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Research Article

Effect of Doping on the Photoelectric Properties of Borophene

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Borophene is a new type of two-dimensional material with a series of unique and diversified properties. However, most of the research is still in its infancy and has not been studied in depth. Especially in the field of semiconductor optoelectronics, there is no related research on the modulation of photoelectric properties of borophene. In this work, we focus on the effect of doping on the photoelectric properties of borophene by using the first-principles pseudopotential plane wave method. We calculate the geometric structure, electronic structure, Mulliken population analysis, and optical properties of impurity (X = Al, Ga) doped α-sheet borophene. The results show that α-sheet borophene is an indirect band gap semiconductor with 1.396 eV. The band gap becomes wider after Al and Ga doping, and the band gap values are 1.437 eV and 1.422 eV, respectively. Due to the orbital hybridization between a small number of Al-3p electrons and Ga-4p state electrons and a large number of B 2p state electrons near the Fermi level, the band gap of borophene changes and the peak value of the electron density of states reduces after doping. Mulliken population analysis shows that the B_0-B bond is mainly covalent bond, but there is also a small amount of ionic bond. However, when the impurity X is doped, the charge transfer between X and B atoms increases significantly, and the population of the corresponding X-B bonds decreases, indicating that the covalent bond strength of the chemical bonds in the doped system is weakened, and the chemical bonds have significant directionality. The calculation of optical properties shows that the static dielectric constant of the borophene material increases, and the appearance of a new dielectric peak indicates that the doping of Al and Ga can enhance the ability of borophene to store electromagnetic energy. After doping, the peak reflectivity decreases and the static refractive index n_0 increases, which also fills the gap in the absorption of red light and infrared light by borophene materials. The research results provide a basis for the development of borophene materials in the field of infrared detection devices. The above results indicate that doping can modulate the photoelectric properties of α-sheet borophene.

1. Introduction

As a representative of the low-dimensional structure of boron, borophene is a new type of two-dimensional material. Therefore, its structure and properties have received strong attention and extensive research.

The theoretical research on the structure of borophene can be traced back to 1995 [1]. At that time, Boustani proposed the presence of quasi-planar boron clusters with pentagonal or hexagonal shape. Later, some researchers successively proved that a single layer of boron with a warped triangular lattice exists and the structure is the most stable [2–7]. During the period, Tang and Ismail-Beigi [8] proposed a kind of single-layer boron with a planar structure composed of a mixture of multiple triangular lattices and hexagonal holes. This structure is called α-sheet borophene. Its characteristic is that all boron atoms are on the same plane, and the energy is lower than the most stable single-layer boron with a warped triangular lattice structure proposed before.

Studies have found that borophene has diversified properties due to its rich structure. Zhou et al. [9] predicted borophene with a Dirac cone structure by theoretical calculations. Mannix et al. [10] proved that the structure of borophene is anisotropic and has high conductivity by experiments. Xu et al. [11] studied the field

emission properties of borophene and the characteristics of fast response and good stability. Penev et al. [12] and Zhao et al. [13] proved that borophene may become a superconductor, respectively, from experimental preparation and theoretical calculation and calculated the superconducting transition temperature. Mortazavi et al. [14] studied the performance of borophene in lithium storage by molecular dynamics methods. Compared with graphene, the study found that borophene has more advantages in the field of lithium-ion batteries. Zhang et al. [15] proposed an infrared plasma sensor based on borophene, which can be applied in next-generation point-of-care diagnostic devices. Feng et al. [16] discovered the existence of Dirac fermions with quantum effects in borophene.

