



**Dielectric Properties of Silicene Functionalized with Monomers, Dimers and Trimers of B, C & N atoms**

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# Electronic & Dielectric Properties of Silicene Functionalized with Monomers, Dimers and Trimers of B, C & N atoms

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First principle calculations have been performed to study geometric, electronic and dielectric properties of low-buckled silicene with the adsorption of monomers, dimers and trimers of B, C and N atoms. Binding energy calculations show that all the adsorbates, except homo N-N dimer, form stable configuration on silicene. The bandgap opening has been achieved for all the C adsorbate; homo dimers of B and N; hetero N-B dimer and B-C-N trimer on silicene. The plasmonic features and static dielectric constants are found to be tunable by various types of adsorbates on silicene which makes functionalized silicene a potential candidate for future nanoelectronics applications.

## 1 Introduction

Performance of electronic devices is inversely proportional to the dimension of devices. It is desirable in device manufacturing, to increase the performance of ICs with the decrease of dimensions of FETs. After the synthesis of mono-layer graphene<sup>1</sup>, an intense research activity has happened around graphene as well as other possible two dimensional layers to achieve this goal. Graphene exists with many novel properties and has been extensively studied both theoretically and experimentally<sup>1–9</sup>. However, because of incompatibility of graphene with existing electronics, researcher's efforts have been to investigate materials with novel properties like graphene. Silicene is one of those 2D stable layers, whose most of the properties resemble graphene<sup>7,11–14</sup>. Among the other monolayers, Silicene a two-dimensional buckled honeycomb silicon structure has attracted much attention since its successful preparation by depositing a mono-layer of silicon on silver substrate<sup>10</sup>. Moreover, it is also compatible with existing Si-based semiconductor devices.

It is found that the silicene sheet is low buckled, zero-gap semiconductor with Dirac cone at Fermi level, which makes it a competitive novel material. However, from a device point of view its gap-less behaviour is not beneficial for application in nanoelectronics<sup>15</sup> and therefore cannot be used in semiconductor devices. Many techniques have been proposed to tailor the band gap of two dimensional honeycomb structures<sup>9,16–23</sup>. Doping by adsorption and defects are two of the most com-

mon and convenient techniques to model electronic structures<sup>16,24–29</sup>. Effects of defects and impurities on electronic properties of graphene have been intensively investigated to tailor band-gap near Fermi level in the last few years<sup>30–32</sup>.

Although there exist theoretical studies on geometric and electronic properties of pristine silicene<sup>33–36</sup>, no detailed study of adsorption of foreign atoms on silicene layer and their influence on structural, electronic and dielectric properties are available in the literature. The adsorption of nonmagnetic 2p elements like B and N can achieve n- and p-type doping due to the injection of additional electrons and holes into the silicene and is expected to give more control over the electronic and optical properties of silicene. The researchers have studied single atom adsorption of B and N on silicene sheet by use of DFT and have found no band gap near Fermi level<sup>27</sup>. In the present work, we have studied a new aspect of doping by adsorption of homo & hetero dimers and trimers of B, C and N atoms.

## 2 Computational Details

Calculations were performed by the SIESTA (Spanish Initiative for Electronic Simulation with Thousand of Atoms) code and method<sup>37</sup> which uses an ab initio pseudopotential based on density functional theory (DFT). We have used Troullier-Martins norm conserving relativistic pseudo-potential<sup>38,39</sup> in fully separable Kleinman and Bylander form. The exchange and correlation energies have been treated within the Local Density Approximation (LDA) according to Ceperly and Alder (CA) parametrization. The charge densities and DFT potential were computed on the real space grid with equivalent plane-wave cutoff energy of 250 Ry. A  $4 \times 4$  supercell has been used for calculation with sufficiently large 20Å vac-

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uum region to separate the two dimensional structures to rule out any interaction among the neighboring layers along c-axis. Throughout geometry optimization, numerical atomic orbitals (NAO's) with double zeta polarization (DZP) basis set with confinement energy of 0.01 Ry were used. Relatively larger radii of the basis orbitals (using smaller value of energy shift parameter) were used for better accuracy. Minimization of energy was carried out using standard conjugate-gradients(CG) technique. Structures were relaxed until the forces on each atom were less than  $0.01\text{eV}/\text{\AA}$ . A  $10\times 10\times 1$  Monkhorst-Pack of k points were used for Brillouin zone integration. The  $90\times 90\times 3$  optical mesh points have been used for integration across Brillouin zone in the direction of reciprocal lattice vectors for optical properties calculations. Optical broadening of 0.2 eV was used for optical spectra. All the unoccupied states have been used for the calculations of optical spectra.

