Silicene beyond mono-layers—different stacking configurations and their properties

C Kamal\(^1\), Aparna Chakrabarti\(^{1,3}\), Arup Banerjee\(^{2,3}\) and S K Deb\(^1\)

\(^1\) Indus Synchrotrons Utilization Division, Raja Ramanna Centre for Advanced Technology, Indore 452013, India
\(^2\) BARC Training School, Raja Ramanna Centre for Advanced Technology, Indore 452013, India
\(^3\) Homi Bhabha National Institute, Department of Atomic Energy, Indore 452013, India

E-mail: ckamal@rrcat.gov.in

Received 23 October 2012, in final form 20 December 2012
Published 31 January 2013
Online at stacks.iop.org/JPhysCM/25/085508

Abstract

We carry out a computational study on the geometric and electronic properties of multi-layers of silicene in different stacking configurations using state-of-the-art \textit{ab initio} density functional theory based calculations. In this work we investigate the evolution of these properties with increasing number of layers (\(n\)) ranging from 1 to 10. Although a mono-layer of silicene possesses properties similar to those of graphene, our results show that the geometric and electronic properties of multi-layers of silicene are strikingly different from those of multi-layers of graphene. We observe that strong inter-layer covalent bonding exists between the layers in multi-layers of silicene as opposed to weak van der Waals bonding which exists between the graphene layers. The inter-layer bonding strongly influences the geometric and electronic structures of these multi-layers. Like bi-layers of graphene, silicene with two different stacking configurations AA and AB exhibits linear and parabolic dispersions around the Fermi level, respectively. However, unlike graphene, for bi-layers of silicene, these dispersion curves are shifted in the band diagram; this is due to the strong inter-layer bonding present in the latter. For \(n > 3\), we study the geometric and electronic properties of multi-layers with four different stacking configurations, namely AAAA, AABB, ABAB and ABC. Our results on cohesive energy show that all the multi-layers considered are energetically stable. Furthermore, we find that the three stacking configurations (AAAA, AABB and ABC) containing tetrahedral coordination have much higher cohesive energy than the Bernal (ABAB) stacking configuration. This is in contrast to the case of multi-layers of graphene, where ABAB is reported to be the lowest energy configuration. We also observe that bands near the Fermi level in lower energy stacking configurations AAAA, AABB and ABC correspond to the surface atoms and these surface states are responsible for the semi-metallic character of these multi-layers.

(Some figures may appear in colour only in the online journal)

1. Introduction

Finding novel materials is one of the prime goals of material science research activity. With the advance of sophisticated experimental methods and characterization techniques, many novel materials have been synthesized and their properties have also been investigated. Graphene is one such material with many novel properties and it has been extensively studied both theoretically and experimentally. The charge carriers in this two-dimensional system behave like massless relativistic Dirac fermions giving rise to a linear dispersion around the Fermi energy at a highly symmetric \(k\)-point (\(K\)) in the reciprocal lattice. This system exhibits various other properties such as anomalous...
integer quantum Hall effect, Klein tunneling, and non-zero minimum DC conductivity [1–4]. Recently, silicon based nanostructures such as silicene (the silicon counterpart of graphene) and silicene nanoribbons have attracted the interest of many researchers [5–28] due to the properties which are similar to those of graphene. Moreover, silicon based nanostructures have some distinct advantages over carbon based nanostructures. The former systems are expected to be compatible with the existing semiconductor industry. Furthermore, it has been theoretically predicted that a band gap can be opened up and tuned in a mono-layer of silicene by applying an external transverse electric field [7–10]. On the other hand, inducing a band gap by applying an electric field is not possible in a mono-layer of graphene. It is interesting to note that, recently, silicene has been grown epitaxially on a close-packed silver surface [20–26] and hence it opens up a possibility of validating the existing theoretical prediction.

