Islamic Azad University

Journal of

Optoelectronical Nanostructures

Winter 2017 / Vol. 2, No. 1

The structural and density state calculation of Boron and Nitrogen doped silicene nano flake

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(Received 26 Dec. 2016; Revised 22 Jan. 2017; Accepted 15 Feb. 2017; Published 15 Mar. 2017)

Abstract: In this paper, we study the effect of single Boron/Nitrogen impurity atom on electronic properties of a silicene nano flake. Our calculations are based on density functional theory by using Gaussian package. Here, one Si atom in silicene nano flake substitutes with a Boron/Nitrogen atom. The results show that substitution of one Si atom with single Boron/Nitrogen atom increases distance of impurity atom with its nearest neighbors and changes hexagonal structure of silicene nano flake. Doping silicene nano flake with a Boron impurity atom makes its structure curved and causes to create a miniband in energy gap, which increases conductance consequently while doping with a Nitrogen atom causes to produce two spin dependent midbands in energy gap which leads to creating a controllable spin dependent conductance with electron energy for silicene nano flake. Therefore, Nitrogen doped silicene nano flake is good material for design of nano electronic and spintronic devices.

Key words: Boron Impurity, Nano flake, Nitrogen Impurity, Silicene**.**

1. INTRODUCTION

Silicene is a single layer of silicon atoms arranged in two-dimensional honeycomb network. Silicene has interesting properties same as graphene. Several experimental works have been done to synthesize it on proper substrate in recent years. Its stability on boron nitride and silicon carbide has been predicted in recent theoretical studies. Silicen has fascinating properties. Its energy gap can be controlled by applying external electric field. This property

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arises from a buckled structure of silicene nano sheet. Comparing to graphene, silicene has a large spin orbit interaction.

In recent years, the effect of impurity atoms on properties and lattice structure of silicene has attracted a huge interest of researchers. In this material, impurity atom can lead to appearance of special and applied properties. Many works have been done to study the effect of impurity atom on silicene nanoribbons. In these investigations silicene system has been considered to nanoribbons form and the effect of the variation in position of impurity atoms throughout the nanoribbon width on its electronic properties has been studied.

In this paper, our aim is to study the electronic and structural properties of silicene nano flakes. There is not regular geometrical structure in nano flakes similar to nanoribbins and comparing to nanoribbons, they have the more edge effects. Based on density functional theory, calculation is done by Gaussian package.

2. Simulation METHOD

A silicene nano flake containing 30 silicene atoms is considered to study the doping effect. The each Si atoms are saturated by hydrogen. Fully optimization is consequently achieved at three steps. a) We used Hartree-Fock method and 3-21G basis set. b) The previous step result are considered as input file in this step and DFT method with 3-21G basis set is used. c) Considering the result of second step as input file, the optimization is finally accomplished with B3LYP and 3-61G(d) basis set. These steps are repeated for doped silicene nano flake.

3. RESULTS AND DISCUSSION

Firstly, we simulate nano flake structure of silicene, which contains 30 Si atoms using reconstruction of graphene network as shown in figure 1. To obtain a planar structure, dangling bonds are terminated by 44 Hydrogen atoms. Values of bond lengths, bond angles and planar angle of bonds that are calculated with geometric method, have been utilized as input files in Gaussian package. Then we chose appropriate calculation method and basic functions to obtain optimized parameters. Our findings are in consistence with experimental calculations.

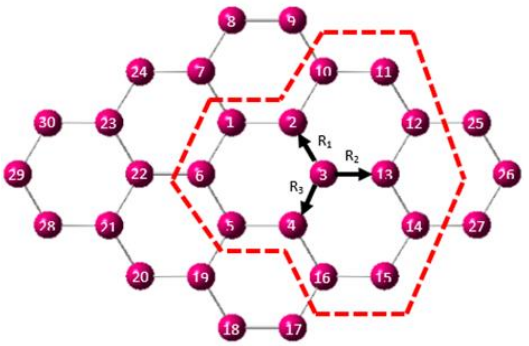


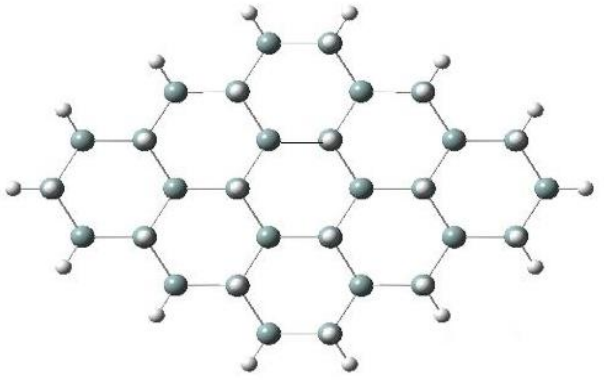
Fig. 1. : Reconstruction schematic of two dimensional honeycomb silicene nanoflake.

Distances of nearest neighbours and bond length values have been displayed in Table 1 in case of with and without doping effect. Each of obtained distances for pristine silicene nanoflake is 2.30 A^o that corresponds with bond length of silicene. Moreover, R_1, R_2 and R_3 distances are equal and symmetric.

