Replacing two As atoms in silicene nanoribbons in the presence of an external electric field

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Abstract. With the continuous development of nanotechnology and science, its life application is extremely large. Silicene nanoribbons (SiNR) are nanostructures with many advantages, replacing another element in SiNR helps to create new materials with many outstanding properties. This work studies the doping of two arsenic (As) atoms at different positions in the unit lattice cell of SiNR, the system is placed in an electric field. The presence of an electric field in the system causes changes in the energy band structure and the density of the state. There are three sites to be doped in here, namely the meta, ortho, and para position. One of these three positions will be the most optimal, the position at which the formation energy is the lowest. The structure diagrams of the energy region and state density will be drawn, compared, and examined.

1. Introduction

The creation of low-dimensional materials in recent years has created momentum for the continued development of science and technology [1-3]. The application of research on low-dimensional materials has resulted in new products with many outstanding features, lighter, smaller, low cost, and high-performance products [4-8]. There is a lot of research on low-dimensional materials such as germanene [5-10], graphene [11,12], and silicene [13-18], making the structure of these structures an important advance in materials science [3]. The study of doping substances in graphene, germanene, and silicene is also of interest to many scientists. Doping these materials with impurity creates structures with more prominent properties and a wider application [3,10,16,18]. The doping of substances to silicene nanoribbons (SiNR) has been studied extensively in recent years [3,16,18]. In this work, the doped substance is arsenic, arsenic is a nonmetal, toxic, and its compound is widely used in life. There are three sites to be studied for arsenic atom doping in SiNR, namely meta, ortho, and para sites. We calculated forming energies for all three positions and came up with conclusions for the most optimal location. Band structure and state density calculations give us an overview of the doping system. The system is placed in a 0.3V/Å electric field, and placing the system in an external electric field induces changes in the band structure and density of states (DOS), which offers applications in controlling the electrical properties of the system. materials using an external electric field. From the research results, we compare the structure of the energy region and the state density of
the system when there is an external field and when there is no external field to clearly see the effect of the external field on the system.

2. Configuration

Silicene nanoribbons that we study here have its configuration shown in figure 1.

![Pristine-configuration of SiNR](image1.png)

**Figure 1.** Pristine-configuration of SiNR

The maximum and minimum distances between Si-Si atoms are $2.23934\text{Å}$ and $2.16769\text{Å}$, respectively. Buckling of SiNR is about $0.8\text{Å}$. The total energy of pristine system is about $-69.408218\text{eV}$.

Configuration of doping systems are shown in Figures 2, 3, 4.

![Meta-As doping configuration](image2.png)

**Figure 2.** Meta-As doping configuration

The meta doped structure is shown in figure 2. In this configuration, the silicon atom is located between two arsenic atoms. The total energy of meta-configuration is about $-69.795159\text{eV}$. In the figure 3, with an ortho configuration, with two As atoms in adjacent positions, the total energy of the system is $-70.218542\text{eV}$. Figure 4 shows the para doping configuration, in this configuration, two As atoms are placed in two symmetrical positions in the hexagonal cell. One As atom is in top position, the other in valley position. The total energy of system is about $-69.991258\text{eV}$. 
All three configurations are optimized for the structure and give us the total formation energy to form as follows [4]: 

\[ \Delta E_f = E_{0t} - E_{0p} + nE_{0Si} - nE_{0As} \]

| Table 1. The formation energy of the systems in the presence of the external electric field |
|---------------------------------|-------------------|----------------|-----------------|-----------------|-----------------|
| Doping systems  | \( E_{0t}(eV) \) | \( E_{0p}(eV) \) | \( E_{0Si}(eV) \) | \( E_{0As}(eV) \) | \( \Delta E_f (eV) \) |
| Ortho       | -70.218542      | -69.408218     | -0.1353442      | -0.09662854     | -0.88775532     |
| Meta        | -69.795159      | -69.408218     | -0.1353442      | -0.09662854     | -0.46437232     |
| Para        | -69.991258      | -69.408218     | -0.1353442      | -0.09662854     | -0.66047132     |

Looking at table 1 we see that the formed energy with the ortho configuration is the smallest (-0.88775532eV), so the ortho configuration is the most optimized configuration corresponding to the As atomic doped SiNR system placed in a the external electric field is about 0.3V/A.
3. Bandstructure and density of states

The band structure and the state density of the undoped system are shown in Figure 5. The undoped system has a band gap of 0.285eV, which is a semiconductor. Figure 2 shows band structure and DOS of the meta-doped structure in the presence of an external electric field, the band gap still exists, the band gap energy is about 0.472eV. Compared to the pristine configuration we see that the band gap is wider, this is a semiconductor, compared with the pristine configuration, these states moved closer to the Fermi level.

Figure 5. Band structure and DOS of pristine-configuration

Figure 6. Band structure and DOS of meta-configuration in the presence of the external electric field

Figure 7. Band structure and DOS of para-configuration in the presence of the external electric field
Figure 7 shows the energy band structure and the state density of the para doped system in the presence of an external electric field. Comparing with pristine system, we can see that the energy gap is now wider, the size of the energy gap is about 0.921eV, the doping system is a semiconductor. The states are more concentrated around the Fermi level.

Figure 8. Band structure and DOS of ortho-configuration in the presence of the external electric field

The energy gap disappears in figure 8, the semiconductor becomes a conductor of electricity, the doped structure is metallic. The collective states are more concentrated at the bottom of the conduction band.

Figure 9. Band structure and DOS of ortho-configuration without the external field

In the absence of an external electric field (figure 9), the ortho doped configuration is still a semiconductor with an energy gap of 0.388eV, compared to the pristine system, the energy gap has been wider.

Figure 10. Total and partial DOS of ortho-configuration in the presence of the external electric field
The total state density and the partial state density in the ortho doped configuration are shown in figure 10 (when the external electric field is present) and figure 11 (when there is no external electric field). The contributions of the states Si-s, Si-p, As-s, As-p are almost unchanged in the presence of an external electric field and when there is no external electric field. The contributions of the Si-p state are essential to the formation of the conduction and valence bands.

4. Conclusions

Nanotechnology science research has many great applications. Doping another atom in a material helps to create materials of scientific value. Doping two arsenic atoms in silicene nanoribbons in the presence of an external electric field has been studied and analyzed. There are three doping configurations studied here, namely meta, ortho, and para configuration. By calculating the forming energy, we have found that the most optimal structure when there is an external electric field of 0.3V/0A is the ortho configuration with the forming energy of -0.88775532eV. The pristine configuration is a semiconductor with a narrow energy gap, when doped with arsenic we find that both meta and para configurations are semiconductors with wider energy gap, especially with ortho, the band gap is lost, and for a conductor of electricity. The contributions of the partial states Si-s, Si-p, As-s, As-p have been studied here, the Si-p state is the state that contributes mainly to the formation of the band structure energy of the ortho optimal system.

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