

Electronic Structures of Silicene Doped with Gallium: First Principle study

Mauludi Ariesto Pamungkas^{1,a}, Wafa Maftuhin^{2,b}
^{1,2} *Jurusan Fisika (Physics Department), Universitas Brawijaya, Indonesia*

Abstract. Following the success of graphene which possesses unique and superior properties, 2D material other than graphene become centre of interest of material scientists. Silicene, which has the same crystal structure as graphene but consist of silicon atoms rather than carbon become intriguing material due to domination of silicon as main material of electronic component. It is common to enhance electronic properties of semiconductor by adding dopant atoms. The electronic properties of Silicene doped with Gallium are investigated using first principle calculation based on density functional theory (DFT). Ga doping changes character of silicene from semimetal to conductor except silicene with Ga doping on S-site (Ga atom substitutes one Si atom) which lead to semiconductor.

1 Introduction

Today, graphene has attracted the most attention of material researchers not only because it is the first 2D material successfully synthesized but also because of its peculiar behaviors and superior properties[1]. Its successful synthesis and potential applications in wide areas have stimulated many researchers to study possibility of elements other than carbon to be formed in graphene structure. Considering domination of silicon in electronic industries owing to its abundant existence in the earth as well as excellent interface with its oxide, investigation of silicene, silicon material with graphene crystal structure (two dimensional honey comb), is paramount important. Theoretical prediction of the existence of silicene had been started even before invention of graphene[2]. Despite possibility of silicene to exist had ever been questioned due to natural sp^3 hybridization of silicon silicene has been successfully synthesized on a Ag (111) substrate[3]. Recently, silicene has been successfully implemented as a channel layer of field effect transistor[4]. Other important research findings from recent theoretical studies have shown that electronic band structure of silicene is similar to that of graphene. However, silicene has larger band gap at Dirac point. In addition, due to its low buckles, band gap of silicene can be controlled by electric fields[5,6]. Like graphene, silicene possesses massless Dirac fermion whose electron velocity is only hundredths of light velocity[7]. Recent first principle study reported existence of quantum hall effect in silicene as it was found in graphene[8]. Considering above mentioned both similarities and differences between graphene and silicene, it is then justified to expect similarities and differences in other properties.

Beside properties of pristine graphene, graphene doped with other elements, particularly from third and

fifth column of periodic table, have been intensively investigated. Doping on graphene influences its electronic structure especially tune its band gap. Therefore it is intriguing to investigate influences of doping on electronic structure of silicene. This work is aimed to investigate influence of Gallium doping on the electronic structure of silicene.

2 Computational Methods

The calculations are performed using Density functional Theory implemented in ABINIT code. The electron-ionic core interaction is represented by norm conserving pseudopotential. Perdew–Burke–Ernzerhof (PBE) formulation of the GGA is chosen to treat electron exchange correlation. Plane wave basis set with cutoff energy of 20 hartree (560 eV) is used. Special $12 \times 12 \times 1$ k -point grid was generated using Monkhorst-Pack scheme.

We studied Silicene with armchair structure and with size of 2×2 cell. Vacuum layer with width of 15 angstrom is implemented to eliminate interaction. One Gallium atom is placed on several most possible positions. The system is then relaxed with Broyden–Fletcher–Goldfarb–Shanno (BFGS) algorithm to lead it into ground state with forces smaller than 0.005 eV/Å.

3 Results and Discussion

At first, we calculated ground state structure and electronic properties of bare graphene and silicene to confirm our calculation parameter. The equilibrium lattice constant of bare graphene and silicene are 2.46 Å and 3.90 Å respectively which are close to the values reported by previous studies[9],[10],[11], [12].

