Interlayer interaction controlling the properties of AB- and AA-stacked bilayer graphene-like BC$_{14}$N and Si$_2$C$_{14}$

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Abstract

We model bilayer graphene-like materials with Si$_2$C$_{14}$ and BC$_{14}$N stoichiometry, where the interlayer interactions play important roles shaping the physical properties of the systems. We find the interlayer interaction in Si$_2$C$_{14}$ to be repulsive due to the interaction of Si-Si atoms, and in BC$_{14}$N it is attractive due to B and N atoms for both the AA- and the AB-stacking. The repulsive interlayer interaction opens up a bandgap in Si$_2$C$_{14}$ while the attractive interlayer interaction in BC$_{14}$N induces a small indirect bandgap or overlapping of the valence conduction bands. Furthermore, the repulsive interaction decreases the Young modulus while the attractive interaction does not influence the Young modulus much. The stress-strain curves of both the AA- and the AB-stackings are suppressed compared to pure graphene bilayers. The optical response of Si$_2$C$_{14}$ is very sensitive to an applied electric field and an enrichment in the optical spectra is found at low energy. The enrichment is attributed to the bandgap opening and increased energy spacing between the $\pi-\pi^*$ bands. In BC$_{14}$N, the optical spectra are reduced due to the indirect bandgap or the overlapping of the $\pi-\pi^*$ bands. Last, a high Seebeck coefficient is observed due to the presence of a direct bandgap in Si$_2$C$_{14}$, while it is not much enhanced in BC$_{14}$N.

Keywords: Energy harvesting, Thermal transport, Graphene, Density Functional Theory, Electronic structure, Optical properties, and Stress-strain curve

1. Introduction

The ability to control physical properties of a material by tuning its bandgap is at the heart of modern electronic devices [1]. Studies have found that an energy gap can be generated in two-dimensional materials, such as a monolayer [2] or a bilayer graphene (BLG) [3]. BLG consisting of two stacked monolayers of graphene is a material in which physical properties can be controlled by tuning the bandgap [4]. It is thus possible to improve the electrical, the thermal and the optical conductivities and modulate the mechanical properties [5]. However, several of the characteristics of BLG are similar to those of a monolayer, but a BLG has interesting underlying physics that holds a potential for electronics applications such as sensors [6], exhibiting high sensitivity [7], stable specificity, and fast response [8].

The electronic properties of a BLG have been studied using density functional theory (DFT), in which the bandgap at the $K$ point in the Brillouin zone depends linearly on the average applied electric field [9, 10]. One of the main approaches to alter the electrostatic potential of a BLG is substitutional doping with foreign atoms [11] such as Boron (B), Nitrogen (N) [12], and Silicon (Si) atoms. For instance, a B- and N-doped BLG results in a p-type or an n-type semiconducting behavior with a shifting of the Fermi energy, respectively. A B and N codoped BLG exhibits a semiconducting material with a small bandgap, where the Fermi energy is located in the bandgap [13]. A substantial bandgap due to Boron and Nitrogen atoms codoped in BLG can be created in which the size of the band gap...
is effectively tuned in the presence of B-N pairs [1]. The created band gap of a boron nitride (BN) BLG by varying an external electric field can be used for investigating photocatalysis [14]. These electronic properties of B or N doped BLG give almost similar result for both the AA- and AB-stackings patterns with respect to the dopant atoms [15].

The doping of graphene with Si, N and B atoms leads to modified bonds in the BLG which in turn effects its mechanical properties. The influence of the Si, N and B doping on the mechanical properties of graphene has been examined and it was shown that it leads to an almost linear decrease of the Youngs modulus. Such doping effects are found to be most significant for silicon, less pronounced for boron, and small or negligible for nitrogen [16]. In addition, molecular dynamics simulations have been done for twisted bilayer of graphene displaying that they possess outstanding mechanical properties. In the linear elastic region, the mechanical strain rate and the presence of cracks have negligible effects, while in the nonlinear mechanical region fracture toughness is seen [17].

