Properties of BC$_6$N monolayer derived by first-principle computation: Influences of interactions between dopant atoms

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Abstract

The properties of graphene-like BC$_6$N semiconductor are studied using density functional theory taking into account the attractive interaction between B and N atoms. In the presence of a strong attractive interaction between B and N dopant atoms, the electron charge distribution is highly localized along the B-N bonds, while for a weaker attractive interaction the electrons are delocalized along the entire hexagonal ring of BC$_6$N. Furthermore, when both B and N atoms are doped at the same site of the hexagon, the breaking of the sub-lattice symmetry is low producing a small bandgap. In contrast, if the dopant atoms are at different sites, a high sub-lattice symmetry breaking is found leading to a large bandgap. The influences of electron localization/delocalization and the tunable bandgap on thermal behaviors such as the electronic thermal conductivity, the Seebeck coefficient, and the figure of merit, and optical properties such as the dielectric function, the excitation spectra, the refractive index, the electron energy loss spectra, the reflectivity, and the optical conductivity are presented. An enhancement with a red shift of the optical conductivity at low energy range is seen while a reduction at the high energy range is found indicating that the BC$_6$N structure may be useful for optoelectronic devices in the low energy, visible range.

Keywords: BC$_6$N, DFT, Electronic structure, Thermoelectric, Optical properties

1. Introduction

The optical behavior of 2D materials such as graphene and silicene have unique tunability through controlling the geometrical configuration, the local excitonic effects, the doping density, and the defects levels [1, 2]. Graphene possesses unique optical transitions and can absorb light over a wide range of frequencies due to the presence of the linear dispersion at the Dirac point. It leads to an exhibition of extraordinary properties such as a constant optical conductivity in the infrared regime and the gate-dependent optical absorbance [3, 4]. The strong optical transitions of a monolayer graphene and the tunability by simple electrical gating hold a promise for new applications in for infrared optics, optoelectronics, and the semiconductor and optical industry [5, 6].

Substitutional doping has been considered as an effective method for tailoring the electronic and optical properties of monolayer graphene nanostructures. This is because the doping helps to tune the work function and the carrier concentration of the nanostructure broadening the range of possible electronic and optical applications [7, 8]. Boron (B) atoms supply an electron to the graphene in the case of a B-doped graphene increasing the Fermi energy due to the low electronegativity of the B atom leading to a p-type semiconductor [10]. In contrast, the N atoms receive electrons from the graphene leading to an n-type semiconductor because the electronegativity of an N atom is higher than that of the carbon, C, atoms [11]. The optical response of both doped systems is sensitive to their electronic structure around the Fermi energy, and the absorption spectrum undergoes changes in low energy range [12, 13]. In the case of BN-codoped monolayer graphene, the optical response evolves from the infrared to the ultraviolet region and shows significant anisotropy for different polarizations [14, 15]. Extra peaks in absorption spectra in addition to the $\pi-\pi^*$ transition peak have been found for BN-codoped graphene in the visible range of the electromagnetic spectrum in the case of parallel polarization [16]. Furthermore, the optical response such as the dielectric function and the reflectivity have been investigated by varying the concentration ratio of the BN-dopant atoms in monolayer graphene, and significant red shift in absorption towards the visible range of the radiation at high doping was found [17].

We believe that information on the influences of the interaction between the B and the N atoms in a graphene...
structure on the optical response is still lacking. We therefore consider the role of the interaction between the B and N dopant atoms in different configuration in a BN-codoped monolayer graphene. We find that the imaginary and real part of the dielectric function, the excitation spectra, the refractive index, the reflectivity, and the optical conductivity are prominently modified due to the interaction between the B and N atoms in the system.

In Sec. 2 the BN-codoped monolayer graphene structure is briefly overviewed. In Sec. 3 the main achieved results are analyzed. In Sec. 4 the conclusion of the results is presented.