It is observed that the electronic structure of silicene possesses linear dispersion around the Dirac point which is similar to that of graphene and hence it is a potential candidate for applications in nanotechnology [5–19]. It is important to note that the geometric structure of a mono-layer of silicene is slightly different from the planar structure of a mono-layer of graphene. The structure of the mono-layer of silicene is buckled and the presence of this buckling results in an increase in the cohesive energy of the system. The buckling is due to the mixing of sp$^2$ and sp$^3$ hybridizations rather than purely sp$^2$ hybridization. This is due to fact that silicon favors sp$^3$ hybridization.

In the literature, there have been many theoretical and experimental studies on bi- and multi-layers of graphene in the recent past [29–39]. The studies on the bi-layer of graphene indicate that it possesses parabolic dispersion around the highly symmetric k-point (K) in the reciprocal lattice as opposed to the linear dispersion in the case of the mono-layer. Though the mono-layer of graphene possesses many interesting properties, the bi-layer structure is much more important from the application point of view. For example, there is no band gap in the pristine mono- and bi-layer of graphene. However, it has been shown both theoretically and experimentally that a band gap can be opened up in the bi-layer of graphene by applying a gate voltage. Further, the value of the band gap can be tuned over a wide range, which may have potential applications in nanoelectronics and nanodevices [29, 30]. It is to be noted that there are numerous studies on bi- and multi-layers of graphene; however, detailed theoretical studies on similar systems of silicene are lacking in the literature. Hence, it may be interesting to study the properties of bi- and multi-layers of silicene, given the importance of silicon based nanostructures. In this work, we carry out a detailed investigation of geometric and electronic properties of bi- and multi-layers of silicene with different stacking configurations using state-of-art ab initio density functional theory based calculations. We also study the evolution of geometric as well as electronic structures of multi-layers of silicene with increasing number of layers (n = 1 to 10). In section 2, we briefly outline the computational methods employed in the present work. The results and discussions are presented in section 3, followed by the conclusion in section 4.

2. Computational details

We perform density functional theory (DFT) [40] based calculations using the Vienna ab initio simulation package VASP [41] within the framework of the projector augmented wave (PAW) method. We use the generalized gradient approximation (GGA) given by Perdew, Burke, and Ernzerhof (PBE) [42] for the exchange–correlation potential. The cutoff for the plane wave expansion is taken to be 400 eV and the mesh of k-points for Brillouin zone integrations is chosen to be $21 \times 21 \times 1$. The convergence for the plane wave cutoff and the number of k-points in the mesh have been checked by varying these parameters. The convergence criteria for energy in SCF cycles is chosen to be $10^{-6}$ eV. All the 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$^{-1}$. We use a super-cell geometry with a vacuum of about 15 Å in the z-direction (direction perpendicular to the plane of silicene) so that the interaction between two adjacent unit cells in the periodic arrangement is negligible. All the geometric structures and charge density distributions are plotted using XCrySDen software [43].

3. Results and discussion

3.1. Geometric structure and cohesive energy

The unit cell of the mono-layer of silicene has two Si atoms (Si1 and Si2) which form a hexagonal lattice with space group of P3m1. In this work, we consider three possible arrangements for these two Si atoms, which are placed at symmetric positions. The geometric structures of these three types are shown in figure 1. These arrangements are (i) A, Si1 (0, 0, 0), Si2 (2/3, 1/3, z), (ii) B, Si1 (0, 0, 0), Si2 (1/3, 2/3, z), and (iii) C, Si1 (2/3, 1/3, 0), Si2 (1/3, 2/3, z). The variable z in the fractional coordinates along the z-axis indicates that the two silicon atoms in the unit cell are not in the same plane and this is due to the effect of buckling. The relative position of Si2 can be below (A, B and C) or above (A, B and C) the Si1 atom. The multi-layers of silicene with different stacking configurations are constructed with these three types. In the present work, we consider the following four different stacking configurations: (1) AAAA—simple hexagonal, (2) AABB—double hexagonal, (3) ABC—rhombohedral, and (4) ABAB—Bernal stacking. The first three stacking configurations lead to a tetrahedral arrangement of Si atoms, which is a favorable configuration for silicon based systems. We would like to mention here that the ABC stacking configuration leads to a multi-layered structure with stacking of the diamond structure of bulk silicon along the (111) direction. In case of multi-layers of

---

4 The VASP 5.2 program package used here is fully integrated in the MedeA platform (Materials Design) with a graphical user interface enabling the computation of the properties.
Figure 1. Three types of mono-layer of silicene in which two Si atoms are at highly symmetric positions: top view (top panel) and side view (middle and bottom panels).