### 3 Results and Discussions

#### 3.1 Structural Properties

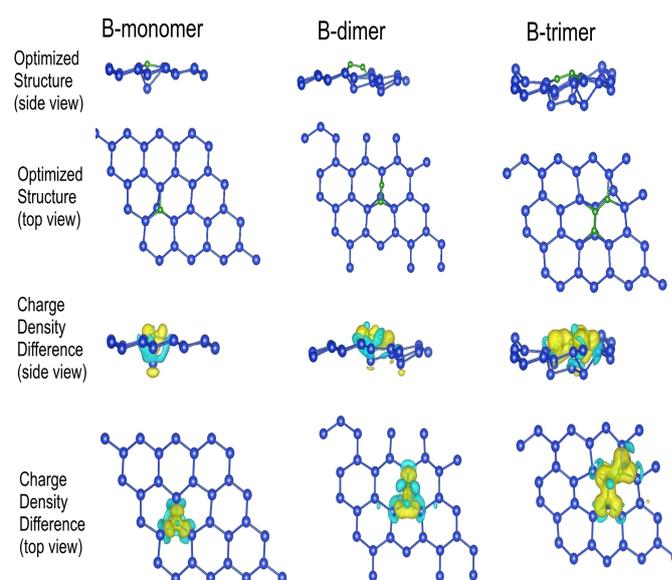
We have taken a supercell of 32 silicon atoms with doped monomer, homo and hetero dimers and trimers adsorption of B, C and N atoms. The optimized bond length of the Si-Si bond is  $2.28\text{\AA}$  in pristine silicene, which agrees with previous studies<sup>40</sup>. The studied structures were fully relaxed and optimized. First, we considered the adsorption of single atom on silicene. There are four possible adsorption sites i.e. hollow, bridge, valley top and hill top; on buckled silicene<sup>27</sup>. However, after total energy optimization, the adsorbate takes its place at minimum energy position. So, we have put adsorbate at any arbitrary position and fully optimized the adsorbate with silicene sheet. The trimers have two possible topologies, one is linear and other is closed triangle. We have considered only linear trimers, because they are energetically more stable than closed triangle trimers. The adsorption energy of monomers, dimers and trimers are defined as:

$$E_{ad} = E_{system} - E_{silicene} - E_{monomer/dimer/trimer} \quad (1)$$

where  $E_{system}$ ,  $E_{silicene}$  and  $E_{monomer/dimer/trimer}$  are the total energy of silicene with adsorbates, silicene alone and adsorbates (monomer/dimer/trimer) alone respectively. The structural properties such as supercell lattice constant, Si-adsorbate bond lengths, adsorbate-adsorbate bond length and adsorption energies are shown in Table 1. The optimized structures of our considered cases are shown in Figure 1. We also present the charge density difference for the studied structures in which yellow regions show charge accumulation, while the blue regions represent charge depletion. The charge density difference is calculated by subtracting the total charge density of silicene with adsorbate from the sum of the charge density of pristine silicene and isolated adsorbate.