2. Computational details

In the present work, the Quantum espresso (QE) package code based on density functional theory (DFT) has been used \cite{28, 29}. The approach is based on an iterative solution of the Kohn-Sham theory of DFT in a plane-wave set with Norm Conserving (NC) pseudopotential \cite{22, 23}. In the calculations, we consider the Perdew-Burke-Ernzerhof (PBE) functional of the GGA approach \cite{22, 23, 24}.

Our model is a 2×2 supercell of monolayer sheets, where the sheets are separated by 20 Å along the perpendicular direction to avoid an interaction between the layers. The plane wave cutoff energy is assumed to be 680 eV, and the Monkhorst-Pack scheme is used to form the Brillouin zone sampling. Our pure and BN-codoped monolayer graphene are fully relaxed with an 8×100 Å mesh, and a very dense k-mesh of k-points, 100×100×1, is used to calculate the electron density of states (DOS) of the system.

The optical properties of the systems are evaluated using the QE package, and a large number of empty bands is taken into account to evaluate the dielectric properties of the systems, ε(ω) = ε1(ω) + iε2(ω), where ε1 and ε2 are the real and imaginary parts of dielectric function. The QE code gives us ε1(ω) and ε2(ω). One can then calculate the complex refractive index, N(ω) = n(ω) + iκ(ω), where n(ω) is the real part of refractive index and, κ(ω) the excitation coefficient, the imaginary part of N via \cite{25}

\[
n(ω) = \frac{1}{\sqrt{2}} \left( \left[ ε_1^2(ω) + ε_2^2(ω) \right]^{1/2} + ε_1(ω) \right)^{1/2}, \quad (1)
\]

and

\[
κ(ω) = \frac{1}{\sqrt{2}} \left( \left[ ε_1^2(ω) + ε_2^2(ω) \right]^{1/2} - ε_1(ω) \right)^{1/2}. \quad (2)
\]

The reflectivity at normal incidence of EM wave on the materials can be obtained from n and κ by

\[
R(ω) = \frac{n(ω) - 1}{n(ω) + 2} \left[ n(ω) + 2 \right]^2 + κ^2(ω). \quad (3)
\]

In addition, the optical conductivity can be computed from

\[
σ_{\text{optical}} = \frac{-i}{4π} \left[ ε(ω) - 1 \right]. \quad (4)
\]

3. Results

In this section, we present the model, dispersion energy, partial density of states, optical response, and thermal properties of the systems.

3.1. Model, Charge distribution, and Interaction energy

We consider three different configurations of BN-codoped graphene based on the distance between the B and N atoms. The electron charge distribution of all the three different BN-codoped graphenes are shown in Fig. 1. A schematic diagram of a hexagonal ring is presented in Fig. 1(a) indicating the ortho-, the meta-, and the para-positions. In the first configuration for our systems, the B atom is doped at an ortho-position and the N atom is at a meta-position identified as BC4N-1, and it’s electron charge distribution is presented in (b). The other two configurations are BC4N-2 (c) and BC4N-3 (d) where the B atom is fixed at an ortho-position, but the N atom is moved to a para-, or a meta-position, respectively. In this way, we define three BC4N structures with different distances and interaction strength between the B and the N dopant atoms. The distance between the B and the N atom in BC4N-1, BC4N-2, and BC4N-3 is 1.41, 2.43, and 2.8 Å, respectively. The interaction energy between the B and the N atoms can be evaluated from the total energy obtained via SCF calculation \cite{28, 29}. The interaction type between the B and the N atoms is attractive as the interaction energy has a negative sign \cite{29}. Our calculations indicate that the strongest interaction between the

![Figure 1](image-url)

Figure 1: Schematic of a hexagonal structure (a) with the ortho-, the meta-, and the para-positions, and the electron charge density for BC4N-1 (b), BC4N-2 (c), BC4N-3 (d).
B and the N atoms is in BC$_6$N-1, which is expected as the distance between the B and the N atoms is then the shortest for all the three configurations. The attractive interaction becomes weaker increasing distance between the B and the N atoms in both BC$_6$N-2, and BC$_6$N-3.