When silicene is doped with Gallium atom in the B-site, Gallium atom whose atomic radius is larger than that of silicon atom is placed in the middle of honey

^a m_ariesto@ub.ac.id, ^b wafamaftukhin@gmail.com

comb structure surrounded by silicon atoms. After relaxation, the closest silicon atom is pushed out to find new stable position so that Si-Si bonding is broken. Closest distance between Ga atom and silicon atom after they reach stable position is within 2.87-2.99 Angstrom. For doping of Ga atom on T-site, namely putted above one Si atom, after the system is relaxed, the closest silicon atom is also repelled away and leads to breaking of Si-Si bond. The closest Ga-Si distance is 2,63 Angstrom. While, for doping at H-site, there is no position of atoms change significantly. In this case, Ga bonds to Si atom with bond length of 2.32 Angstrom. Differ from other Ga position, doping of Ga atom on S-site, Ga atom replaces one Si atom position.

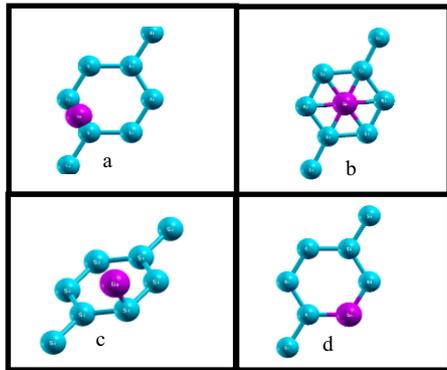


Figure 1. Position of Ga atom on silicene, a. Brige (B-site), b. Hollow (H-site), c. Top (T-site), and d. Substitute (S-site)

Table 1 Structure and formation energy of silicene doped with Ga atom.

Position of Ga atom doping	Si-Si (Angstrom)	Si-Ga (Angstrom)	Ef (eV)	Eg
GA top site	2.29	2.94	-15,24	-
GA bridge site	2.12-2.18	2.87-2.99	-14,22	-
GA Hollow site	2.3175	2.32	-14,81	-
Substitution GA	2.22-2.26	2.25	-15,79	0,275

Table 1 shows that silicene with doping of Ga atom at S-site is the most stable state. Formation energy is calculated based on this equation :

$$E_{\text{formation}} = (E_{\text{total}} - E_{\text{silicene}} - E_{\text{adatom}} + \mu_{\text{total}} - \mu_{\text{Si}}).$$

4 Band Structure

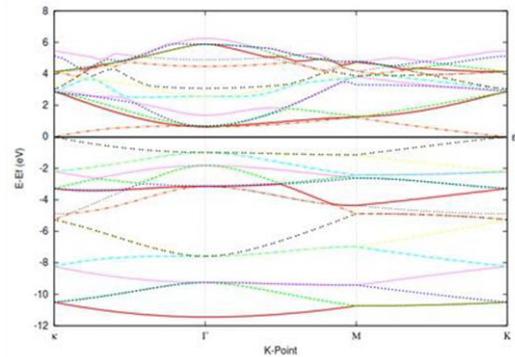


Figure 2. Band structure of pristine silicene with supercell 2x2.

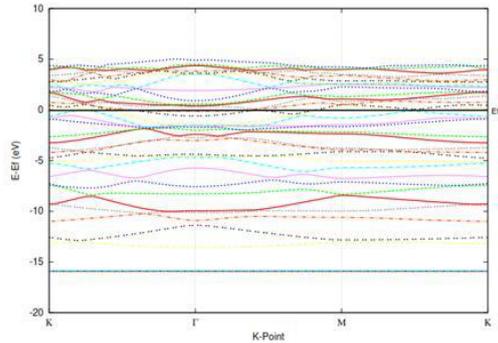


Figure 3. Band structure of silicene doped by Ga atom at B-site

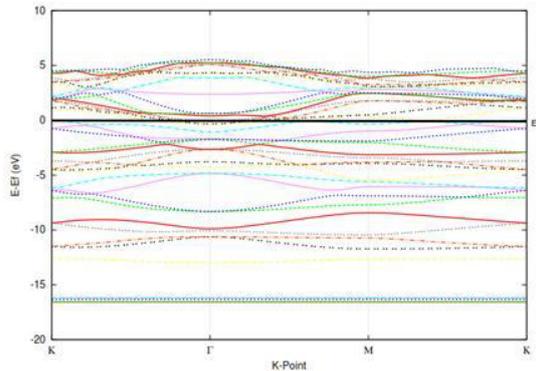


Figure 4. Band structure of silicene doped with Ga atom at H-Site.