#### 3.1.1 Boron monomer, dimer and trimer adsorption

Adsorption of Boron monomer i.e the single B atom, pushes the Si atom downwards and takes its place so that Si atom looks like an adsorbate i.e. the displaced Si-atom goes to valley top position. The measured average Si-B bond length of  $1.98\text{\AA}$  is in good agreement with other DFT result  $1.95\text{\AA}$ <sup>27</sup>. The top and side view of optimized structures and charge density differences are shown in Figure 1. The charge density difference shows that the charge gets depleted from near the Si-atom and accumulated between Si and B atoms resulting in stable structure with adsorption energy of  $-5.95\text{eV}$ . Further, adsorption of B-dimers and trimers is studied. B-dimer optimizes on silicene surface with Si-B average bond length of  $1.96\text{\AA}$  which shows stronger bonding and leads to higher adsorption energy of  $-7.80\text{eV}$  as compared to single B-adsorption. In case of B-trimer adsorption, the edge atoms of B-dimers makes bond with two Si-atoms and middle B atom makes bond with one Si atom. The adsorption energy ( $-8.22\text{eV}$ ) of B-trimer is higher than the mono and dimer adsorbate, however, the bond lengths of Si-B and B-B atoms increases slightly to  $2.02\text{\AA}$  and  $1.70\text{\AA}$  respectively (Table 1).

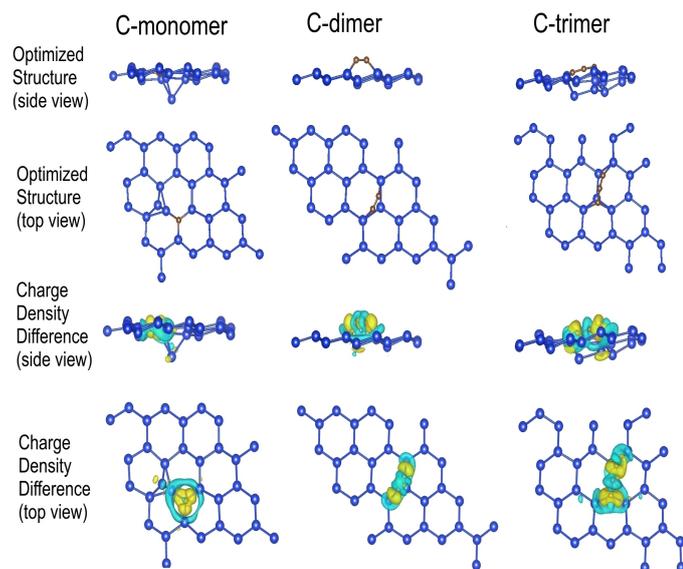


**Fig. 1** Top and side view of optimized structures with charge densities difference profiles for various types of B-adsorbate on silicene.

#### 3.1.2 Carbon monomer, dimer and trimer adsorption

Similar to B-monomer adsorption, C-atom also takes the position in the sheet making bonds of  $1.87\text{\AA}$  with three Si-atoms shown in Figure 2. However, here the difference is that the displaced Si-atom goes below the nearby hexagon and allows making bonds with the three neighboring Si atoms. The

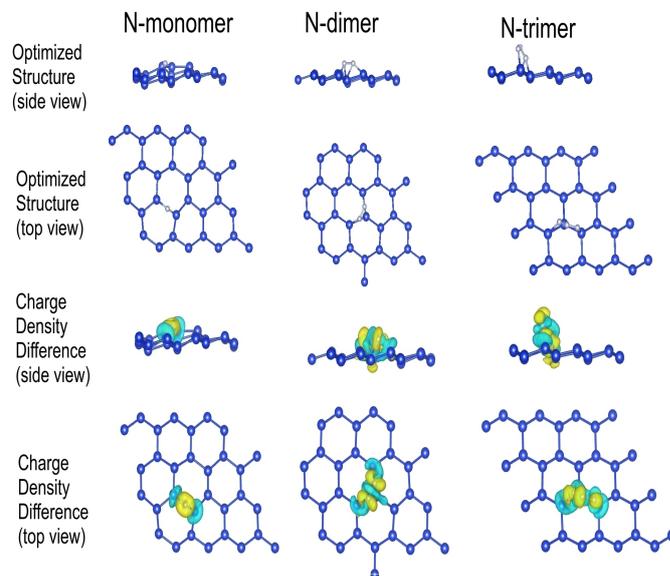
charge density difference in Figure 2 shows that the charge gets depleted from Si-atoms and gets accumulated between Si and C-atoms, revealing a stronger bonding and high stability with adsorption energy of  $-7.97$  eV, which is higher as compared to B-adsorption. The C-dimer adsorption also shows similar bond length between C and Si of silicene sheet. The charge density difference shows that the charge gets accumulated between C and Si atoms by depletion of charge both from C and Si atoms. However, for C-trimer adsorption, the Si-C bond length increase upto  $1.90$  Å while C-C bond length is  $1.36$  Å and the adsorption energy decreases to  $-5.57$  eV. This decrease in binding energy is due to the decrease in the bonding strength between the adsorbate and the layer.