Figure 2. The optimized geometric structures of multi-layers \((n = 10)\) with four stacking configurations: (a) ABC, (b) AABB, (c) AAAA and (d) ABAB.

Figure 3. Variation of the cohesive energy per atom with the increasing number of layers for the four stackings ABAB (with triangle symbol), AAAA (with diamond symbol), AABB (with square symbol) and ABC (with circle symbol). The dashed line indicates the value of cohesive energy per atom of bulk silicon (diamond structure).

dashed line indicates the value of cohesive energy per atom \((4.553 \text{ eV/atom})\) of bulk silicon (diamond structure). We observe that all the multi-layered structures considered in this work are energetically stable. Our calculations suggest that the rhombohedral stacking (ABC) is the minimum energy configuration. However, the values of cohesive energy of ABC stacking are much closer to those of AAAA and AABB stackings. The cohesive energies per atom of ten layers in AABB and AAAA stackings are 7 and 15 meV/atom lower than that of ABC stacking, respectively. The cohesive energies per atom of three stacking configurations, AAAA, AABB and ABC increase smoothly with the number of layers. Interestingly, the cohesive energy of the Bernal stacking (ABAB) is much lower than those of all the other stackings. In the case of 10 layers, the cohesive energy per atom of the ABAB stacking configuration is 236 meV/atom lower than that of ABC stacking. This result is in contrast to that of multi-layers of graphene, where ABAB stacking is the lowest energy configuration. We also observe an oscillation in the values of cohesive energy of Bernal stacking. In order to understand these results for cohesive energies of multi-layers of silicene, we carry out a detailed investigation on the geometric structures of all the multi-layers of silicene.

3.1.1. Mono-layer. In mono-layer of silicene, the two Si atoms have three nearest neighbors with bond length of 2.279 Å and hence these atoms make three strong \(\sigma\) bonds and one weak \(\pi\) bond with their nearest neighbors. Furthermore, the \(\pi\) bonds in silicene are weak due to the large internuclear distance between Si atoms (\(d_{\text{Si-Si}}\) is much larger than \(d_{\text{C-C}} = 1.42\) Å in graphene). In table 1, we compile the results for the lattice constant, bond length and bond angle corresponding to the optimized structures of mono- and bi-layers of silicene. For comparison, we have also included the bond length and bond angle between Si atoms in bulk silicon (diamond structure) in table 1. We note that these results agree well with...
Table 1. The results of optimized geometries of mono- and bi-layers of silicene obtained by DFT with the PBE exchange–correlation functional.

| System            | Lattice constant (Å) | Bond lengths (Å) | Bond angles (deg.) | Buckling length (Å) |
|------------------|----------------------|------------------|-------------------|---------------------|
| Mono-layer       | 3.867                | 2.279            | 116.08            | 0.457               |
| Bi-layer AB      | 3.851                | 2.321, 2.528     | 112.10, 106.69    | 0.667               |
| Bi-layer AA      | 3.858                | 2.324, 2.464     | 112.21, 106.57    | 0.663               |
| Bulk silicon     | 5.468                | 2.368            | 109.47            | —                   |

those available in the literature [5, 6]. It is important to note that the hybridizations in graphene (sp$^2$) and silicene (mixture of sp$^2$ and sp$^3$) are different due to the presence of buckling.