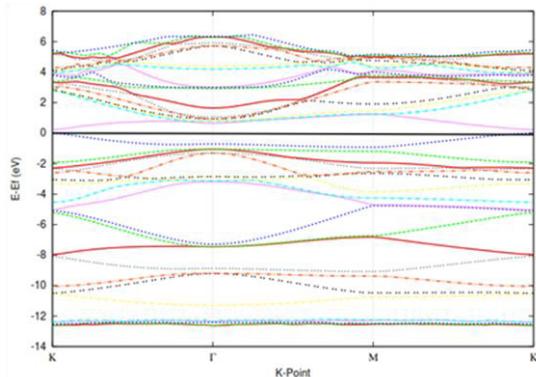


Figure 5. Band structure of silicene doped with Ga atom at S-Site.

Figure 2 shows that there is no gap between valence band and conduction band (zero band gap) at Fermi energy. There is also no overlap between valence band and conduction band. The two bands meet at K point. One can conclude that pristine silicene is a semimetal.

After silicene is doped with Ga atom, its band structure changed. For Ga atom at H-Site, B-Site, and T site (Figure 3, 4 and 5 respectively) there is no gap at Fermi energy, several energy levels overlap. Therefore, there is no Dirac point. It can be inferred that silicene doped at those sites is a conductor. While, silicene doped with Ga atom at S-site (Figure 6) possesses a small gap at Fermi energy. It is a direct gap of 0.275 eV which means silicene doped with Ga atom at S-site is a semiconductor.

5 Conclusion

In summary, Ga doping on silicene at B-site, T-site and H-site changes it from semimetal to conductor. While at S-site, Ga atom changes silicene from semimetal to semiconductor with an energy gap of 0.275 eV.

References

1. A.H.C. Neto and K. Novoselov, *REPORTS Prog. Phys.* 74, (2011).
2. S. Fagan, R. Baierle, R. Mota, A. da Silva, and A. Fazzio, *Phys. Rev. B* 61, 9994 (2000).
3. P. Vogt, P. De Padova, C. Quaresima, J. Avila, E. Frantzeskakis, M.C. Asensio, A. Resta, B. Ealet, and G. Le Lay, *Phys. Rev. Lett.* 108, 155501 (2012).
4. L. Tao, E. Cinquanta, D. Chiappe, C. Grazianetti, M. Fanciulli, M. Dubey, A. Molle, and D. Akinwande, *Nat. Nanotechnol.* 10, 227 (2015).
5. N.D. Drummond, V. Zólyomi, and V.I. Fal'ko, *Phys. Rev. B* 85, 075423 (2012).
6. Z. Ni, Q. Liu, K. Tang, J. Zheng, J. Zhou, R. Qin, Z. Gao, D. Yu, and J. Lu, *Nano Lett.* 12, 113 (2012).
7. L. Chen, C.-C. Liu, B. Feng, X. He, P. Cheng, Z. Ding, S. Meng, Y. Yao, and K. Wu, *Phys. Rev. Lett.* 109, 056804 (2012).
8. C.-C. Liu, W. Feng, and Y. Yao, *Phys. Rev. Lett.* 107, 076802 (2011).
9. R. Brako, D. Šokčević, P. Lazić and N. Atodiresei, 2010 *New J. Phys.* 12 113016(2010).
10. S. Lebegue and O. Eriksson, *Phys. Rev. B* 79, 4 (2009).
11. B. Feng, Z. Ding, S. Meng, Y. Yao, X. He, P. Cheng, L. Chen, and K. Wu, *Nano Lett.* 12, 3507 (2012).
12. A.H.C. Neto, *Rev. Mod. Phys.* 81, 109 (2009).