The optical characteristics of BLG are interesting for optoelectronics devices and graphene-based photodetectors [18]. Inter- and intraband transitions in graphene have been studied using infrared spectroscopy finding a strong intraband absorption in the terahertz frequency range [19, 20, 21]. The foreign atoms can be used to control the optical properties as a function of the doping as has been demonstrated in an electrostatically gated BLG [22]. The roles of the doping atoms on the $\pi - \pi$ interactions was studied and a systematic red shift and a broadening of the lowest excitations in the optical absorption was demonstrated [23]. Furthermore, the Si doping opens the band gap of graphene and enhances its optical conductivity [24, 25].

The pure monolayer and bilayer graphene structures are generally not good candidates for thermoelectric based devices because of the vanishing bandgap [26, 27]. In the pure material the Seebeck coefficient, $S$, and the thermoelectric figure of merit, $ZT$, are thus very limited. In order to enhance $S$ and $ZT$, one may thus introduce B and N doping atoms in the graphene structures. It has been shown that graphene/BN heterostructures provide the possibility to tune and decrease strongly the phonon thermal conductivity, which is a very favourable feature to enhance the thermoelectric properties such as $S$ and $ZT$ [28, 29, 30].

In this work, we consider Si, B, and N atoms doped AA- and AB-stacked BLG represented by BC$_{14}$N and Si$_2$C$_{14}$ structures. The electronic, mechanical, optical and thermal characteristics are investigated using density functional theory. A comparison between the AA- and the AB-stacked BLG will be shown with detailed mechanisms of improving these two BLG structures by Si and BN impurity atoms.

In Sec. 2 the structure of BLG is briefly over-viewed. In Sec. 3 the main achieved results are analyzed. In Sec. 4 the conclusion of the results is presented.

## 2. Computational details

The present results have been worked out by using the Quantum Espresso (QE) package [31], which encompasses tools for first-principles calculations and materials modeling for electronic structure simulations based on DFT. A full structure relaxation is obtained by including van der Waals interactions in the exchange (XC) functional of the DFT model, where the $k$-point grid is $12 \times 12 \times 1$ [32]. The Perdew-Burke-Ernzerhof functional (PBE) within the framework of the generalized gradient approximation is employed for the calculations of geometry optimizations and the electronic properties [33]. For the Brillouin zone sampling and the calculations of the density of state (DOS), a $12 \times 12 \times 1$ and a $77 \times 77 \times 1$ grids are used, respectively. The energy cutoff for the plane wave expansion is set to be 1088.45 eV for all the calculations. Pure BLG and doped BLG graphene structures are iteratively optimized and the calculations are considered converged when the force on each atom is less than $10^{-6}$ eV/Å.

The crystalline and molecular structure visualization program (X CrySDen) is employed to visualize all the structures [34]. In addition, the Boltzmann transport properties software package (BoltzTraP) is used to investigate the thermal properties of the systems [35]. The BoltzTraP code uses a mesh of band energies and has an interface to the QE package [36]. The optical characteristics of the systems are obtained by the QE code.
3. Results

We approach the AA- and AB-stacked BLG with a $2 \times 2$ supercell. Two types of doping are considered: Si doped BLG and BN-codoped BLG. These two types of atom doping are expected to form BLG-like semiconductor materials.

3.1. AA- and AB-stacked structures

We consider an AA- and an AB-stacked BLG in our study as are shown in Fig. 1. The AA-stacked BLG is composed of two layers that are exactly aligned, while in the AB-stacked BLG (Bernal stacking), the carbon atoms belonging to different sublattices, A and B, form the AB stacking pattern between the layers (atoms belonging to the A sublattice in one layer are stacked directly above the atoms of the B sublattice from the other layer).

Based on interaction effects between atoms or the interlayer interaction, we consider two types of doping arrangements in the BLG with Si dopant or BN-codopant atoms. The Si-doped BLG identified as Si$_2$C$_{14}$ for both the AA- and the AB-stackings shown in Fig. 1 (Middle panel). In addition, a BN-codoped BLG that is labeled as BSi$_{14}$N for the AA- and the AB-stackings. In a $2 \times 2 \times 1$ super-cell of Si$_2$C$_{14}$, one Si (golden) atom in each layer is doped while in BSi$_{14}$N we assume one B (blue) atom in the top layer and one N (red) atom in the bottom layer. The Si atom in top(bottom) layer is doped in the para(meta) position, while the B(N) atom is located at the ortho(para) position [37, 38, 30].

