



# Ab initio investigation on hybrid graphite-like structure made up of silicene and boron nitride



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## ABSTRACT

In this work, we report our results on the geometric and electronic properties of hybrid graphite-like structure made up of silicene and boron nitride (BN) layers. We predict from our calculations that this hybrid bulk system, with alternate layers of honeycomb silicene and BN, possesses physical properties similar to those of bulk graphite. We observe that there exists a weak van der Waals interaction between the layers of this hybrid system in contrast to the strong inter-layer covalent bonds present in multi-layers of silicene. Furthermore, our results for the electronic band structure and the density of states show that it is a semi-metal and the dispersion around the Fermi level ( $E_F$ ) is parabolic in nature and thus the charge carriers in this system behave as *nearly-free-particle-like*. These results indicate that the electronic properties of the hybrid bulk system resemble closely those of bulk graphite. Around  $E_F$  the electronic band structures have contributions only from silicene layers and the BN layer acts only as a buffer layer in this hybrid system since it does not contribute to the electronic properties near  $E_F$ . In case of bi-layers of silicene with a single BN layer kept in-between, we observe a linear dispersion around  $E_F$  similar to that of graphene. However, the characteristic linear dispersion becomes parabola-like when the system is subjected to a compression along the transverse direction. Our present calculations show that the hybrid system based on silicon and BN can be a possible candidate for two-dimensional layered system, akin to graphite and multi-layers of graphene.

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## 1. Introduction

There has been a lot of interest in layered systems, such as two-dimensional (2D) graphene-like honeycomb structure made up of materials other than carbon, because of the novel properties associated with these 2D systems and also due to their potential applications in nanotechnology. The important property associated with the layered systems is that they have a strong in-plane bonding and a weak van der Waals (vdW) bonding in a direction perpendicular to the plane which leads to an anisotropic bonding arrangement in the systems [1]. Among these graphene-like systems, *silicene*, the graphene analog of silicon, has been extensively studied by both theoreticians and experimentalists in recent past [2–29]. Silicene possesses many physical properties which are similar to those of graphene. For example, silicene is a semi-metal and the charge carriers in this 2D material behave like massless Dirac-Fermions due to the presence of linear dispersion around

the Fermi level ( $E_F$ ) at a symmetry point  $K$  in the reciprocal lattice [2,3]. Presence of linear dispersion in silicene has been recently confirmed by ARPES measurement [20]. Moreover, it has been observed that a band gap can be opened up and tuned in a monolayer of silicene by applying an external transverse electric field [6–9] which is, however, not possible in monolayer of graphene.

Although the properties of monolayer of silicene resemble those of monolayer of graphene, the properties of multi-layers of silicene are drastically different from those of multi-layers of graphene. It has been observed from our recent studies [4,5] that the multi-layers of silicene possess strong inter-layer covalent bonds in contrast to the weak van der Waals interaction between the layers of graphene multi-layers and bulk graphite. Presence of inter-layer strong covalent bond influences many properties of multi-layers of silicene. Due to this strong inter-layer covalent bonding, the multi-layers of silicene can no longer behave like a layered system. The reason for differences in properties between carbon and silicon based systems is due to the different energetically favorable hybridizations present in these two systems in spite of the fact that

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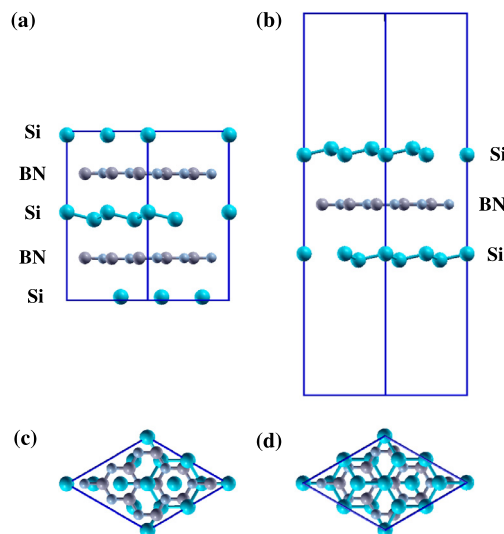
these two atoms contain same number of electrons in the valence shell. Most favorable hybridization in silicon system is  $sp^3$  whereas carbon system can exist in  $sp$ ,  $sp^2$ , as well as  $sp^3$  hybridizations. It is important to note that the difference in the values of energy levels between the two valence sub-shells namely 3s and 3p in Si atom is smaller than the corresponding value between 2s and 2p sub-shells in C atom. This leads to the preference of  $sp^3$  hybridization in Si because 3s can easily mix with all the sub-shells  $3p_x$ ,  $3p_y$  and  $3p_z$ .