In order to improve the performance of borophene materials, researchers usually use adsorption and doping. Wang et al. [17] studied the hydrogen storage performance of borophene and found that the hydrogen storage effect of borophene modified with Ca can reach 12.68 wt%. Chowdhury et al. [18] studied the electronic and optical properties of borophene doped with hydrogen, lithium, beryllium, and carbon by using density functional theory. The study found that the Dirac point was split and moved after doping, which changed the optical properties accordingly. Ishaq et al. [19] investigated the nonlinear optical properties of superhalogen doped borophene in electronic devices by the first principle study. Chen et al. [20] stimulated P doped borophene as anode materials for lithium-ion batteries by density functional theory. Thanh et al. [21] investigated the charge doping effects on the mechanical strength of borophene. Tu et al. [22] investigated that Li doped borophene can significantly improve the adsorption performance and electronic properties for SO_2. Zhang et al. [23] studied the electronic and magnetic properties of borophene intercalated by 3D transition metal atoms.

Due to the unique properties and wide application of borophene, efforts to modulate hydrogen storage effect, Li storage effect, the adsorption performance, the electronic properties, magnetic properties, and optical properties of borophene are still in their infancy; further research focusing on the properties modulation of borophene is still necessary. Especially in the field of semiconductor optoelectronics, there is no related research on the modulation of photoelectric properties of borophene.

In this work, we focus on the effect of doping on the photoelectric properties of borophene by using the first-principles pseudopotential plane wave method. We investigate that the borophene is the α-sheet borophene with the most stable structure and a semiconductor structure. The selected doping elements are aluminum (Al) and gallium (Ga) that are in the same main group as boron (B). The above is the novelty of our work. The specific task is to analyze the electronic structure and optical properties of borophene before and after doping. It is hoped that the research results can provide a theoretical basis for the application of borophene in the field of semiconductor optoelectronics.

2. Calculation Model and Method

2.1. Calculation Model. The calculation model is α-sheet borophene, and the lattice constants are $a = 0.5050$ nm, $b = 0.5050$ nm, and $c = 3$ nm [24]. The model of α-sheet borophene contains 48 B atoms, as shown in Figure 1(a). The models of the impurity doped borophene are shown in Figures 1(b) and 1(c). These models are obtained by substituting an impurity atom X (X = Al, Ga) for a B atom whose coordinates are (0.44, 0.67, 0.50) in Figure 1(a).

2.2. Calculation Model and Method. The calculation method is the first-principles pseudopotential plane wave method. The ultrasoft pseudopotential [25] is used to deal with the interaction between ionic cores and electrons, and the PBE functional [26] of generalized gradient approximation is used to deal with the exchange correlation energy between electrons. Set $E_{\text{cut-off}} = 240$ eV, the precision is 1.0×10^{-6} eV/atom, and the valence electrons involved in the calculation are selected as follows: B $2s^2 2p^1$, Al $3s^2 3p^1$, and Ga $3d^{10} 4s^2 4p^1$. The Brillouin zone integration adopts the symmetrical special k-point method in the form of $2 \times 3 \times 1$ Monkhorst-Pack [27] and sets $72 \times 45 \times 135$ FFT grid parameters. Considering that the value of band gap calculated by GGA is small, scissors correction is performed when calculating the electronic structure and optical properties, and scissors are set as 1.37 eV.

The expression of binding energy $\mathbf{E_b}$ [28] is as follows:

$$\mathbf{E_b} = \frac{\left[\mathbf{E_T} - \mathbf{n_B E(B)} - \mathbf{E(X)}\right]}{\mathbf{n}}, \tag{1}$$

where $\mathbf{E_T}$ is the total energy of the doped system, $\mathbf{n_B}$ is the number of B atoms in the system, $\mathbf{E}$ ($\mathbf{B}$) is the energy of a single isolated B atom, $\mathbf{E}$ ($\mathbf{X}$) is the total energy of a single isolated doped atom X, and $\mathbf{n}$ is the total number of atoms in the system.

3. Results and Discussion

3.1. Geometric Structure. Table 1 lists the structural parameters and binding energy of impurity X doped α-sheet borophene, where $\mathbf{d_{B0\text{-}B}}$ represents the average length of six B-B bond lengths, which are adjacent to the central atom B_0 of the hexagon when borophene is undoped, $\mathbf{d_{X\text{-}B}}$ represents the average length of six X-B bond lengths, which are adjacent to the impurity atom X when borophene is doped, and $\mathbf{E_b}$ is the binding energy of the system.