The interlayer distance of both the AA- and the AB-stacked BLG are found to be 3.6 and 3.4 Å, respectively, which are a good agreement with experimental [39] and theoretical [1] results. The lattice constant, a, the interlayer distance, $l$, the distance between the B-N ($d_{BN}$), the distance between the Si-Si atoms ($d_{Si-Si}$), the C-C, C-B, C-N and the C-Si bond lengths are all presented in Tab. 1. It is known that the repulsive force between the two layers in the case of the AA-stacking is much stronger than that in the AB-stacking. This is attributed to the fact that half of the atoms of the first layer are located in the center of hexagon of the second layer, and the other half of the atoms of the first layer lies directly above atoms of the second layer in the AB-stacking. Therefore, a higher binding energy is required for the AA-stacking compared to the AB-stacking. Based on that, the AB-stacking is a more stable arrangement compared to the AA-stacking. The repulsive interaction between the layers of the AA-stacking leads to a larger interlayer distance.

Another observation of the data in Tab. 1 is that the average lattice constant of both Si$_2$C$_{14}$, and BC$_{14}$N is larger than that of BLG in both cases of an AA- and an AB-stacking indicating a super-cell expansion due to the dopant atoms. This is attributed to the larger atomic radii of the B and Si atoms compared to the C atom. In addition, the super-cell expansion for the doped AB-stacked structure is slightly larger than that of the AA-stacked. This may be referred to the interlayer interaction which is stronger for the AB-stacked doped systems as the interlayer distance of AB-stacked is smaller.

Furthermore, the inter-layer distance in Si$_2$C$_{14}$ is large, but in BC$_{14}$N it is small compared to BLG for both the AA- and AB-stackings. This reveals a repulsive interaction between layers in Si$_2$C$_{14}$ [40], but an attractive interaction between the layers in BC$_{14}$N. These repulsive and attractive interactions arise due to presence of the dopant atoms.

Several methods have been used to analyse the components or the sources of the interlayer interactions in BLG. First, the interaction that emerges due to the sp$^3$ bonding between the two layers of BLG. This type of interaction is studied by incrementally moving two atoms with the same planar coordinates (one in the upper layer and the other one in the lower layer) to the sp$^3$ bond distance which is about 1.54 Å [41]. Second, non-bonding potentials are used to describe the van der Waals interactions between the layers of BLG [42, 43, 44]. The Van der Waals interaction is a dipole-dipole interaction that is effective if the distance between dipoles is around 4-5 Å. Third, the non-bonding interaction energy between the layers of a BLG [45]. In this case the interaction energy determines the type of the interlayer interaction that could be either a repulsive or an attractive interaction.

In our work, the non-bonding interlayer interaction energy between the layers of the BLG is considered, where the dopant atoms play an essential role [46]. The interaction energy between the dopant atoms in graphene can be determined or obtained from the total energy of the system using DFT calculation. The interaction energy be-
between two dopant atoms in a structure can be defined as

$$\Delta E = E_2 - E_0 + 2 \times E_1,$$

where $E_0$, $E_1$ and $E_2$ are the total energies of the systems with zero, one and two substitutional dopant atoms, respectively. The interaction energy between the Si atoms in the different layers of the AA- and that AB-stacked Si$_2$C$_{14}$ is found to be 2.11 eV and 1.34 eV, respectively, revealing a stronger repulsion interaction between the two substitutional Si atoms in the AA-stacking. The interaction is repulsive as the interaction energy has a positive value in both cases.

Even though the Si atoms in the AA-stacking do not lie directly above each other, the repulsive interaction is still stronger between the layers just like in the pure AA-stacked BLG. We can say that the AB-stacked Si$_2$C$_{14}$ is more stable than AA-stacked because the repulsive interaction in the AB-stacked is smaller leading to a smaller binding energy. This interactions between the Si atoms in a monolayer [47] and a bilayer [40] graphene have been studied an a repulsive interaction between the Si atoms has been confirmed.