3.1.2. Bi-layers. In the case of bi-layers of silicene, our results on geometric structures show that there exists a strong coupling between the layers of silicene as opposed to a weak van der Waals interaction, which exists in the multi-layers of graphene and graphite. For bi-layers, there are only two possible stackings, namely AA and AB. We perform geometry optimization of the bi-layers of silicene with starting inter-layer separation equivalent to that of bi-layers of graphene. The optimized structures of these bi-layers are displayed in figure 4. These results show that the two layers are covalently bonded with each other. Consequently, the $E_c$ per atom for bi-layers of silicene increases significantly from that of mono-layers. It is also observed that AB stacking is lower in energy as compared to the AA stacking and the difference in cohesive energy between these two structures is 34 meV/atom. In order to further examine the nature of bonding between the two layers of silicene, we study the valence charge density distributions of bi-layers. In figure 5, we show the valence charge density distributions of AA and AB stacked bi-layers of graphene ((a) and (b)) and silicene ((c) and (d)). The analysis of valence charge density distribution in both AA and AB stackings of silicene corroborates the results of optimized geometries discussed above. The significant charge density distribution around the inter-layer bonds establishes the covalent nature of these bonds. This is different from a weak van der Waals coupling which exists between two graphene layers (see figures 5(a) and (b)). We also observe that the buckling and the bond lengths in both AA and AB stacked bi-layers have increased compared to corresponding results for the mono-layer of silicene. Furthermore, the results presented in table 1 clearly show that there is a reduction in the values of bond angles between atoms in the same layer (intra-layer) and there is an increase in the values of bond angles between atoms in two layers (inter-layer). These results suggest that the contribution of sp$^3$ hybridization has increased as compared to that for the mono-layer of silicene.

3.1.3. Multi-layers. Now, we discuss the results for optimized geometry and cohesive energy of multi-layers of silicene with four different stacking configurations. In figure 2, we show the optimized structures of multi-layers ($n = 10$). This figure clearly elucidates the existence of an inter-layer covalent bonding in the multi-layers of silicene similar to the case of bi-layers. As discussed above, the cohesive energies of multi-layers with the three stacking configurations AAAA, AABB and ABC are significantly higher than that of the structure with ABAB stacking. This can be attributed to the fact that all the inner layers are
covalently bonded with the adjacent layers in these three stackings. Due to this inter-layer bonding, all the silicon atoms in these three stackings, except those on surfaces, have four nearest neighbors (three intra-layer and one inter-layer) in nearly tetrahedral configurations. Hence, all the valence electrons in the silicon atoms (except ones on the surface) make four sigma bonds with their nearest neighbors, which leads to sp³-like hybridization in these stackings. On the other hand, in ABAB stacking, the Si1 atom in layer A makes a fourth inter-layer sigma bond with the Si1 atom in layer B along the z-direction (see figure 2; both the atoms are at the same (x, y)) and hence these atoms assume nearly tetrahedral configuration. However, Si2 atoms in layers A and B do not have strong sigma bonds with each other (they are at different (x, y)) and the Si2–Si2 distance is more than 3 Å. Each set of AB layers is well connected by Si1–Si1 bonds but there are two Si2 atoms which lack the fourth nearest neighbors to form the sigma bond. Therefore, the number of sigma bonds in this stacking is less and hence they have the lowest cohesive energy as compared to those of AAAA, AABB and ABC stacking configurations. The reason for the closeness of the cohesive energies of AAAA, AABB and ABC stacking configurations is the similar bonding environment of each Si atom in these three stackings.

Having discussed the geometric properties of multi-layers of silicene, we now present the results for the valence charge density distribution of these multi-layers. In figure 6, we plot the valence charge density distributions for six layers with ABC and ABAB stacking configurations. This figure clearly brings out the differences in bonding properties in these two configurations, which are consistent with our results obtained from the optimized geometries of these multi-layers. Furthermore, we note here that the cohesive energy of the ABAB stacking configuration shows oscillations with increasing number of layers. This can be explained by examining the charge density distribution of this stacking configuration as shown in figure 6(b). It is observed that each bi-layer (AB) in ABAB stacking is strongly connected by inter-layer Si1–Si1 covalent bonds. However, the bonding between two adjacent AB bi-layers is weak and they are connected by the inter-layer Si2 atoms. The valence charge density presented in figure 6(b) confirms the presence of strong Si1–Si1 and weak Si2–Si2 bonds. Hence, the structures with even numbers of layers have large cohesive energy as compared to the structures with odd numbers of layers. This leads to an oscillation in cohesive energy per atom in ABAB stacking.