Due to the above mentioned reason, it is not possible to have bi- and multi-layers of silicene analogous to the bi- and multi-layers of graphene. Furthermore, the graphite-like layered structure of silicon cannot be constructed by directly stacking one silicene layer over another since they readily form inter-layer covalent bonds [4,5]. However, it is desirable to obtain graphene-like silicon based layered systems possessing similar exciting and novel properties of multi-layer of graphene since the former has an important advantage over carbon based systems because of their compatibility with the existing semiconductor industry. Keeping these points in mind, in the present work, we propose that there is a possibility of creating a graphite-like layered structure of silicon by inserting a buffer layer in between the multi-layers of silicene. The buffer layer prevents the strong inter-layer covalent bonds between the layers of silicene. Moreover, the buffer layer is expected not to alter the electronic properties of the multi-layers of silicene around  $E_F$ . For this purpose, we consider a hybrid graphite-like layered system made up of alternate layers of honeycomb silicene and honeycomb boron nitride. It has been shown in existing theoretical studies that interaction between monolayer of silicene and boron nitrate substrate is due to weak van der Waals [30–33]. We study the geometric and electronic structures of the hybrid graphite-like layered system by employing *ab initio* density functional theory (DFT) [34] based calculations. In this case, BN layer acts as a buffer layer. We want to probe whether it would be possible to have an energetically stable hybrid system with physical properties similar to those of bi-layers of graphene as well as bulk graphite.

The present paper has been arranged in the following manner. We give the details of the computational methods employed in our calculations in the next section. The results of the properties of hybrid graphite-like structure have been discussed in Section 3, and then followed by the conclusion in Section 4. Effect of vdW interaction on the geometric and electronic properties of the hybrid system is studied in Appendix A.

## 2. Computational details

Density functional theory (DFT) [34] based calculations have been performed using Vienna ab-initio simulation package (VASP) [35] within the framework of the projector augmented wave (PAW) method. We employ generalized gradient approximation (GGA) given by Perdew–Burke–Ernzerhof (PBE) [36] for exchange–correlation (XC) functional. The plane waves are expanded with energy cut of 400 eV. We use Monkhorst–Pack scheme for k-point sampling of Brillouin zone integrations with  $10 \times 10 \times 5$  and  $11 \times 11 \times 1$  for bulk and bi-layer systems respectively. The convergence criteria for energy in SCF cycles is chosen to be  $10^{-6}$  eV. The geometric structures are optimized by minimizing the forces on individual atoms with the criterion that the total force on each atom is below  $10^{-2}$  eV/Å. For bi-layer, we use a super cell geometry with a vacuum of about 15 Å in the z-direction (direction perpendicular to the plane of silicene/BN) so that the interaction between two adjacent unit cells in the periodic arrangement is negligible. The geometric structures and charge density distributions are plotted using XCrySDen software [37].



**Fig. 1.** (Color online.) The optimized geometric structures of hybrid graphite-like structures made up of silicene and boron nitride layers. Bulk system ( $Si_{16}B_{18}N_{18}$ ): (a) side and (c) top views. Bilayer of silicene with a single boron nitride layer ( $Si_{16}B_9N_9$ ): (b) side and (d) top views.

## 3. Results and discussions

### 3.1. Geometric structures and charge density distributions

In this section, we start our discussion on the geometric properties of the hybrid graphite-like bulk system ( $Si_{16}B_{18}N_{18}$ ) with alternate layers of honeycomb silicene and BN. The space group of the hybrid bulk system is  $P3m1$ . The unit cell contains two silicene and two BN (buffer) layers. The super cell of  $(2 \times 2)$  of honeycomb silicene is lattice matched with  $3 \times 3$  of honeycomb BN with the deviation of only about 1.7%. Each layer of silicene (BN) contains 8 silicon (9 boron and 9 nitrogen) atoms. The calculated optimized geometric structures of the hybrid graphite-like structure are shown in Figs. 1(a) and (c). Our results on geometric structure obtained by DFT based calculation with PBE XC functional show that the hybrid system has a value of lattice constant about 7.554 Å along  $a$  axis (which is denoted by  $A$ ). The calculated values of Si–Si and B–N bond lengths in the basal plane are 2.246 and 1.454 Å respectively. We observe that the amount of buckling present in silicene layer in the hybrid system is slightly increased to 0.543 Å from its free standing value [4] of 0.457 Å. The reason for increase in the buckling length is due to the interaction of silicene layer with the other layers present in the bulk system. Moreover, the increase in the value of buckling leads to a higher contribution of  $sp^3$ -like hybridization in Si atoms in silicene of the hybrid system as compared to that of Si atoms in free standing silicene. Our calculations with PBE XC functional give 14.695 Å for the value of lattice constant along  $c$  axis (which is denoted by  $C$ ). Thus, the inter-layer distance, denoted by  $D$ , between the silicene and BN layers becomes 3.674 Å (in this case,  $D = C/4$ , see Fig. 1(a)). We also perform similar calculations for bi-layer of silicene with a single BN layer kept in between ( $Si_{16}B_9N_9$ ). The optimized geometry of bi-layer is given in Figs. 1(b) and (d). In this case, the lattice constant ' $A$ ' and inter-layer distance of the hybrid bi-layer are estimated to be 7.607 and 4.011 Å respectively. We observe from these results that for hybrid bi-layer both the values of lattice constant and inter-layer distance slightly increase from the corresponding values in hybrid bulk system. Furthermore, our calculations of cohesive energy of the hybrid systems show that they are energetically stable. We find that the cohesive energy per atom for the hybrid bulk and bi-layer systems are 6.07 and 5.57 eV/atom respectively. These results indicate that the

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