The C, B and N atoms can be ordered from the higher to lower electronegativity as follows: N $>$ C $>$ B. The B atom gives an electron to the C atoms, and the N atom receives electrons from the C atoms due the difference in their electronegativity [34]. Consequently, one can see that the electron charge distribution around the N atom is high and around the B atom is low comparing to the C atoms in all three configuration structures shown in Fig. 1. In BC$_6$N-1, electrons are directly transferred from a B atom to an N atom leading to a higher electron charge distribution in the B-N bonds near to the N atom comparing to the C-B and C-N bonds. This confirms the strong attractive interaction between the B and N atoms. In both BC$_6$N-2 and BC$_6$N-3, electrons are not directly transferred from a B atom to an N atom, but an N atom receives electrons from the C atoms along all the three C-N bonds in the hexagonal, and a C atoms receives electrons from the B atoms. As a results, the electron delocalization along the C-C, C-B and C-N bonds is indicative for electron transport along the entire ring of the hexagonal structure. This gives rise a higher electron charge distribution between the C-C, C-B, and C-N bonds of the BC$_6$N-2 and BC$_6$N-3 structures comparing to the BC$_6$N-1 structure.

The stability of the structures can be determined by the bonding between the C, B and N atoms, and the number of C-C, C-B, C-N, and B-N bonds in a structure will affect its stability. The binding energies of the C-C and B-N bonds are higher than those of the C-B and C-N bonds. So, a structure with a higher number of C-C and B-N bonds has a higher binding energy [31,32]. We can therefore confirm that the BC$_6$N-1 structure is the most energetically stable structure.

3.2. Dispersion energy and PDOS

The electronic dispersion energy for the BC$_6$N structures (b-d) are displayed in Fig. 2 together with that of pure graphene (a). The band structure of pure graphene (PG) is re-plotted for the sake of comparing it with the band structure of BC$_6$N.

A bandgap opens in the presence of the B and N atoms reflecting the sublattice symmetry breaking. The bandgap is 0.13, 1.2 and 1.26 eV for BC$_6$N-1, BC$_6$N-2, and BC$_6$N-3, respectively. In spite of the sublattice symmetry breaking, the Dirac cone of the BC$_6$N structures remains preserved. One notices that the opening of a bandgap is larger for the structures whose B and N atoms are doped at both A- and B-sites of the hexagonal ring such as BC$_6$N-1 and BC$_6$N-3. If the B and N atoms are doped at either a A- or a B-site such as in BC$_6$N-2, the bandgap is small indicating smaller symmetry breaking. This has been previously explained and confirmed by Zhu and et al. [34], and Chang and et al. [35] where they have connected the opening up of a bandgap to the number of $\pi$-bands or $\pi$-electrons, and aromaticity of the structures, respectively.

They show that there is an odd number of $\pi$-electron or $\pi$-bands if the B and N atoms are doped at either a A- or a B-site producing a small bandgap, while an even number of $\pi$-electrons is found for a structure with the B and N atoms doped at a A- and a B-site leading to a larger bandgap. We draw the attention to that the dispersion energies of these structures are also presented in [36], where the mechanical and thermal properties of the systems were investigated.

The partial density of states (PDOS) for BC$_6$N-1 (a), BC$_6$N-2 (b), and BC$_6$N-3 (c) structures are demonstrated in Fig. 3. It can be seen from the PDOS that both the B and N atoms contribute to the opening up of a bandgap as the PDOS of the B and N atoms have a high contribution around the Fermi energy, and the maxima and minima of the valence and conduction band edge in the energy range from −2.5 to 2.5 eV. The PDOS around the Fermi energy for both the B and N atoms are p$_z$-components indicating the $\pi$-states of a B and N atoms. Furthermore, the distance between the $\pi$-peak and the $\pi^*$-peak in the PDOS around the Fermi energy for BC$_6$N-1 and BC$_6$N-3 is 3.289 and 4.17 eV, respectively. These are larger than for BC$_6$N-2: 3.068 eV, confirming the larger bandgaps of these two structures.