It can be seen from Table 1 that after the c-axis is fixed and the structure is optimized, the errors of the lattice constants a and b between borophene and [24] are not more than 0.2% and 0.4%. At the same time, the average length of $\mathbf{d_{B0\text{-}B}}$ is 0.1693 nm, and the error in 0.167 nm obtained in [29] is not more than 1.4%. The above two points indicate that the calculation model is reliable.

As Figure 1 shows, after doping with impurity X, α-sheet borophene still has a two-dimensional planar structure, but the structure is distorted after doping. These changes can be directly seen by the changes in the bond length of $\mathbf{d_{X\text{-}B}}$ given

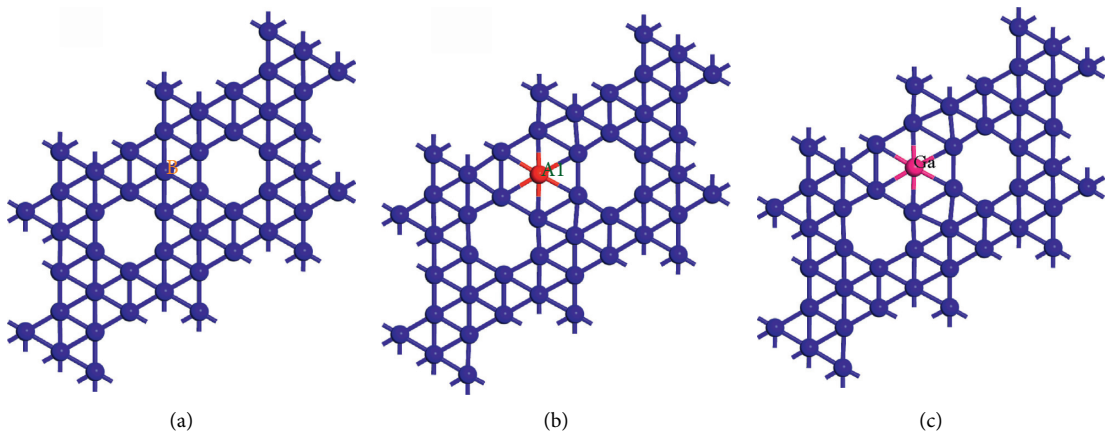

Figure 1: Model of α-sheet borophene. (a) Undoped; (b) Al doped; (c) Ga doped.

Table 1: Structural parameters and binding energy of α-sheet borophene (X = Al, Ga).

Sample	a (nm)	b (nm)	$d_{B0\text{-}B}$ (nm)	$d_{X\text{-}B}$ (nm)	E_b (eV)
Borophene	0.5060	0.5070	0.1693	—	−5.267
Al doped borophene	0.5120	0.5128	—	0.1880	−5.393
Ga doped borophene	0.5127	0.5134	—	0.1896	−5.146

in Table 1. The reason for the changes in bond length is that the covalent radii of each atom are different. For example, the covalent radii of B, Al, and Ga are 0.084 nm, 0.121 nm, and 0.122 nm, respectively. Since the covalent radius of the impurity atom X is larger than that of B, the bond length of $\mathbf{d_{X\text{-}B}}$ is larger than that of $\mathbf{d_{B0\text{-}B}}$. Moreover, since the covalent radius of Ga is larger than that of Al, the structural distortion caused by Ga doping is more serious than that of Al doped.

According to the binding energy values of the borophene system listed in Table 1, the values of $\mathbf{E_b}$ are both negative after Al and Ga doped, which are close to those of undoped system. It indicates that the structure of X doped borophene system is stable.

3.2. Electronic Structure. Figures 2–4 show the band structure and the electronic density of states of borophene before and after doping.

As Figure 2 shows, α-sheet borophene is an indirect band gap semiconductor with 1.396 eV, and the electronic density of states also shows the characteristics of the band gap. It is very consistent with the calculated value of 1.40 eV [24], indicating that the calculation method and accuracy in this paper are reliable. Therefore, the α-sheet borophene expands the application of borophene in the preparation of new nanooptoelectronic devices.