**Fig. 2** Top and side view of optimized structures with charge density difference profiles for various types of C-adsorbate on silicene.

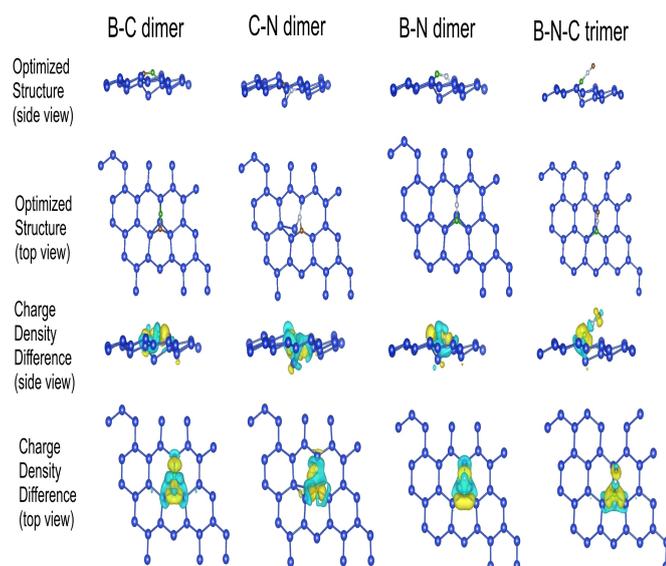
**3.1.3 Nitrogen monomer, dimer and trimer adsorption** In the case of N-monomer adsorption, N atom breaks the bond between two Si atoms and adjust itself between them making a bridge between two Si-atoms shown in Figure 3. The Si-N bond length  $1.64$  Å is in very good agreement with previously reported result  $1.63$  Å<sup>27</sup>. Charge density difference profile shows that the charge accumulated around N atom which is depleted from nearby two Si-atom that reveals a high adsorption energy of  $-8.16$  eV and stable structure. But for N-dimer adsorption, the system is energetically not favorable. The N-Si bond length is found higher,  $1.93$  Å, as compared to  $1.78$  Å of N atom adsorption. The charge density difference profile in Figure 3 also shows that the charge gets accumulated away from the Si-N bonds and the positive dimer adsorption energy,  $+1.43$  eV, can be attributed to a energetically unstable

structure. However, the N-trimer adsorption is slightly stable with adsorption energy of  $-3.01$  eV. The bond length of  $1.85$  Å has been calculated between N and Si atoms.



**Fig. 3** Top and side view of optimized structures with charge densities difference profiles for various types of N-adsorbate on silicene.

**3.1.4 Hetero dimer and trimer adsorption** Here we present results corresponding to the three possible hetero-dimers of B, C and N atoms which are B-C, C-N and B-N. Also we have one hetero-trimer B-N-C. All hetero-dimers on silicene are optimized resulting in structures shown in Figure 4. However, the adsorption energies are different. For B-C adsorption on silicene, C atom gets bonded with two Si atoms with bond length of  $1.91$  Å and B atom makes bond with only one Si atom of bond length  $1.93$  Å. The charge density difference in Figure 4 shows charge accumulation at C-Si and B-Si bonds. Adsorption energy of dimer  $-8.05$  eV makes it an energetically stable structure. But for C-N dimer adsorption, the charge accumulation has taken place on one side only because of depletion from other side of the dimer, which leads to a less stable structure with adsorption energy  $-3.82$  eV. In B-N dimer adsorption, B is bonded to two Si atoms and N is bonded to one Si atom. Charge depletes from B-N bond and accumulates at B-Si and N-Si bonds, which leads to a higher adsorption energy of  $-6.53$  eV. The hetero-trimer B-N-C adsorbs on silicene linearly with bonding of B with two Si atoms and the other edge of trimer ending with dangling C-atom. The charge density difference in Figure 4 also shows a high accumulation of charge at B-Si bond and one sided attachment with layer leads to slightly lower adsorption energy of  $-3.81$  eV.