In addition, an attractive interaction between the B and the N atoms is observed in both the AA- and the AB-stacked BC$_{14}$N as the interaction energy has a negative value, $-3.2$, and $-2.5$ eV, respectively. The attractive
interaction between the B and the N atoms leads to a decrease the the interlayer distance which is 3.05 Å for AA-stacking and 2.9 Å for AB-stacking. Furthermore, the the B atom in the top layer and the N atom in the bottom layer are slightly moved toward each other indicating an attractive interaction between these two atoms. We conclude that the AB-stacking is more stable because of higher attractive interactions. The attractive interaction between the B and the N atoms in graphene has been studied in two dimensional systems such as in monolayer graphene and in silicene nanosheet [48, 49].

3.2. Electronic Band structure

The electronic band structure is plotted in Fig. 2 for an AA-stacked BLG (a), Si$_2$C$_{14}$ (c), and BSi$_{14}$N (e), and AB-stacked BLG (b), Si$_2$C$_{14}$ (d), and BSi$_{14}$N (f). In the AA-stacked BLG, the electron distribution pattern has a hexagonal symmetry which is almost the same as for a monolayer graphene. It thus generates a linear dispersion of a valence band ($\pi$) and conduction band ($\pi^*$) intersecting the at K-point. In the AB-stacked BLG, parabolic bands are found near the Fermi level due to the asymmetric interactions between the upper and the lower layers. The lowest valence band and the conduction band only have a weak overlap near the K-point. It means the density of free carriers is very low. In both the AA- and the AB-stackings, the $\Gamma$-point determining the π-band width corresponds to the maximum and minimum π-band energy levels. The energy states are affected by interlayer atomic interactions at the M-point [50].

![Electronic band structure of AA-stacked BLG (a), Si$_2$C$_{14}$ (b) and BC$_{14}$N (c). Fermi energy is set at 0 eV.](image)

Furthermore, the energy spacing between $\pi_2^*$ and the $\pi_1^*$ near the K-point is 0.11, and 0.07 eV for the AA- and the AB-stackings, respectively, which are equal to the corresponding energy spacing of the $\pi_2-\pi_1$, where $\pi_2$ and $\pi_1$ refer to the double states of the π-bands. The linear dispersion of the AA-stacked BLG has been experimentally confirmed [51].

The dopant atoms in BLG induce a symmetry breaking and the interlayer interactions result in a bandgap. Band gaps also appear due to the interactions of dopants arising from their lateral periodicity. We therefore see a bandgap at the the K-point for the AA- and AB-stacked Si$_2$C$_{14}$ and AA-stacked BSi$_{14}$N [52]. The repulsive interaction in the AA- and the AB-stacked Si$_2$C$_{14}$ induces a direct bandgap which is 0.66, and 0.72 eV, respectively. Thus, both systems exhibit a semiconductor behavior. The attractive interaction in the AA-stacked BSi$_{14}$N generates a very small indirect bandgap, 0.025 eV indicating semiconductor property. The B/N atoms change the position of the Dirac cone along the $M-K$ direction. The Fermi energy crosses the valence band maxima and the conduction band minima in the AB-stacked BSi$_{14}$N revealing a degenerate semiconductor behavior. Furthermore, The energy spacing between the $\pi_2$ and the $\pi_1$ bands is increased in Si$_2$C$_{14}$, while the double states of the π-bands in BSi$_{14}$N totally disappears. This is in a good agreement with recent results for BN-codoped BLG in which the BLG is doped with one N atom in one layer and one B atom in the other [1].

3.3. Stress-Strain curves

The mechanical properties of a structure can be determined by the stress-strain curve. A uniaxial tensile strain is applied to the atoms of both layers in the zigzag and the armchair directions. In the DFT calculation, the system is extended by small displacement increments, 0.02, to the atoms at both ends. After each elongation, the system is relaxed to reach a new equilibrium state with both ends fixed. The elongation and relaxation procedures are repeated until the desired tensile strain is reached. The same mechanism has been applied for BLG using MD simulation [53].