It can be seen from Figures 3 and 4 that, after Al and Ga doping, the top position of the valence band remains unchanged, and the bottom position of the conduction band moves up slightly, which makes the band gap of the doped

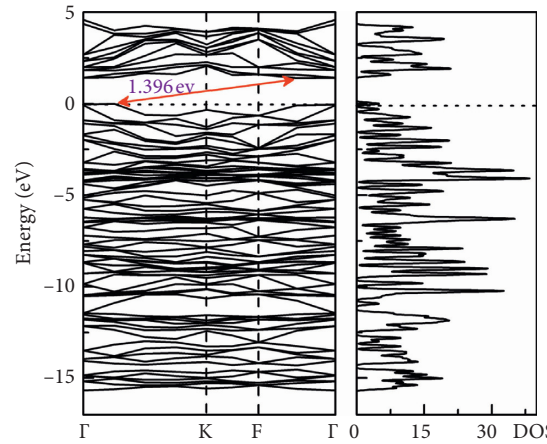

Figure 2: Electronic structure of borophene.

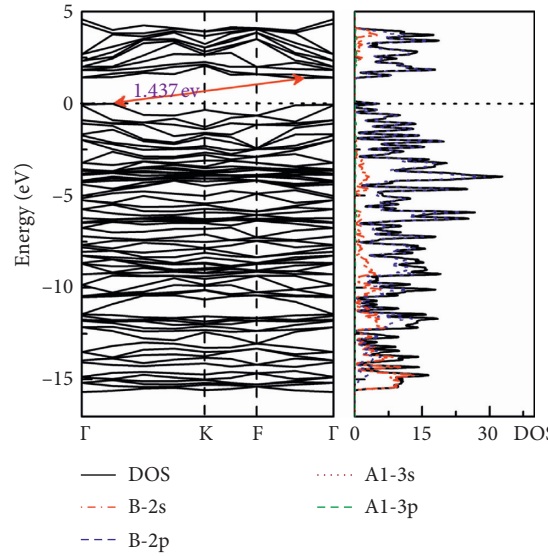

Figure 3: Electronic structure of Al doped borophene.

system wider and the band gap values are, respectively, 1.437 eV and 1.422 eV. It is known that the valence electron arrangement of B is $2s^2 2p^1$, Al is $3s^2 3p^1$, and Ga is

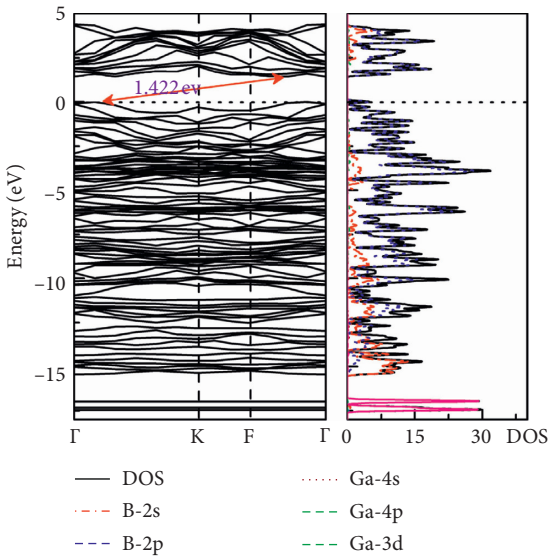

Figure 4: Electronic structure of Ga doped borophene.

$3d^{10}4s^24p^1$. It can be seen from the electronic density of states that, compared with the contribution of the s-state electron of each atom, the contribution of the p-state electron in the outermost layer is larger. In the vicinity of the Fermi level, since a small number of Al 3p-state electrons and Ga 4p-state electrons and a large number of B 2p-state electrons have orbital hybridization, this causes a change in the band gap and a decrease in the peak of electronic density of states of borophene after doping. In addition, due to the introduction of Ga 3d state electrons, Ga doped borophene has five new energy levels between the deep levels of −18 eV to −16 eV.