We also study the evolution of the structural properties of multi-layers with increasing number of layers. To this end, we plot in figure 7 the variations of (a) lattice constant, (b) thickness and (c) difference of thickness of multi-layers with AAAA, AABB and ABAB stackings with respect to that of ABC stacking with increasing number of layers.
the lattice constant of ABC stacking is always higher than those of AAAA and AABB. Consequently, the geometric structure of the multi-layer with ABC stacking is slightly more relaxed in the lateral direction than for AAAA and AABB stacking configurations. For a given number of layers the ABC stacked structures are thick as compared to AAAA and AABB structures. The slightly higher relaxation in the lateral and the compression in the transverse direction of the ABC stacked structures may have led to the small increase in the cohesive energy of this stacking as compared to those of AAAA and AABB stackings.

3.2. Electronic structures

Having discussed the results for optimized geometric structures of multi-layers of silicene in the previous section, we now focus our attention on the electronic properties of these systems. For this purpose we calculate and study the band structure of multi-layers of silicene with number of layers ranging from 1 to 10.

3.2.1. Band structure of mono-layer. First, we start our discussion on the results of the band structure which are already established in the literature [5, 6]. The plot of the band structure of a mono-layer of silicene along the highly symmetric \( k \)-points in the Brillouin zone is given in figure 8(a). This result clearly shows linear dispersion around the high symmetry \( k \)-point (K) near the Fermi level \( E_F \) (see enlarged dispersion in figure 8(d)). We infer that the mono-layer of silicene is a semi-metal with the valence and conduction bands touching each other at the highly symmetric \( k \)-point (K). From the analysis of angular momentum (f) projected bands (not shown here), we confirmed that the valence and conduction bands near \( E_F \) are mainly due to \( \pi \) and \( \pi^* \) orbitals respectively. It is also observed that there is a small mixing of \( \pi \) and \( \sigma \) states (or mixture of sp\(^2\) and sp\(^3\) hybridizations) which leads to a buckling of the mono-layer of silicene. Our results on the mono-layer match well with those available in the literature [5, 6].

3.2.2. Band structure of bi-layers. As mentioned earlier, there are two possible stacking structures, namely AB and AA, for bi-layers of silicene. The band structures for AB and AA stackings are shown in figures 8(b) and (c) respectively. It is clearly seen from the figures that dispersions around \( E_F \) for these two cases are different and hence the electronic properties strongly depend upon the nature of the stacking. For AA configuration, it is observed that there exists linear dispersion along two directions, namely \( 0-K \) and \( 0-M \) (see figure 8(e)). Each of these dispersion curves crosses at two points, denoted by P and Q in the band diagram (\( E-k \)). On the other hand, for the AB stacked bi-layer we obtain a dispersion which is parabolic in nature (see figure 8(f)). These two dispersion curves also cross each other at two points, namely R and S, in the \( E-k \) diagram. It is interesting to note that none of these four points coincide with the Fermi level. In particular, the points P and R lie above \( E_F \) while the points Q and S lie below \( E_F \). The presence of linear and parabolic dispersions in AA and AB stacked bi-layers respectively is similar to that in bi-layers of graphene [35]. However, in the case of bi-layers of graphene, all these crossing points (P, Q, R and S) lie at \( E_F \). The differences in the band structures of bi-layers of silicene from those of graphene may be due to the presence of strong inter-layer covalent bonding in bi-layers.
Figure 9. Variation of band structures of AA and AB stacked bi-layers of silicene with different inter-layer separations. A closer look reveals that, for an inter-layer separation of about 3.73 Å, the band structures of silicene become similar to those of bi-layers of graphene. In order to verify this, we carry out calculations of band structure for both AA and AB stacked bi-layers of silicene with different inter-layer separations and these results are presented in figure 9.

