Pb Doping in Silicene Nanoribbons in the Presence of an External Electric Field

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Abstract. Silicene nanoribbons (SNRs) are one-dimensional materials that have been extensively studied in recent years. The SNRs studied here have hydrogen-modified edges, having 12 silicon atoms and 4 hydrogen atoms per unit cell. In the work of doping Pb in SNRs, three configurations have been studied as top configuration, valley configuration, and one-to-one configuration. Research has shown that Pb doping is responsible for the change in band gap and state density of the system. The appearance of the electric field is also the cause leading to the change in the energy band structure of the doped system. The work uses density functional theory (DFT) to study, the formation energy of the system is calculated based on this theory. The doped structures are stable after optimization.

1. Introduction
Silicene is a low-dimensional material that has received much research attention in recent years, and its compatibility with silicon semiconductor devices creates useful applications in the future [1-3]. Like graphene, silicene is a material with a honeycomb structure, but silicene is not a planar structure, it has a warped structure [4-7]. Silicene was first studied and applied in semiconductor technology, semiconductor technology is the foundation of electronic technology [8].

Doping other atoms into silicene creates many new materials and helps to tune the band gap. The hybridization between silicon and other atoms creates a diverse energy band structure. The appearance of an external electric field is also responsible for the change in the band gap [9-13].

Silicene nanoribbons (SNRs) are one-dimensional materials made from silicene with edges modified by atoms, there have been many research works on SNRs and hopefully a lot of promise [14-17]. The combination of other element doping and the external electric field is a way to create more diversity for the energy band structure of the material.

Lead is a good conductor of electricity, is ductile, and is an element found in many alloys. Doping lead into SNRs creates a new material, the system is placed in an external electric field that helps to regulate the electrical properties of the material.
2. Configurations

Figure 1. The pristine-configuration

Figure 2. The top configuration

Figure 3. The valley configuration

Figure 4. The 1-1 configuration

Figure 1 is the unit cell of the undoped SNRs, the unit cell consisting of 12 silicon atoms and 4 hydrogen atoms on either side. The buckling of this configuration is 0.538 Å. Figures 2, 3, and 4 are the top, valley, and 1-1 doped configurations. These configurations are stable after being optimized in an electric field of 0.2 V/Å.

The formation energy of the system is calculated by the formula [18]:
\[ E_f = E_t - E_p + n^*E_{Si} - n^*E_{Pb} \]  
(1)

Here \( E_f \) is the formation energy; \( E_t \) is the doped configuration; \( E_{Si}, E_{Pb} \) are the energy of the free atoms Si and Pb, respectively.

**Table 1.** The formation energy of the systems in the presence of the external electric field

| Doping systems | \( E_t \) (eV) | \( E_p \) (eV) | \( E_{Si} \) (eV) | \( E_{Pb} \) (eV) | \( \Delta E_f \) (eV) |
|----------------|---------------|---------------|-----------------|-----------------|-----------------|
| Top            | -69.739162    | -69.408218    | -0.13534420     | -0.1320471      | -0.3342411      |
| Valley         | -69.796856    | -69.408218    | -0.13534420     | -0.1320471      | -0.3919351      |
| 100            | -70.923018    | -69.408218    | -0.13534420     | -0.1320471      | -1.5345826      |

Table 1 shows the formation energies of the doped systems. If only one Pb atom is doped, the valley configuration is the more optimal configuration.

3. **Band structure and density of states**

![Figure 5. Band structure and DOS of the pristine configuration](image)

![Figure 6. Band structure and DOS of the top configuration](image)

The pristine configuration is a semiconductor with a band gap of 0.325eV. The states extend from the conduction band to the valence band with a relatively thick density.

All three top, valley, and 1-1 configurations are semiconductors with bandgaps of 0.414eV, 0.432eV, and 0.675eV, respectively. Compared to the pristine configuration, these configurations all have a more extended forbidden zone. Of the three configurations, the 1-1 configuration has more states extending from the conduction band to the valence band. Thus we can see that under the influence of external electric field and Pb doping, the band gap of the system is widened.
Figures 9, 10, 11 respectively show the contributions of the partial states Si(s), Si(p), Pb(s), Pb(p) in the top, valley, and 1-1 configurations. We see that the contributions of the Si(s), Si(p) partial states in the top and valley configurations are much larger than the contributions of the partial states Pb(s), Pb(p), which is understandable because the density of Si particles in these configurations is large. In contrast, for the 1-1 configuration, the contributions of the partial states of Pb are larger than those of Si even though the densities of these two particles are equal. Lead and silicon belong to group 4, but lead is metal while silicon is a semiconductor, the larger contribution of Pb to the formation of the energy band structure of the 1-1 configuration represents the mobility of electrons in the outermost shell of Pb.
4. Conclusions
The work is focused on replacing Pb doping in SNRs, the system being placed in an external electric field. There are three configurations studied as top configuration, valley configuration, and 1-1 configuration. Use DFT theory to calculate the formation energy, and the energy band structure of the system. The configurations are stable after being optimized. The contributions of partial states are also studied here. The s states mainly help to form the valence band bottom while the experimental states help form the band structure around the Fermi level. Lead-doping and placing the system in an electric field widens the band gap of SNRs and creates a new type of semiconductor with different properties.

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