3.3. Optical properties

It was seen in the previous section that the B-N dopant atoms can significantly tune the dispersion energy and PDOS of BC$_6$N-monolayer structures. This modification of the band structure and PDOS alter the optical properties of systems. In this section, we focus on the main results of the dielectric function, the refractive index, the reflectivity, the electron energy loss spectra, EELS, and the
optical conductivity of BC$_6$N-monolayer structures emerging due to the B and N dopant atoms. In general, the optical response rather depends on the position of the B and N atoms doped at either the same or different sites in the hexagonal structure of graphene.

The imaginary part of dielectric function that expresses the damping of the wave and the dissipation of energy is presented in Fig. 4 with both parallel, $E_\parallel$ (a) and perpendicular, $E_\perp$ (b), polarization of the electric field vector of external EM field. In order to clearly see the modification of the optical response, we re-plot the dielectric function of PG. In the case of $E_\parallel$, two main peaks in imaginary part of dielectric function (black), $\varepsilon_2$, are observed for PG at $\approx 4.16$ and $14.59$ eV corresponding to the $\pi$-$\pi^*$ and $\sigma$-$\sigma^*$ transitions, respectively. The position of the first peak is close to the experimental value observed at 4.16 eV. The slight different in the peak position stems from the neglect of the interaction between the monolayer graphene and the substrate in our calculation. The position of the second peak agrees very well with an experimental value, 14.6 eV, obtained for free-standing monolayer graphene. In addition to the two peaks, a strong peak at zero energy is seen due to the vanishing bandgap of PG. In the case of $E_\perp$ shown in Fig. 4(b), two peaks at 11.46, and 14.83 eV for PG are seen associated with the $\pi$-$\sigma^*$, and $\sigma$-$\pi^*$ transitions, respectively.

In the presence of the BN-dopant atoms, the Fermi level shifts and a bandgap is introduced at Fermi level so the energy peak at 4.16 eV is prominently shifted. In addition to the two main peaks, a pronounced peak starting from 1.2 (red), or 1.26 eV (green) is found in the visible region for BC$_6$N-1, and BC$_6$N-3, respectively, in the case of $E_\parallel$. These energy values coincide with the bandgap of the two structures, BC$_6$N-1, and BC$_6$N-3. So, the peak in the visible region is caused by the opening up of a bandgap. Furthermore, a very strong peak at 0.1 eV is seen for BC$_6$N-1 indicative of the transition around small bandgap of the structure. In general, for both $E_\parallel$ and $E_\perp$, the intensity of both main peaks is decreased for all three BN-codoped graphene structures indicating a weaker damping or dissipation of the wave compared to PG. This reflects the increased localization of the electrons occurring in these structures.

The imaginary part of a refractive index (excitation spectra) shown in Eq. (2), $\kappa(\omega)$, is related to the absorption coefficient. The excitation spectra is qualitatively very similar to the imaginary part of the dielectric function for both $E_\parallel$ (a) and $E_\perp$ (b) displayed in Fig. 5 for PG and BN-codoped graphene. Similar information can be read from $\varepsilon_2$, a significant red shift of the two main peaks of the excitation spectra towards the visible range of the electromagnetic radiation is observed for BN-codoped graphene structures in the case of $E_\parallel$, while a reduction in the peaks without any pronounced shift is seen in the case of $E_\perp$. A peak caused by the opening up of a bandgap is also seen for $E_\perp$.

Further interesting information about optical response is associated with the real part of dielectric function, $\varepsilon_1$, which is presented in Fig. 6 for both parallel, $E_\parallel$ (a) and perpendicular, $E_\perp$ (b), polarization of the external electric
The $\varepsilon_1$ is indicative of the ability of materials to store electrical energy related to the polarization. The value of $\varepsilon_1(0)$ is defined as a static dielectric constant or the value of dielectric function at zero energy. The value of $\varepsilon_1(0)$ of PG is 4.81, and 1.23 for $E_\parallel$ and $E_\perp$, respectively, which is in a good agreement with the recent results of $\varepsilon_1(0)$ for both directions of polarized electric field calculated via DFT [38], and in a fair agreement with [17] for $E_\parallel$, where 7.6 and 1.25 are obtained. The different values of $\varepsilon_1(0)$ for PG may be influenced by the number of bands taken in the DFT calculations or choice of pseudopotentials. When the value of $\varepsilon_1$ is zero or very small, and $\varepsilon_2$ is also small, the electron energy loss spectra (EELS) shown in Fig. 7 starts to display a peak. This frequency is the plasma frequency for collective electron oscillations, $\omega_p$, and the energy of plasma frequency is defined as $E = \hbar \omega_p$. The energy of the plasmon oscillation for PG is found to be 4.25 and 14.95 eV for $E_\parallel$ and $E_\perp$, respectively, agreeing very well with [38].