It can be clearly observed from figure 9 that these four crossing points (P, Q, R and S) slowly move toward each other in the $E-k$ diagram (both $E$ and $k$ undergo change) and finally merge with each other at $E_F$ for a distance larger than 7 Å between the two layers. Furthermore, the band structures of both AA and AB stacked bi-layers are reduced to that of mono-layer, since there is no interaction between the layers at a distance larger than 7 Å. We also observe, during the evolution of the band structure of bi-layers of silicene with increasing inter-layer separation, that the band structures become similar to those of bi-layers of graphene for the intermediate inter-layer distances of about 3–4 Å. Therefore, we note that the origin of the differences in the band structures of bi-layers of silicene and graphene is indeed due to the presence of strong inter-layer coupling in the former. To estimate the strength of coupling, we calculate the splitting of energies of the topmost valence bands at the highly symmetric $k$-point $\Gamma$. Note that the first and second valence bands are degenerate and the case for the third and fourth bands at the $\Gamma$ point is similar. Therefore, we estimate the amount of splitting by calculating the difference in the energies between the first and third bands at the $\Gamma$ point. The values of splitting for AA and AB stacked bi-layers are found to be 0.748 and 0.502 eV respectively. These values indicate that the splitting is greater in AA stacking and hence experiences much stronger inter-layer interaction as compared to that in AB stacking. These results are consistent with our results on the geometric structure, that the inter-layer bond length in AA stacking (2.464 Å) is shorter than that in AB stacking (2.538 Å).

3.2.3. Band structure of multi-layers. The interesting trends found in the bi-layer prompt us to probe the band structures of multi-layers of silicene with more than two layers in four different stacking configurations, namely AAAA, AABB, ABC and ABAB. For each stacking configuration, we plot the
Figure 11. Evolution of band structures of AABB stacked multi-layers of silicene with increasing number of layers.

Figure 12. Evolution of band structures of ABC stacked multi-layers of silicene with increasing number of layers.

band structure with increasing number of layers \((n = 3–10)\) and these are displayed in figures 10–13. LH in figures 10–13 indicates that the multi-layers are terminated with hydrogen atoms. We wish to point out that we do not include the results for multi-layers containing seven to nine layers since the trends in the band structures with increasing number of layers are similar. We observe from figures 10–13 that for a given number of layers \((n)\) the band structures of multi-layers with AAAA, AABB and ABC stacking configurations are quite similar, and on the other hand they are different from those of a multi-layer of silicene with Bernal stacking (ABAB). The similarity of the band structures in AAAA, AABB and ABC is due to the similar local environments of the silicon atoms in tetrahedral configurations in these stackings. However, they are different from those of the multi-layer with ABAB stacking due to different arrangement of silicon atoms in this stacking. Furthermore, for a given number of layers, we observe that there exist more bands with characteristic dispersion of \(\sigma\) bonds between Si atoms in multi-layers of silicene with AAAA, AABB and ABC stackings as compared to those in ABAB structures. Moreover, it can be observed that there exist two bands in multi-layers with AAAA, AABB and ABC stackings which always cross the Fermi level. The width of these bands decreases with number of layers and hence they tend to be dispersionless as \(n\) goes beyond 6. These bands are due to the surface states since they correspond to Si atoms which are present on the surface layers. To verify the nature of these two bands, we hydrogenate the multi-layers of silicene and study the effect of hydrogenation on their band structure. The band structures of hydrogenated multi-layers of silicene with six layers are also plotted in figures 10–13 (see bottom-most right panel) for comparison with bare multi-layers. These plots clearly show the absence of bands corresponding to surface states and thus a transition from a semi-metallic to a semiconductor state takes place.