3.3. Mulliken Population Analysis. The Mulliken population analysis of the B atom adjacent to the impurity atom X is listed in Table 2.

As Table 2 shows, the charge transfer between the B_0 and B atoms is only 0.01 in borophene, indicating that the B_0-B bond is mainly a covalent bond, but there are also a small number of ionic bond components. However, when the impurity X is incorporated, the charge transfer between X and B atoms is significantly increased, indicating that the covalent strength of the X-B bond is weakened, the ionicity is enhanced, and the chemical bond has significant directionality. The characteristics of the chemical bond of X doped borophene system can also be directly seen from the population analysis in Table 3.

As Table 3 shows, the population of the B_0-B bond is 0.54 in borophene. After doping with the impurity X, the population of X-B bond reduces, and the value reaches 0.08 (Al) and 0.28 (Ga), respectively. The decrease of the population indicates that the covalent bonding strength of the chemical bonds in the doping system is weakened, while the ionic bonding strength is increased. The above Mulliken population analysis shows that the introduction of impurities can diversify the properties of the chemical bonds between atoms in doped borophene system.

Table 2: Mulliken population analysis of atoms around the impurity atom.

Sample	Atom	*s*	*p*	*d*	Total	Charge (e)
Borophene	B	0.69	2.31	0	2.99	0.01
	B_0	0.63	2.38	0	3.01	−0.01
Al doped borophene	B	0.91	2.53	0	3.44	−0.44
	Al	−0.02	0.18	0	0.16	2.84
Ga doped borophene	B	0.85	2.45	0	3.30	−0.29
	Ga	0.35	0.53	9.97	10.86	2.44

Table 3: Mulliken population analysis of bands around the impurity atom.

Sample	Band	Population
Borophene	B_0-B	0.54
Al doped borophene	Al-B	0.08
Ga doped borophene	Ga-B	0.28

3.4. Optical Properties. In order to explore the influence of doping on the optical properties of α-sheet borophene, the complex dielectric functions, reflectivity, refractive index, absorption, and loss function of borophene before and after doping are further calculated.

Figure 5 shows the complex dielectric functions of borophene. It can be seen from Figure 5(a) that the static dielectric constant of borophene ε_1 (0) = 2.60. After Al doping, ε_1 (0) increases to 3.21. After Ga doping, ε_1 (0) increases to 3.57. It can also be seen that when undoped, ε_1 (ω) obtains a dielectric peak at $E = 1.95$ eV, which is caused by the interband transition of the B 2p-state electrons from −4.08 eV to −2.13 eV in Figure 2. When Al and Ga are doped, a new dielectric peak appears at $E = 1.28$ eV and $E = 1.34$ eV respectively, and they become the first main peaks. These two new dielectric peaks are mainly contributed by the interband transition of the B 2p-state electrons from −5.91 eV to −4.63 eV and from −5.99 eV to −4.65 eV, as well as a small number of the Al 3p-state electrons and Ga 4p-state electrons. The dielectric peak at $E = 1.91$ eV is significantly reduced, and it retreats to the second dielectric peak. This is because a small number of Al 3p-state electrons and Ga 4p-state electrons and a large number of B 2p-state electrons have been orbitally hybridized; therefore, the transition between bands is weakened. It can be seen from Figure 5(b) that, after Al and Ga doping, the main peak ε_2 (ω) of the imaginary part of the complex dielectric function of borophene at $E = 4.79$ eV is significantly reduced, and a new dielectric peak appears in the low-energy direction. The increase in static dielectric constant and the appearance of new dielectric peaks indicate that Al and Ga doping can enhance the ability of borophene to store electromagnetic energy. The above results indicate that doping can modulate the dielectric properties of borophene.