In the presence of BN dopant atoms the value of $\varepsilon_1(0)$ does not change appreciably for $E_\perp$ polarization. However, for $E_\parallel$ polarization, the values of $\varepsilon_1(0)$ and $\varepsilon_1(\omega)$ below 5 eV change significantly in the presence of B and N atoms doped at the A- and B-sites of the hexagon, BC$_6$N-1, and BC$_6$N-3. This is caused by the stronger symmetry breaking of the sub-lattice symmetry when both the A- and B-sites are doped. The value of $\varepsilon_1(0)$ is reduced to 3.19 and 2.39 for BC$_6$N-1, and BC$_6$N-3, respectively, in the case of $E_\parallel$ indicating the weaker ability of these structures to store electrical energy at nearly zero-energy of an applied electric field, and it is a slightly increased in the case of $E_\perp$ (inset of Fig. 6). On the other hand, for BC$_6$N-2 where both the B and N atoms are doped at the A- or the B-sites resulting in less breaking of the sub-lattice symmetry, the value of $\varepsilon_1(0)$ is found to be 4.13, which is relatively close to that of PG. We therefore see that the ability of BC$_6$N-2 to store energy is almost similar to PG. Furthermore, the plasma oscillation is only seen at 3.06 eV for BC$_6$N-2 in the case of $E_\parallel$ while the plasma oscillation vanishes for both BC$_6$N-1, and BC$_6$N-3.
the electron charge density distribution shown in Fig. 1, the ultra violet (UV) region at a frequency of
reduction ratio in the refractive index is higher for BC
6
PG are found at 4 of the BC
6
for the reflectivity for PG in both directions of electric
energy range, 10-20 eV, are activated leading to the reduc-
tivity located between 10 to 20 eV for both directions of
In the case of E
∥
and BC
6
be 1 peaks at 12.
Figure 8: Refractive index, real part of complex refractive index, for PG (black), BC
6
N-1 (red), BC
6
N-2 (blue), and BC
6
N-3 (green) for both parallel, E
∥
(a) and perpendicular, E
⊥
(b), polarization of electric field vector of external EM field.

The real part of refractive index of PG near to zero en-
ergy, n(0), is found to be 2.19 for E
∥
and 1.109 for E
⊥
. In the presence of the attractive interaction between the B
and N atoms, no noticeable change is found corresponding
to the n(0) value the peak positions for the E
⊥
polarization. In the case of E
∥
, the value of n(0) is observed to be 1.78, 2.07, and 1.71 indicating that the refractive
index is reduced by 18.73%, 5.43%, and 21.92% for BC
6
N-1, BC
6
N-2, and BC
6
N-3, respectively, compared to PG. The
reduction ratio in the refractive index is higher for BC
6
N-1 and BC
6
N-3 where both the B and N atoms are doped at
different atomic sites indicating less transmittance behav-
iors near zero-energy.

After obtaining the frequency dependent refractive index,
we compute the reflectivity of the PG and BN-
codoped graphene for both E
∥
(a) and E
⊥
(b) polarization shown in Fig. 8. Two main peaks in the reflectivity of PG are found at 4.32 and 14.76 eV for E
∥
, and two main peaks at 12.02 and 15.47 eV for E
⊥
. The peak positions
for the reflectivity for PG in both directions of electric
field are well agree with [39]. For all three configurations
of the BC
6
N structures, the peak intensity of the reflectiv-
ity located between 10 to 20 eV for both directions of
E-field is reduced irrespective of the strength of the at-
tractive interaction between the B and N atom, and the
position of the B-N atoms. The collective oscillations of
free electrons and the valence electrons in the selected en-
ergy range, 10-20 eV, are activated leading to the reduc-
tivity of the BC
6
N structures. In contrast, an enhancement of the reflectivity is seen for BC
6
N-2 in the ultra violet (UV) region at a frequency of < 6.0 eV for E
∥
. This is in agreement with our previous explanation of the electron charge density distribution shown in Fig. 8.