**Fig. 4** Top and side view of optimized structures with charge densities difference profiles for different types of hetero-dimers and hetero trimer on silicene.

From Table 1, it can be easily concluded that the N-monomer adsorption is most stable among the single atom adsorptions, while N-dimer is most unstable. Adsorption of B-C and N-N dimers are respectively most stable and least stable in dimer adsorptions. Among hetero dimers/trimer (B-C, C-N, B-N and C-B-N), B-C adsorption is energetically most favorable. Furthermore, with increase in the coverage by clusters (from monomer to trimer) on the surface of silicene, the hexagonal honeycomb structure of silicene gets deformed as shown in Figures (1-4), that have significant influence on the electronic properties.

### 3.2 Electronic Properties

The electronic band structure is calculated along the high symmetry  $\Gamma$ -M-K- $\Gamma$  direction of the Brillouin zone. In silicene,  $\sigma$  and  $\pi$  bonds are formed by  $(3s, 3p_x, 3p_y)$  and  $3p_z$  orbitals respectively. The linear dispersion relation at high symmetric point K for monolayer silicene is mainly due to the  $3p_z$  orbitals making a node at the Fermi energy with zero density of states<sup>36</sup>.

#### 3.2.1 Boron monomer, dimer and trimer adsorption

The electronic band structure for B-monomer, dimer and trimer adsorbed on silicene is shown in Figure 5(a-c) respectively. B-monomer adsorption shows a p-type band structure shifted below the Fermi energy level which agrees with previous results<sup>27</sup>. This is due to the deficiency of one electron

**Table 1** Calculated parameters for monomers, dimers and trimers adsorbed on silicene: lattice constant ( $a$ ); Si-adsorbate bond distance ( $d_{Si-X}$ ); adsorbate-adsorbate bond distance ( $d_{X-X'}$  where X and X' may or may not be the same); and adsorption energy per monomer/dimer/trimer ( $E_{ad}$ )

System	$a$ Å	$d_{Si-X}$ Å	$d_{X-X'}$ Å	$E_{ad}$ eV
Silicene	15.40	-	-	-
B	15.28 (15.16) <sup>a</sup>	1.98 (1.95) <sup>a</sup>	-	-5.95 (-5.85) <sup>a</sup>
B-B	15.27	1.96	1.58	-7.80
B-B-B	14.85	2.02	1.70	-8.22
C	15.26	1.87	-	-7.97
C-C	15.42	1.87	1.30	-7.02
C-C-C	15.18	1.90	1.36	-5.57
N	15.48 (15.30) <sup>a</sup>	1.64 (1.63) <sup>a</sup>	-	-8.16 (-5.54) <sup>a</sup>
N-N	15.47	1.93, 1.78	1.38	+1.43
N-N-N	15.43	1.85	1.25, 1.37	-3.01
B-C	15.25	1.91, 1.93	1.44	-8.05
C-N	15.20	1.90, 1.68	1.39	-3.82
N-B	15.32	1.71, 2.08	1.37	-6.53
B-C-N	15.28	2.01	1.44, 1.20	-3.81

<sup>a</sup>Ref. <sup>27</sup>.

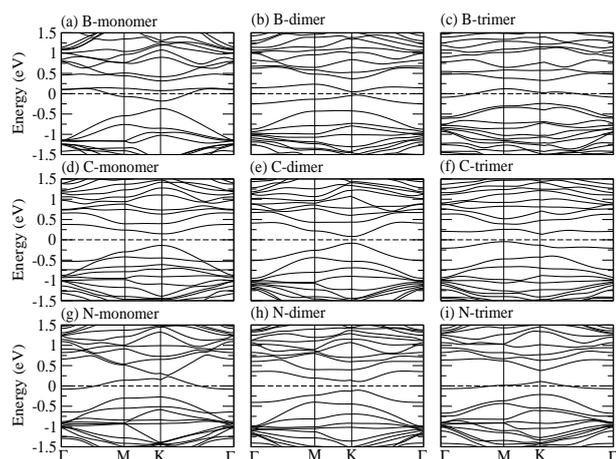
in B outer shell as compared to Si atom outer shell. But for B-dimer, a energy band gap 0.081 eV is observed at high symmetric point K around Fermi level. For B-trimer adsorption, a band line near Fermi level is found, which is mainly contributed by the bonding of B and Si atoms and leads to metallic behavior.