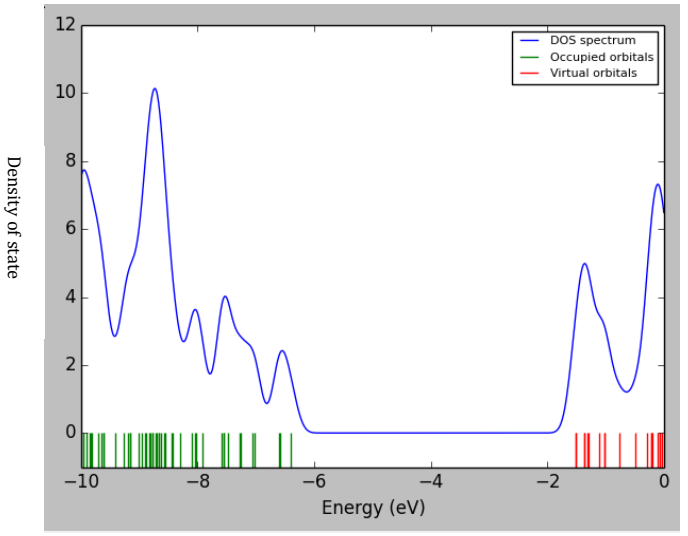
TABLE I
DISTANCES OF NEAREST NEIGHBOR AND BOND LENGTH

Bond	Bond length befor doping	Bond length after B doping	Bond length after N doping
R_1	2.30	2.05	1.77
R_2	2.30	2.15	3.29
R_3	2.30	2.05	1.77

Figure 2(a) shows silicene nano flake after the act of optimization. In order to study electronic properties of the considered system, investigation of density of state graph as a function of energy can be valuable. Figure 2(b) shows density of state graph as a function of energy for pristine nano flake. As can be seen in this Figure, density of state for considerable range of energy, $-6.2<E_f<-2.5$ is equal to zero. In other words, the nano flake can be assumed as a semiconductor. This result originates from conductance and valence bands variation due to cutting silicene sheet, which leads to constructing silicene nano flake. In fact, edge effects in nano flake are more effective relative to nanoribbon.



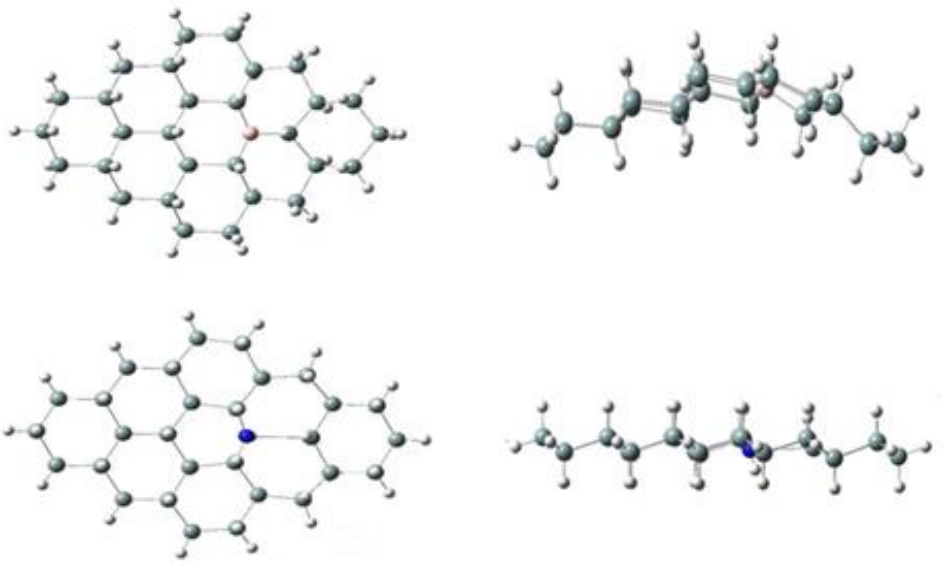
(a)



(b)

Fig. 2: (a) Schematic structure of silicene nano flake without impurity, (b) Density of state as function of energy.

In this research, we have substituted one Si atom, which is labeled by Number 3, with a Boron (Nitrogen) atom. Doping silicene nano flake with Boron impurity atom leads to decreasing of bond lengths (i.e. R_1, R_2 &R_3) and lack of symmetry in distance of nearest neighbor atoms with impurity atom. As can be observed in Table 1, substitution of one Si atom with a Boron atom in silicene nano flake has affected significantly on its honeycomb structure. It is seen that not only the distance of nearest neighbor atoms with Boron atom varies because of doping, but also the distance of next-nearest atom with Boron atom changes, drastically. Nano flake structure in presence of Boron or Nitrogen atom is shown in Fig. 3(a). Pink (blue) sphere represents Boron (Nitrogen) atom. As shown in Fig. 3(a), hexagonal structure of the nano flake has been disorder due to presence of impurity atom. Actually, Boron impurity atom absorbs its nearest Si atoms, which decreases distance of nearest neighbors.
Consequently, form of other hexagonals constructing silicene nano flake that are located around Boron impurity atom changes. Doping silicene nano flake with single Boron atom makes its structure curved while Nitrogen impurity atom cannot create curvature and is observed out of silicene nano flake plane (see Figure 3(b)).