The stress-strain curves are shown in Fig. 3 for both the AA- and the AB-stacked BLG (green), Si$_2$C$_{14}$ (blue), and BSi$_{14}$N (red) in the zigzag (a and c) and the armchair (b and d) directions. In a pure AA-stacked BLG, the tensile strain linearly increases in a small regime of strain in which the system experiences enlargements linearly up to
≤ 5%. This linearity is measured by the Young moduli, which is calculated as the initial slope of the stress-strain curve. The linear part of the curves is also called the elastic region. Table 2 presents the Young modulus (YM), the tensile strain (TS), and the fracture strain (FS) of undoped and doped BLG. The first column in Tab. 2 shows the structures, the column 2 to 4 are the values in the zigzag direction, and the last three column are the values in the armchair direction. The stress-strain relationship of the AA- and the AB-BLG reveal a Young modulus of 974 and 864 GPa, respectively, which are very close to the Young moduli obtained in reports of experimental [54] and theoretical [55] work. At a large strain, the stress of the system responds non-linearly to the strain until the systems failure, determining the fracture strain. The ultimate tensile strength is defined as the maxima in the stress-strain curve. The corresponding strain is introduced as the fracture strain here as there is no stretching in the structure after the fracture strain [56]. The same behavior of the stress-strain curve is found for the armchair direction, where the Young modulus is the same for both the AA- and the AB-stackings.

In the AA- and the AB-stacked Si2C14 and BC14N the stress-strain curves are modified due to the presence of dopant atoms. The bond energies of C-Si, C-B and C-N are smaller than those of C-C [57, 58]. The bonds can be generically arranged from high to low energy as: C-C, C-N, C-N and Si-C. We therefore see a reduction in the stress-strain curves of Si2C14 and BC14N which are caused by the small bonding energies of the dopant atoms with the C atoms [57]. In addition, the super-cell expansion due to the dopant atoms mentioned before is another reason why the Si2C14 and BC14N bilayers need less tensile stress.

Even though the repulsive interlayer interaction is increased in both the AA- and AB-stacked Si2C14 the Young modulus still decreases. This indicates that the binding energy between C and Si atoms is dominant in controlling the elastic properties of the system. The same scenario can be applied for BC14N where an attractive interaction between the layers exists.

Another observation is that the doped systems experience enlargements in a linear fashion till ≤ 4% in the AA-stacking, which demonstrates less elastic properties compared to the AA-stacking in both the zigzag and the armchair directions (see Tab. 2).

### 3.4. Optical absorption spectra

In general, bilayer graphene has much richer spectral features in comparison with monolayers. We therefore present here the optical response of the AA- and the AB-stacked systems. We find that the optical response of the dielectric function of a BLG can be manipulated by the influence of repulsive or attractive interlayer interactions. The imaginary part of dielectric function $\varepsilon_2$ is shown in Fig. 4 for the AA- (a and b) and the AB-stackings (c and d) in the case of an in-plane, $E_{in}$, (left panel) and an out-of-plane, $E_{out}$, (right panel) electric field.

It well known that in the case of $E_{in}$ the AA-stacked BLG has two main peaks in dielectric function at 3.95 and
13.87 eV formed by the π to π* and the σ to σ* transitions, respectively. Furthermore, in E_{out} the two main peak are generated by transitions from the σ to π* at 11.22 eV and the π to σ* at 14.26 eV. The anisotropic behaviour is clearly observed for the two different polarizations [50]. The AB-stacked BLG has the peaks at almost the same energy values with less intensity since it’s interlayer distance is close to the AA-stacking.

In the AA- and the AB-stacked Si_2C_{14} two main features in ε_2 are observed in the case of E_{in}. First, double peaks for each π → π* and σ → σ* transitions appear. This is attributed to increased energy spacing between the π_{1,2}, the π_{1,2}^*, the σ_{1,2}, and the σ_{1,2}^* as is shown in Fig. 2(c and d). Second, a red shift towards lower energy for both peaks is seen. The red shift of the peaks occurs by decreased energy spacing between the π and the π*, and the σ and the σ* a long the Γ − M and the M − K directions. It is interesting to note that the peak intensity at lower energy is enhanced. The peak intensity for the AA-stacking is higher than that of the AB-stacking. The peaks of Si_2C_{14} in the case of out-of-plane electric field are not red shifted and the intensity of the peaks is almost the same for the AA-stacking, while it is slightly decreased for the AB-stacking.