Before concluding this section, we wish to make a few comments on the band structures of multi-layers with Bernal stacking. The results presented in figure 13 clearly indicate that the band structures of ABAB stacked multi-layers are different from the corresponding results for other stackings. For Bernal stacking, we observe that there exist fewer bands corresponding to \(\sigma\) bonds while more bands correspond to the weakly bound \(\pi\) bonds as compared to those of the other three stackings. These \(\pi\) bands arise from Si atoms present on every layer of the multi-layers of silicene. Therefore, the saturations of Si on surface layers with hydrogen atoms do not cause the system to undergo a transition from semi-metallic to semiconductor state.
4. Conclusion

In this work, we perform studies on geometric and electronic properties of multi-layers of silicene with four different stacking configurations using density functional theory based calculations with the GGA-PBE exchange–correlation functional. The evolution of these properties of multi-layers of silicene with increasing number of layers has been studied.

We observe from the band structures of bi-layers of silicene that they exhibit linear and parabolic dispersions around the Fermi level, as in graphene, for AA and AB stackings respectively. However, the dispersion curves are displaced with respect to the Fermi level along both \( E \) and \( k \) directions in the band diagram of silicene. The calculations on multi-layers with more than three layers show that out of four different stacking configurations considered here, namely AAAA, AABB, ABAB and ABC, the multi-layer of silicene with ABC configuration possesses minimum energy. This is in contrast to the case of multi-layers of graphene, where ABAB stacking is the lowest energy configuration. Furthermore, our results show that all the stackings with tetrahedral coordination (AAAA, AABB and ABC) have much higher cohesive energy than Bernal (ABAB) stacking. We also observe that the surface atoms on the multi-layers of silicene contribute to the bands near the Fermi level in the lower energy stacking configurations AAAA, ABBB and ABC. These surface states are responsible for the semi-metallic character of the multi-layers of silicene studied here.

From our calculations, it is clear that the major differences in the properties of bi- and multi-layers of silicene from those of graphene arise due to the presence of strong inter-layer covalent bonding between the layers of the former as opposed to the weak van der Waals interaction which exists between the layers of graphene.

Acknowledgments

The authors thank Dr P D Gupta for encouragement and support. The support and help of Mr P Thander and the scientific computing group, Computer Centre, RRCAT, is acknowledged. AB wishes to thank Dr P K Gupta for his support and encouragement.

References

[1] Geim A K and Novoselov K S 2007 Nature Mater. 6 183
[2] Novoselov K S, Geim A K, Morozov S V, Jiang D, Katsnelson M I, Grigorieva I V, Dubonos S V and Firsov A A 2005 Nature 438 197
[3] Zhang Y B, Tan Y W, Stormer H L and Kim P 2005 Nature 438 201
[4] Novoselov K S, McCann E, Morozov S V, Falko V I, Katsnelson M I, Zeitler U, Jiang D, Schedin F and Geim A K 2006 Nature Phys. 2 177
[5] Cahangirov S, Topsakal M, Akturk E, Sahin H and Ciraci S 2009 Phys. Rev. Lett. 102 236804
[6] Sahin H, Cahangirov S, Topsakal M, Bekaroglu E, Akturk E, Senger R T and Ciraci S 2009 Phys. Rev. B 80 155453
[7] Ni Z, Liu Q, Tang K, Zheng J, Zhou J, Qin R, Gao Z, Yu D and Lu J 2012 Nano Lett. 12 113
[8] Drummond N D, Zolyomi V and Falcko V 2012 Phys. Rev. B 85 075423
[9] Ezawa M 2012 New J. Phys. 14 033003
[10] Kamal C 2012 arXiv:1202.2636
[11] Ezawa M 2012 Phys. Rev. Lett. 109 055502
[12] Ezawa M 2012 Phys. Rev. B 86 161407
[13] Liu C C, Feng W and Yao Y 2011 Phys. Rev. Lett. 107 076802
[14] Houssa M, Pourtois G, Afanasev V V and Stesmans A 2011 Appl. Phys. Lett. 97 112106
[15] Lebegue S and Eriksson O 2009 Phys. Rev. B 79 115409
[16] Dzade N Y et al 2010 J. Phys.: Condens. Matter 22 375502
[17] Jose D and Datta A 2011 Phys. Chem. Chem. Phys. 13 7304
[18] Spencer M J S, Morishita T, Mikami M, Snook I K, Sugiyama Y and Nakano H 2011 Phys. Chem. Chem. Phys. 13 15418
[19] Osborn T H, Farajian A A, Pupyrevska O V, Aga R S and Voon L C 2011 J. Phys. D: Appl. Phys. 44 112101
[20] Lalmi B, Oughaddou H, Enriquez H, Kara A, Vizzini S, Ealeet B and Aufray B 2010 Appl. Phys. Lett. 97 223109
[21] Aufray B, Kara A, Vizzini S, Oughaddou H, Leandri C, Ealeet B and Lay G L 2010 Appl. Phys. Lett. 96 183102
[22] Vogt P, Padova P D, Quadresima C, Avila J, Frantzeskakis E, Asensio M C, Resta A, Ealeet B and Lay G L 2012 Phys. Rev. Lett. 108 155501
[23] Enriquez H, Vizzini S, Kara A, Lalmi B and Oughaddou H 2012 J. Phys.: Condens. Matter 24 314211
[24] Lay G L, Padova P D, Resta A, Bruhn T and Vogt P 2012 J. Phys. D: Appl. Phys. 45 392001