#### 3.2.2 Carbon monomer, dimer and trimer adsorption

The C-monomer, dimer and trimer show a different electronic behavior as compared to other group III and IV adsorbates on silicene. C and Si are both group IV elements, therefore, the outer shell has the same number of electrons. The electronic band structures are shown in Figure 5(d-f) for C-monomer, dimer and trimer adsorption respectively. For all C-monomer, dimer and trimer adsorbed structures of silicene electronic band gap near Fermi level is found. Adsorption of C-monomer results into a band gap opening of 0.288eV, whereas carbon homo-dimer adsorption shows band gap opening of 0.168 eV. Interestingly the band gap for C-trimer (linear) adsorbed on silicene is an indirect band gap of 0.182 eV in the direction of M-K high symmetric k points.

#### 3.2.3 Nitrogen monomer, dimer and trimer adsorption

The electronic behavior of N-monomer, dimer and trimer adsorption is of same pattern as Boron adsorption. The electronic band structures of N-single atom, dimer and trimer are shown in Figure 5(g-i) respectively. The Dirac cone in silicene with N-monomer adsorption gets shifted to upper side of Fermi level, which is due to the presence of an additional electron in outer shell of N as compared to Si-atom. A band



**Fig. 5** Electronic band structures for adsorption of (a) B-monomer, (b) B-dimer, (c) B-trimer, (d) C-monomer, (e) C-dimer, (f) C-trimer, (g) N-monomer, (h) N-dimer and (i) N-trimer on silicene. The energies are relative to the Fermi level ( $E_F=0$ ).

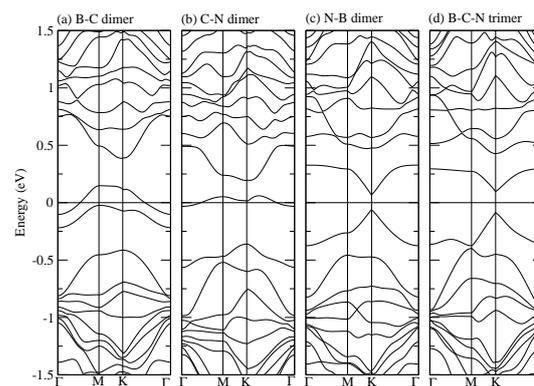
gap of 0.210 eV is found for N-dimer adsorption. For N-trimer adsorption system is metallic with one band line found around Fermi level.

**3.2.4 Hetero-dimer and trimer adsorption** The electronic band structure of hetero-dimers and trimer of B, C and N adsorbed on silicene is shown in Figure 6. In hetero-dimer adsorptions, only B-N adsorption on silicene shows band opening of 0.129 eV near Fermi energy retaining its Dirac cone character and for other two cases i.e. B-C and C-N adsorption, the band lines cross the Fermi energy level. For hetero-trimer (B-N-C) adsorption a band gap of 0.182 eV is found.

An increase in the coverage by adsorbate from monomer to trimer of different species on silicene results in the modification of electronic bands in the respective band structures. However, no systematic trends are observed as far as the shift in the energy bands near the Fermi energy is concerned. In order to get further insight of adsorbate adsorption on silicene, we have calculated the partial density of states as given in Figures S1, S2, S3 and S4 of the supplementary information. On analyzing the PDOS, the strong hybridization between adsorbate and Si- atoms of sheet has been found, which results in deformation of Dirac cone of pristine silicene.

