Effects of Boron Nitride on the optical properties of Silicene: density functional theory calculations

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Abstract. Two dimensional materials with honeycomb lattice have attracted researcher's attention owing to their several superior properties. Silicene which is the most compatible 2D materials with silicon-based nano-electronic industry. Density functional theory was performed to investigate optical properties of silicene doped with Boron Nitride. With the addition of Boron Nitride (BN), the refractive index value of silicene decreases with the highest value achieved in the position of bridge with a value of 1.783, and reaches the peak at lower energy.

1. Introduction
Graphene and its various fascinating properties, including massless Dirac fermion transport[1], near-ballistic transport[2], and high speed mobility[3] have aroused curiosity of researchers and hope to find the similar superior properties from other two-dimensional materials with the same crystal structure and different elements[4]. Especially elements from the same group of carbon (group IV). We prefer to study silicon 2D material not only because silicon is abundant in nature, but also its compatibility with current silicon-based semiconductor technology. Silicene is a monolayer of silicon with honeycomb lattices [5,6,7].

Like other 2D materials, silicene is also known to be a gapless material [8,9]. Several treatments are expected to modify the electronic structure, which also affects their optical properties. Treatments that have proven successful in altering the electronic structure including stress and electric fields. In addition, impurity atoms are the most common. As a Group IV element, the commonly used impurities are Group III elements as acceptors and Group V as electron donors[6]. Therefore, dopants of boron (B) and nitrogen (N) were selected in this study.

2. Methods
The optical properties of silicene are calculated by using the ABINIT Simulations Package [10], which is based on the density-functional theory (DFT). The Perdew–Burke–Ernzerhof (PBE) form of the generalized gradient approximation is adopted to describe the exchange correlation interaction [11]. All self-consistent calculations are performed with the plane-wave cutoff energy of 816 eV on a 10 x 10 x 1 Monkhorst–Pack k-point mesh [12]. Due to periodic boundary condition used in ABINIT code, to model two dimension material, 3D boundary condition was employed with third dimension consisting of a finite slab and large vacuum layer to reduce surface-surface interactions.

We consider the binding of the B/N adatom on three most possible sites: the hollow (H) site in the center of a hexagon (Hollow site), at the midpoint of Si-Si bond (bridge site), and directly above a Si atom (top site) as described in Figure 1. Refractive index of lossy material is complex function of light...
wave and frequency. The complex refractive index which is usually denoted by $n^*$, with real part $n$ and imaginary part $K$.

Figure 1. Three possible position of B/N adatom on silicene: Hollow site (H), Bridge site (B), and Top (T) site.

In this simulation of the optical properties, the ABINIT code produces data of frequency dependent. Using this data set, the related optical properties of the silicene systems.

3. Results and Discussion

We compared refractive index of pristine silicene and that of Boron nitride doped silicene with several combination of B/N atom position. Figure 1.b shows the refractive index for silicene doped by BN in the bridge-bridge position. In the refractive index in the energy range of 0 - 1.4 eV the value increases to 1.783 then decreases because the extinction coefficient has increased to an energy range of 1.8 eV. Then the refractive index value increases again due to a decrease in the extinction coefficient. In the energy range of 3.5 eV, the refractive index value decreases due to the increasing extinction coefficient value. The decrease in the refractive index indicates the dispersion because of the phase velocity of refraction of light decreases. The increase in coefficient indicates an increase in absorption. Increased absorption occurs from the energy range of 3.5 - 5.5 eV with a peak value of 0.733 and then again decreases and fluctuates. Figure 2.b shows the refractive index for silicene doped by BN in the bridge-bridge position and the refractive index for pristine silicene are clearly different. For pristine silicene (Figure 2.a), from 0 to 3 eV, the refractive index is nearly constant. There is a peak (maximum value) at about 6.2 eV. While refractive index of BN doped silicene, with all combination of B/N atom position in silicene, as depicted by figure 2.b, 2.c, and 2.d, have several peaks and the first peaks appear earlier than at pristine silicene.

For silicene doped BN with B atom and N atom at hollow site and bridges site respectively (Figure 2.c and 3.c), the combination of positions on the refractive index value decreases fluctuated because the value of the coefficient extinction also experienced a fluctuating increase. Fluctuations due to the refractive index will decrease if there is an increase in the extinction coefficient and vice versa. However, at 3 eV the increase in the refractive index is slightly visible to the energy of 3.5 eV and back down again. Because in the energy range of 3.5 - 4 eV the extinction coefficient reaches its peak with a value of 0.581. This shows an increase in absorption. After that, the extinction coefficient decreases due to fluctuations from reflection to energy of 6 eV.

In silicene systems with the addition of B at the bridge position and N at the top position, an increase in the refractive index in the energy range of 0 - 1.2 eV until it reaches a peak of 1.642, then decreases due to an increase in the extinction coefficient. The refractive index drops to an energy of 3.2 eV as does the extinction coefficient. This shows that for the decrease in the refractive index, light dispersion occurs, while for the extinction coefficient, there is a decrease in the absorption value. In the range of 3.2 - 6.5 eV an increase in the value of the refractive index and the coefficient of extinction. The peak coefficient of extinction reaches 0.746 at 3.9 eV energy. Then in the energy range of 4 - 6.5 eV, there is a decrease in the fluctuation of the refractive index and the extinction constant.
For silicene with both B atom and N atom at bridge site (figure 4.b), the reflection occurred at 0.038 and then changed to the same increase as the extinction coefficient graph. This shows an increase in reflection when there is a decrease in the refractive index. Then in the energy of 3.2 eV the reflection value has increased fluctuated due to the activity of the refractive index. At 5.6 eV the reflection value reaches a peak value of 1.118. There is an increase in the refractive index so that the reflection values decrease.
Figure 3. Imaginary part of refractive index of silicene system, namely: a. pure/pristine silicene, b. Silicene doped with both B atom and N atom at bridge site of silicene layer, c. Silicene doped with B atom at bridge site and N atom at hollow site of silicene layer, d. Silicene doped with B atom at bridge site and N atom at top site of silicene layer.

Figure 4. Reflection coefficient of silicene system, namely: a. pure/pristine silicene, b. Silicene doped with both B atom and N atom at bridge site of silicene layer, c. Silicene doped with B atom at bridge site and N atom at hollow site of silicene layer, d. Silicene doped with B atom at bridge site and N atom at top site of silicene layer.
As shown by Figure 4.d the value of constant reflection is at 0.035. Then it increases until it drops back from the energy range of 0 - 3.2 eV. Like the refractive index and the extinction coefficient, the reflection value rises again to the peak of 0.107 at the point of energy of 3.9 eV. There is a similarity between the refractive index, the extinction coefficient which represents absorption, and reflection. Indicates that the incoming light is transmitted. So that a decrease in the value of the energy range of 4 - 6.5 eV (in the ultra violet range) due to transmission. A significant increase in reflection value indicates that the material is high reflection and when it goes down it experiences a low reflection.

4. Conclusion
The doping effect of Boron (B) and Nitrogen (N) on the optical properties of the density function approach has been calculated. Based on these results it can be concluded that doping of BN change optical properties of silicene significantly. In Boron Nitrid (BN) doped silicene the refractive index value decreases with the highest value achieved at the bridge position with a value of 1.783.

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