Figure 13. Evolution of band structures of ABAB stacked multi-layers of silicene with increasing number of layers.
[25] Jamgotchian H, Colignon Y, Hamzaoui N, Ealet B, Hoarau J Y, Aufray B and Biberian J P 2012 J. Phys.: Condens. Matter 24 172001
[26] Padova P D, Kubo O, Olivieri B, Quaresima C, Nakayama T, Aono M and Lay G L Nano Lett. 12 5500
[27] Kara A, Vizzini S, Leandri C, Ealet B, Oughaddou H, Aufray B and Lay G L 2010 J. Phys.: Condens. Matter 22 045004
[28] Padova P D et al 2010 Appl. Phys. Lett. 96 261905
[29] Zhang Y, Tang T, Girit C, Hao Z, Martin M, Zettl A, Crommie M, Shen Y and Wang F 2009 Nature 459 820
[30] Oostinga J B, Heersche H B, Liu X, Morpurgo A F and Vandersypen L M K 2008 Nature Mater. 7 151
[31] Castro E V, Novoselov K S, Morozov S V, Peres N M R, Lopes dos Santos J M B, Nilsson J, Guinea F, Geim A K and Castro Neto A H 2007 Phys. Rev. Lett. 99 216802
[32] Trickey S B, Muller-Plathe F, Diercksen G H F and Boettger J C 1992 Phys. Rev. B 45 4460
[33] Ohta T, Bostwick A, Seyller T, Horn K and Rotenberg E 2006 Science 313 951
[34] McCann E 2006 Phys. Rev. B 74 161403
[35] Tabert C J and Nicol E J 2012 Phys. Rev. B 86 075439
[36] Manes J L, Guinea F and Vozmediano Mara A H 2007 Phys. Rev. B 75 155424
[37] Ohta T, Bostwick A, McChesney J L, Seyller T, Horn K and Rotenberg E 2007 Phys. Rev. Lett. 98 206802
[38] Latil S, Meunier V and Henrard L 2007 Phys. Rev. B 76 201402
[39] Mak K F, Sfeir M Y, Misewich J A and Heinz T F 2010 Proc. Natl Acad. Sci. USA 107 14999
[40] Hohenberg P and Kohn W 1964 Phys. Rev. 136 B864
Kohn W and Sham L J 1965 Phys. Rev. 140 A1133
[41] Kresse G and Furthmuller J 1996 Phys. Rev. B 54 11169
Kresse G and Joubert D 1999 Phys. Rev. B 59 1758
[42] Perdew J P, Burke K and Ernzerhof M 1996 Phys. Rev. Lett. 77 3865
[43] Kokalj A 2003 Comput. Mater. Sci. 28 155 Code available from www.xcrysden.org/