where the electron delocalization in BC
6
N-2 is high lead-
ing to higher reflectivity in the UV region. The reflectivity
for PG and all the BN-codoped structures is very small or
close to zero in the energy range 7-10 eV for both direc-
tions of E-field while the refractive index is close to unity
in this energy range.

Last, the real part of the optical conductivity is shown in
Fig. 10 for both a parallel, E
∥
(a) and a perpendicu-
lar, E
⊥
(b) electric field. The optical conductivities starts
with a gap in the case of E
∥
, which is due to the semi-
conducting properties of the BC
6
N-1 and BC
6
N-3. A very
small zero value of optical conductivity of BC
6
N-2 is seen
in the low energy range < 0.15 eV indicative of the small
bandgap of the structure. For PG, two main peaks in the
optical conductivity are seen at 4.33 and 14.75 eV for E
∥
indicating the \( \pi^-\pi^+ \) and \( \sigma^-\sigma^+ \) transitions, respectively,
and 12.02 and 15.47 eV for E
⊥
showing \( \pi^-\pi^+ \) and \( \sigma^-\sigma^+ \), respectively. As we have mentioned, the peak intensity
of the optical conductivity located between 10 to 20 eV for
both directions of an E-field is reduced irrespective of
the strength of attractive interaction between the B
and N atom, and the position of B-N atoms. In contrast, the
peak position in the energy range of 3-6 eV is shifted to-
wars a lower energy for BC
6
N-1 and BC
6
N-2 due to the
shrinking of bands along the \( \Gamma-K-M \) path as is seen in Fig.
10(b-c). The peak here is due to optically active interband
excitations through the Dirac point. Consequently, the
transition from \( \pi \) to \( \pi^+ \) needs less energy, and the peak
appears at a lower energy. In addition, a slightly enhance-
mint in the optical conductivity is seen for BC
6
N-2, which
will be useful for applications in photovoltaic cells.

3.4. Thermal Properties
In this section, thermal properties such as the electronic
thermal conductivity (a), the electrical conductivity (b),
the Seebeck coefficient (c), and the figure of merit (d)
are investigated and displayed in in Fig. 11. The thermal calculations are carried out in the temperature range of \( T = 20-150 \) K where the electron contribution to the transport is dominant and the phonon participation can be neglected because the electron and lattice temperature are decoupled in this temperature range \([40, 41]\). Boltztrap software can be thus used to investigate the thermal properties under the above condition \([42]\). The Boltztrap is based on the Boltzmann theory which is used to calculate the semiclassical transport coefficients. The code uses a mesh of band energies and is interfaced to the QE package \([13]\).

4. Conclusions

To conclude, we have used density functional theory to study the structural, thermal, and optical properties of monolayer graphene doped with boron and nitrogen atoms where the influences of an attractive interaction between the dopant atoms are highlighted. We have assumed few atomic configurations forming different BC\(_6\)N structures based on the interaction between the B and N atoms. We have found that the static dielectric constant is decreased, and the plasmon oscillation is reduced or vanishes in the presence of an attractive interaction between the B and N atoms compared to the pristine monolayer graphene. Furthermore, the refractive index indicating the transmittance behavior is enhanced in the case interactions between the B and N atoms in the low energy ranges while the reflectivity is decreased. In addition, a high Seebeck coefficient and a high figure of merit have been found for BC\(_6\)N where the B and N atoms are doped at different atomic sites of the hexagon structure. We can thus confirm that the thermal and the optical properties of BC\(_6\)N can be improved by controlling the interaction between the dopant atoms which may be useful for thermoelectric and optoelectronic devices.

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