### 3.3 Dielectric Properties

Dielectric functions are important parameters to explore the dielectric properties of materials. In the present work, dielectric function calculations have been performed using the simplest approach based on the dipolar transition matrix elements between different eigenfunctions of the self consistent Hamil-



**Fig. 6** Electronic band structures for adsorption of hetero-dimers (a) B-C, (b) C-N, (c) N-B and (d) hetero-trimer B-C-N. The energies are relative to the Fermi level ( $E_F=0$ ).

**Table 2** Energy band gap, static dielectric constant ( $\epsilon_s$ ) and plasmons energy for  $E \perp c$ .

System	Band gap (eV)	$\epsilon_s$	Plasmons energy (eV)
Silicene	–	34.33	2.16, 7.59
B	–	26.27	2.24, 9.26
B-B	0.081	33.02	2.14, 7.62
B-B-B	–	12.19	2.13, 8.20
C	0.288	13.39	2.11, 7.87
C-C	0.167	18.90	2.15, 7.62
C-C-C	0.182*	26.32	2.11, 7.68
N	–	7.98	2.21, 7.91
N-N	0.210	16.92	2.10, 7.55
N-N-N	–	13.55	2.15, 7.44
B-C	–	25.59	2.14, 7.61
C-N	–	16.71	2.13, 8.05
N-B	0.129	29.25	2.13, 7.59
B-C-N	0.182	26.01	2.14, 7.40

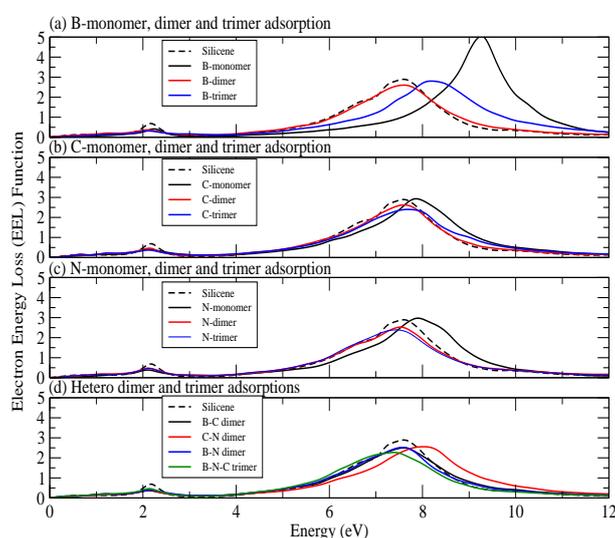
\* Indirect band gap

tonian<sup>37</sup>. Electron energy loss (EEL) function is one of the important properties which corresponds to the collective excitations of electrons of system and is proportional to inverse of dielectric function. EEL function was calculated for silicene with adsorption of B, C and N monomers and their dimers (B-B, C-C, N-N, B-C, C-N and B-N) and trimers (B-B-B, C-C-C, N-N-N and B-N-C) and compared with the previous reported results of pristine silicene<sup>36</sup>. For materials with hexagonal layered symmetry, dielectric properties can be calculated with electric vector  $E$  perpendicular to  $c$  axis. EEL function has been calculated from the real ( $\epsilon_1$ ) and imaginary parts ( $\epsilon_2$ ) of the dielectric function as defined below:

$$-Im \left\{ \frac{1}{\epsilon(\omega)} \right\} = \frac{\epsilon_2(\omega)}{\epsilon_1^2(\omega) + \epsilon_2^2(\omega)} \quad (2)$$

The electron energy loss function for in-plane ( $E \perp c$ ) polarization is plotted in Figure 7 for B, C and N based monomer, dimer and trimer adsorptions on silicene. The measured plasmons energy from graphs for in-plane polarization (perpendicular to c-axis) are also given in Table 2. The low energy weak plasmon peaks around 2-3 eV are due to the excitations of  $\pi$  electrons. Significantly higher energy pronounced peaks above 6 eV may have both  $\pi$  and  $\sigma$  electrons contributions. The most change in the peaks are found for B-adsorption. i.e. two times enhanced structure peak with blue shift of 1.67 eV (at 9.26 eV). The significant shifts are also found for B and N-monomer adsorption. The plasmons energies are blue shifted from yellow to yellow green energy region for B and N monomer adsorption. For other adsorptions, plasmonic features lie in the yellow energy region similar to that of pristine silicene. This tunable EEL spectra may have importance in optical biosensing applications.