Figure 6 shows the optical properties of the α-sheet borophene before and after the impurity X doping. As Figure 6 shows, the reflectivity of the borophene material can reach more than 50%, and the static refractive index $n_0 = 1.61$. Borophene has the best absorption effect on green

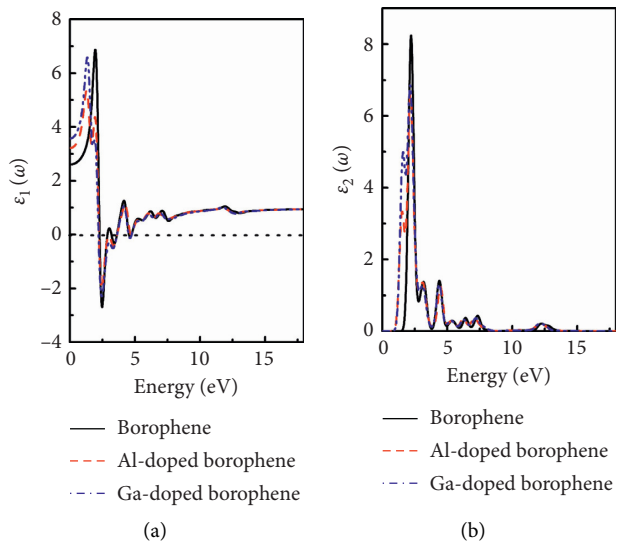

Figure 5: Complex dielectric functions of borophene. (a) $\varepsilon_1(\omega)$; (b) $\varepsilon_2(\omega)$.