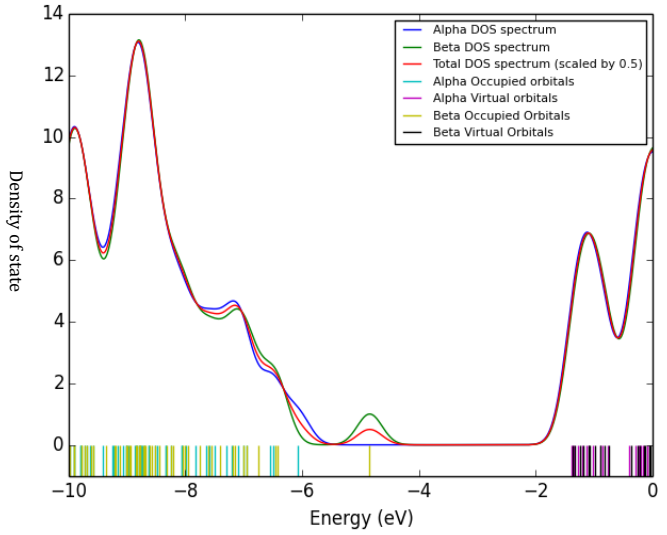
(a) (b)

Fig. 3. : Schematic structure of doped silicene nano flake with Boron and Nitrogen, (a) with perpendicular view,(b) with planar view.

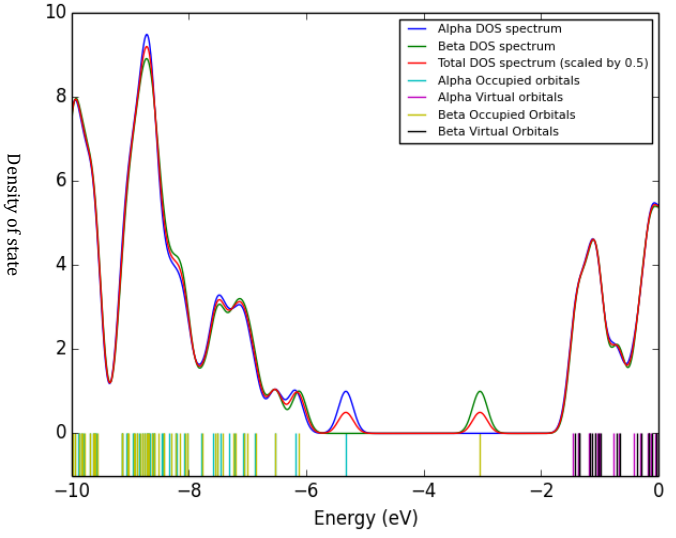
Density of state as a function of energy for doped silicene nano flake with single Boron/Nitrogen atom is demonstrated in Fig. 4. It is observed that doping silicene nano flake with Boron atom decreases energy gap a little and makes a midband in this region, which can be occupied with electrons. Blue-colored and green-colored graphs represent density of state as functions of energy for spin-up and spin-down electrons. Comparing Figs. 2(b) and 4(a), we find that presence of impurity atom leads to creating spin-down dependent states in energy gap. In other words, a spin dependent band is created in energy gap that spin-down electrons can be excited to it and makes spin-down dependent conductance. Note that there is no band for spin-up electrons in this region. Due to existence of the mentioned midband, total density of state without considering state of electron spin can be defined which is demonstrated as a red-colored graph in Figure 4(a). Thus, electrons can be localized at this state and conductance increases relative to the case of no doping. Moreover, it is observed that in Fig. 4(b) doping silicene nano flake with Nitrogen atom has no considerable effect on energy gap region. It only causes to produce two midbands in energy gap region which can be occupied with electrons. With comparing Figs .2(b) and 4(b), we observe that substitution of one Si atom by a Nitrogen atom in silicene nano flake creates spin dependent states in energy gap region. Electron with both of spin states can be excited to these states. Also it is seen that spin dependent density of state is controllable with electron energy.

4. CONCLUSION

Distance of nearest neighbor atoms changes with substitution of impurity in silicene nano flake arising from interaction between silicon atoms and impurity atom. Distance of impurity atom with its nearest neighbors increases and changes hexagonal structure of silicene nano flake by substituting one Si atom with single Boron/Nitrogen atom. Also, doping silicene nano flake with a Boron impurity atom makes its structure curved and causes to create a miniband in energy gap. Therefore, the conductance increases respect to in the absence of impurity atom. While doping with a Nitrogen atom causes to produce two spin dependent midbands in energy gap which leads to creating a controllable spin dependent conductance with electron energy for silicene nano flake. Conductance of electron with up spin and down spin state can take place at -5.34 eV and -3.06 eV, respectively.



(a)



(b)

Fig. 4. : Density of state as function of energy for (a) Boron doped nano flake, (b) Nitrogen doped nano flake.

5. References

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