Furthermore, the static dielectric constants ( $\epsilon_s$ ) have been calculated which have importance in device modeling. The static dielectric constant is given by the value of real part of dielectric function at zero energy or frequency. It is worth noting that zero frequency in this context means a frequency low compared to interband transitions but higher than the phonon frequencies. The calculated values are listed in Table 2. Our calculated value of  $\epsilon_s$  for pristine silicene is 34.33 which gets reduced on adsorption of various types of adsorbate.



**Fig. 7** Electron energy loss function for various types of adsorbates (monomers, dimers and trimers) on silicene.

## 4 Conclusions

In summary, structural, electronic and dielectric properties of monolayer silicene with adsorption of monomers of B, N and C and their dimers and trimers are presented. Our results of structural and electronic properties of B and N doped silicene match well with the results available in literature<sup>27</sup>. N-monomer adsorption shows most stable structure while N-dimer adsorption shows least stable structure. B and N-monomer adsorption and their homo-trimers do not show any bandgap opening, while for other cases like C-monomer adsorption and their trimer adsorption a significant band gap near Fermi energy is found. Homo-dimers of B, C and N shows a semi-conductor behavior and hetero-dimers B-C and C-N show metallic behavior. C-monomer adsorption shows a highest direct band gap opening of 0.288 eV and C-trimer adsorption shows an indirect band gap of 0.182 eV. The band gap opening in silicene by means of adsorption may be very useful in nanoelectronics applications. The significant shift in plasmons energy are found for B and N-monomer adsorption, in which plasmons are blue shifted from yellow to yellow green energy region. The static dielectric constants are also found to be tunable with the functionalization of silicene.

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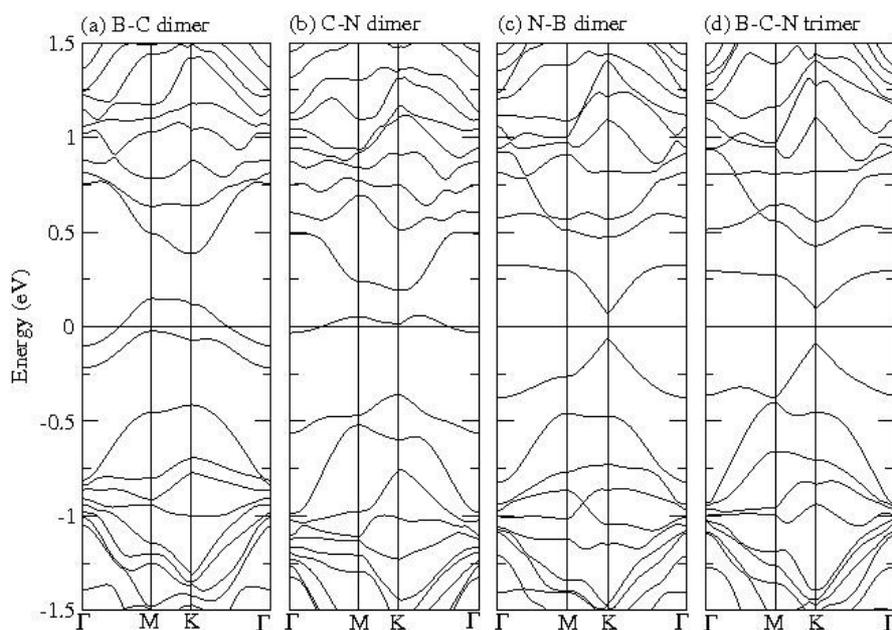
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# Electronic & Dielectric Properties of Silicene Functionalized with Monomers, Dimers and Trimers of B, C & N atoms

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## Abstract:



*Illustration 1: Electronic band structures for adsorption of hetero-dimers (a) B-C, (b) C-N, (c) N-B and (d) hetero-trimer B-C-N. The energies are relative to the Fermi level ( $E_F = 0$ ).*