The properties of the imaginary dielectric function for BC_{14}N is very different for both the in- and the out-of-plane electric fields. The intensity of the peaks is decreased due the overaping of the valence and the conduction bands. In the in-plane electric field, double peaks for both the AA- and the AB-stacking are not seen any more because of the absence the double states in the band structure. It also seems that the peak intensity is almost the same for the AA- and the AB-stacking. In the case of the out-of-plane electric field, the right peak is red shifted for the AA- and the AB-stacking while the left peak is diminished. In addition, a strong peak at a very low energy is observed. These are attributed to extreme decreasing of the energy spacing between the π and the π*, and the σ, and the σ* along the Γ − M and the M − K directions (see Fig. 2(e and f)).

3.5. Seebeck coefficient

We investigated the thermal properties of our model at the low temperature ranging from 20 to 160 K, where the phonons are not active [60, 61]. So, the electrons deliver the main contribution to the thermal behavior. It is know that a good thermoelectric material should have a high electrical conductivity, Seebeck coefficient, S, and low thermal conductivity. The thermoelectric performance of monolayer and bilayer graphene is poor because of closed bandgaps, leading to a small Seebeck coefficient [62, 63]. This can be clearly seen in Fig. 5, where the S versus temperature is plotted for both the AA- (a), the AB-stacking (b), for pure BLG (green), Si_2C_{14} (blue), and BC_{14}N (red). The Seebeck coefficient is very small for pure BLG.

The key point to enhance the S is the opening up of the bandgap. Since the bandgap in Si_2C_{14} is much larger than that of BC_{14}N, a much higher S of Si_2C_{14} is observed for both the AA- and the AB-stacking. Therefore, one can expect to have a higher thermoelectric performance for the Si_2C_{14} structure. The electronic and thermal properties of doped BLG may be of fundamental interest and can play an important role in the performance of nanoscale devices.
4. Conclusion

We investigate the interaction energy, the electronic band structure, the mechanical, the optical and the thermal characteristics of AA- and AB-stacked BLG, Si$_2$C$_{14}$, and BC$_{14}$N structures. We show that interlayer interaction effects have a crucial influence on the properties of both the Si$_2$C$_{14}$, and the BC$_{14}$N structures. The Si atoms in Si$_2$C$_{14}$ and the B and N atoms in BC$_{14}$N induce repulsive and attractive interactions between the layers, respectively. We find that the influence of the repulsive interactions on the stress-strain curves in Si$_2$C$_{14}$ is larger compared to the attractive interactions in BC$_{14}$N. Therefore, the stress-strain curves are more suppressed for Si$_2$C$_{14}$ in both the zigzag and the armchair directions. The imaginary dielectric function of Si$_2$C$_{14}$ induces a red shift at high energy while only a reduction in the imaginary dielectric function of Si$_2$C$_{14}$ is observed in both the zigzag and the armchair directions. We investigate the interaction energy, the electronic band structure, the mechanical, the optical and the thermal characteristics of AA- and AB-stacked BLG, Si$_2$C$_{14}$, and BC$_{14}$N structures. We show that interlayer interaction effects have a crucial influence on the properties of both the Si$_2$C$_{14}$, and the BC$_{14}$N structures. The Si atoms in Si$_2$C$_{14}$ and the B and N atoms in BC$_{14}$N induce repulsive and attractive interactions between the layers, respectively. We find that the influence of the repulsive interactions on the stress-strain curves in Si$_2$C$_{14}$ is larger compared to the attractive interactions in BC$_{14}$N. Therefore, the stress-strain curves are more suppressed for Si$_2$C$_{14}$ in both the zigzag and the armchair directions. The imaginary dielectric function of Si$_2$C$_{14}$ induces a red shift at high energy while only a reduction in the imaginary dielectric function of Si$_2$C$_{14}$ is observed in both the zigzag and the armchair directions.

5. Acknowledgment

This work was financially supported by the University of Sulaimani and the Research center of Komar University of Science and Technology. The computations were performed on resources provided by the Division of Computational Nanoscience at the University of Sulaimani.

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