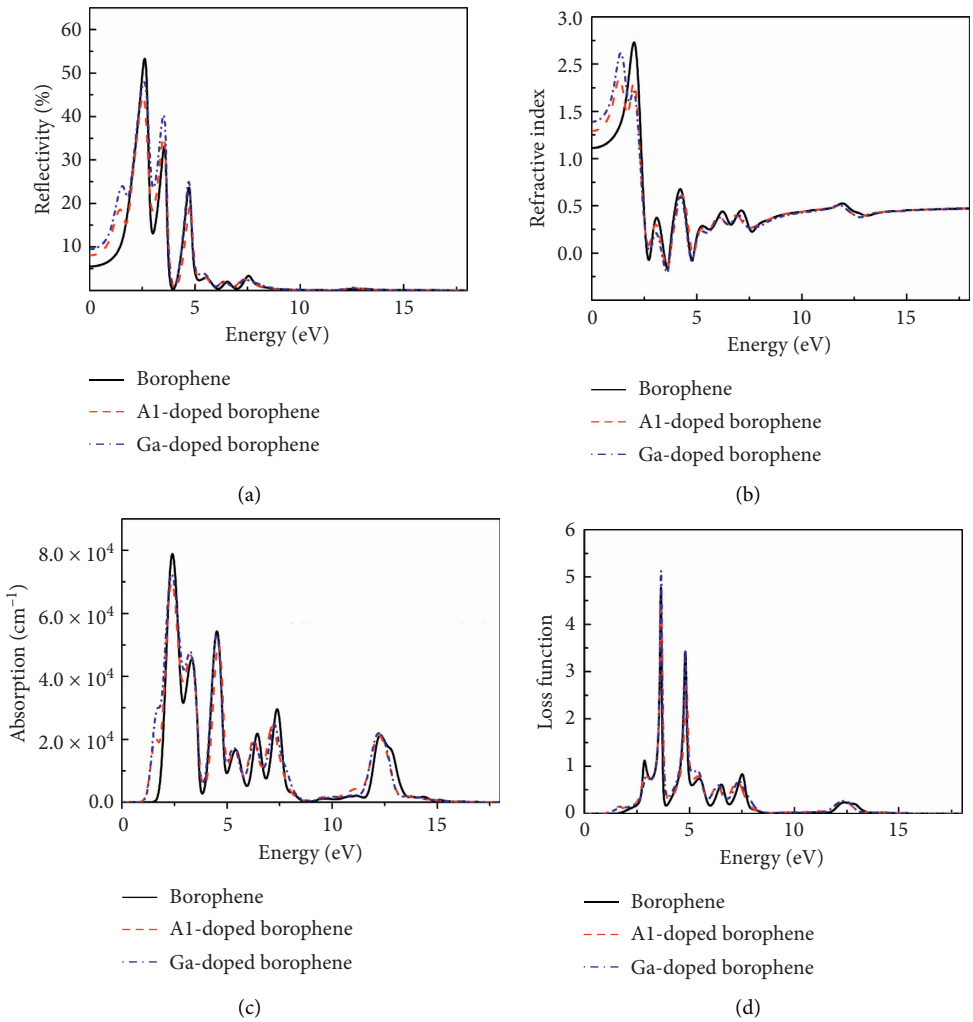

Figure 6: Optical properties of borophene. (a) Reflectivity. (b) Refractive index. (c) Absorption. (d) Loss function.

light with a wavelength of 516 nm in visible light, followed by absorption effect on ultraviolet light with a wavelength of 274 nm, and basically does not absorb red light and infrared light. The peak of the loss function of the borophene is obtained in a very narrow area near $E = 3.64$ eV, indicating that the borophene can be used as a light storage material.

After Al and Ga doping, the peak reflectivity of borophene is reduced to below 45%. After Al doped n_0 increases to 1.79 and after Ga doping, n_0 increases to 1.89. The absorption effect for green light is obviously weakened, and the absorption effect for ultraviolet light is almost unchanged, but it fills the gap in red and infrared absorption after doping. Therefore, the doped borophene system can be used to develop infrared detectors. In the vicinity of $E = 3.64$ eV, the peak of loss function decreases after Al doping, while the peak of loss function increases after Ga doping, but the light loss is limited to a narrow energy range for the doped borophene system. It shows that the doped borophene material can also be used as a light storage material.

4. Conclusion

We have investigated the effect of impurity (X = Al, Ga) doping on the photoelectric properties of α-sheet borophene by using the first-principles pseudopotential plane wave method. The results show the following:

(1) The structure of the borophene is distorted after impurity doping, but the structure of the doped system is stable.

(2) The α-sheet borophene is an indirect band gap semiconductor with 1.396 eV. After Al and Ga doping, the position of the top of the valence band remains unchanged, and the position of the bottom of the conduction band moves up slightly, which makes the band gap of the doped system wider, and the band gap values are 1.437 eV and 1.422 eV, respectively.

(3) In the vicinity of the Fermi level, a small number of Al 3p-state electrons and Ga 4p-state electrons and a large number of B 2p-state electrons have orbital hybridization, the band gap of borophene changes, and the peak value of the electron density of states reduces after doping.

(4) Mulliken population analysis shows that the B_0-B bond is mainly covalent bond, but there is also a small amount of ionic bond. However, when the impurity X is doped, the charge transfer between X and B atoms increases significantly, and the population of the corresponding X-B bonds decreases from 0.54 to 0.08 (Al), 0.28 (Ga), indicating that the covalent bonding strength of the chemical bonds in the doped system is weakened, and the chemical bonds have significant directionality.

(5) The calculation of optical properties shows the following: the increase from 2.60 to 3.21 (Al) and 3.57 (Ga) in static dielectric constant and the appearance of new dielectric peaks indicate that Al and Ga doping can enhance the ability of borophene to store electromagnetic energy. The reflectivity of the borophene material can reach more than 50%, and the static refractive index $n_0 = 1.61$. After doping, the peak of reflectivity decreases to 45% and the static refractive index n_0 increases from 1.61 to 1.79 (Al) and 1.89 (Ga). At the same time, it fills the gap of red light and infrared absorption by the doped borophene system. The research results provide a basis for the development of borophene materials in the field of infrared detection devices. The light loss is limited to a narrow energy range around 3.64 eV for the doped borophene system, indicating that the introduction of Al and Ga does not affect the use of borophene materials as light storage materials.

The above results indicate that doping can modulate the photoelectric properties of α-sheet borophene materials.

Data Availability

The data used to support the findings of this study are included within the article.

Conflicts of Interest

The authors declare that there are no conflicts of interest.

Acknowledgments

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