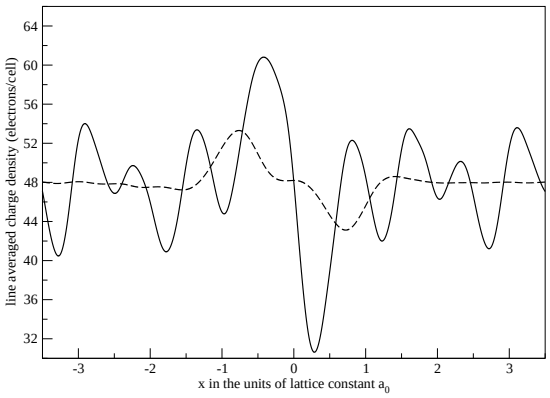

FIG. 9. The BN/C zigzag-short structure showing the dipole across the junction. The line-averaged charge density $\tilde{n}(x)$ as a solid line and the macroscopic average $\tilde{\tilde{n}}(x)$ as a dashed line.

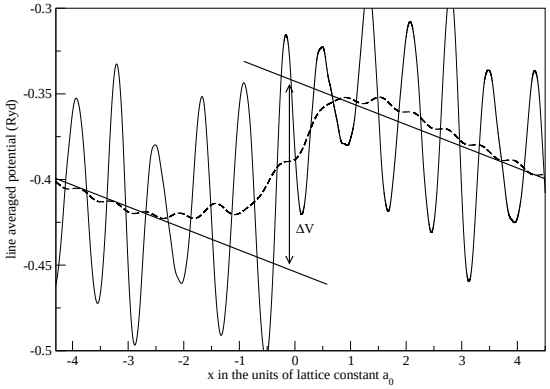

FIG. 10. The BN/C zigzag-short structure showing the band-offset. The line-averaged potential $\tilde{V}(x)$ as a solid line and the macroscopic average $\tilde{\tilde{V}}(x)$ as a dashed line.

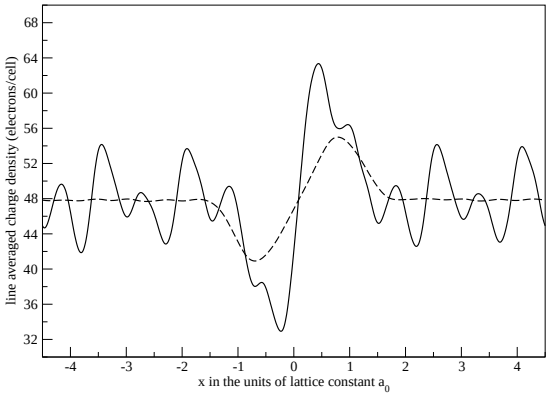

FIG. 11. The BN/C zigzag-long structure showing the dipole across the junction. The line-averaged charge density $\tilde{n}(x)$ as a solid line and the macroscopic average $\tilde{\tilde{n}}(x)$ as a dashed line.

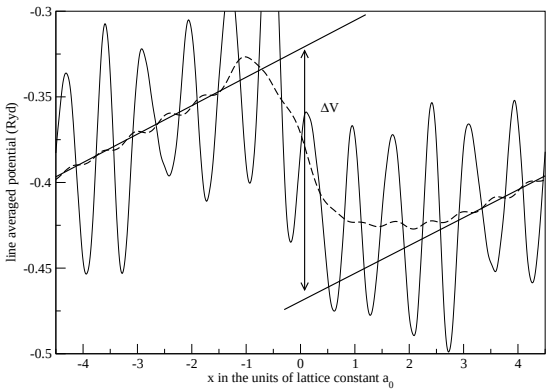

FIG. 12. The BN/C zigzag-long structure showing the band-offset. The line-averaged potential $\tilde{V}(x)$ as a solid line and the macroscopic average $\tilde{\tilde{V}}(x)$ as a dashed line.

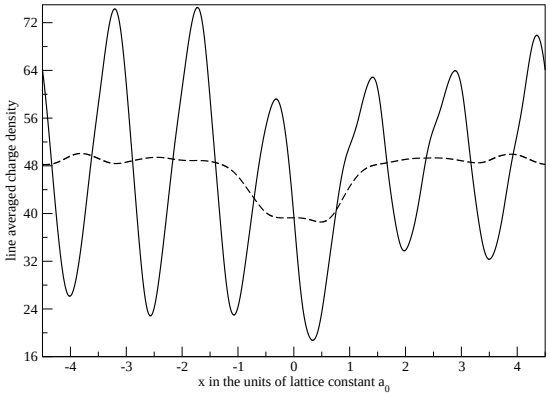

FIG. 13. The BN/C zigzag structure with a single line of C-substituted B atoms showing the line-averaged charge density $\tilde{n}(x)$ as a solid line and the macroscopic average $\tilde{\tilde{n}}(x)$ as a dashed line. There is an accumulation of electronic charge at the interface.

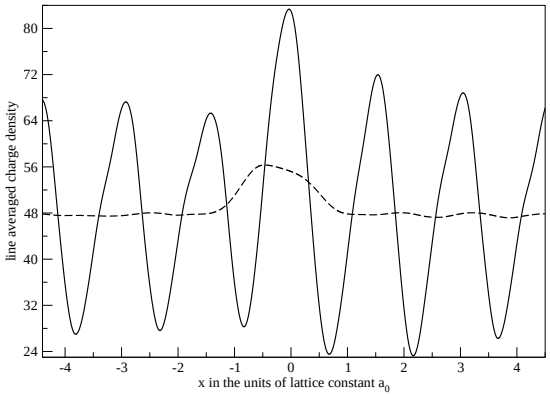

FIG. 14. The BN/C zigzag structure with a single line of C-substituted N atoms showing the line-averaged charge density $\tilde{n}(x)$ as a solid line and the macroscopic average $\tilde{\tilde{n}}(x)$ as a dashed line. There is a depletion of electronic charge at the interface.