

Research Article

Effect of Co-Doping on the Photoelectric Properties of the Novel Two-Dimensional Material Borophene

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Borophene is a novel two-dimensional material with abundant crystal structure and photoelectric properties. We focus on the effect of co-doping on the electronic structure and optical properties of borophene using the first-principles method. The results show that the structure of Al and Ga co-doped borophene is obviously distorted because Al and Ga atoms have formed bonds with a bond length of 2.378 Å, and the two B atoms that bond together with Al and Ga are no longer formed bonds. However, it is also a two-dimensional planar structure after co-doping. After co-doping, the band gap width of the borophene system is narrowed from 1.409 eV to 1.376 eV, and the band gap is narrowed by 0.033 eV. Mulliken population analysis shows an obvious charge transfer between Al-B and Ga-B atoms in the co-doped borophene. The calculation of optical properties shows that the static dielectric constant ε_1 (0) increases from 5.08 to 7.01, and $\varepsilon_2(\omega)$ is larger than that of the undoped sample in the low-energy range. Thus, the co-doping of Al and Ga can enhance the electromagnetic energy storage capacity and the visible light absorption ability. Although the reflectance of borophene is reduced by codoping (the peak of the reflectivity can be decreased from 71% to 61% at E = 2.94 eV), it still presents metallic reflection characteristics. The static refractive index n_0 can be increased from 2.25 to 2.65 by co-doping. The extinction coefficient shows strong band edge absorption at the low-energy range with an absorption edge of 0.85 eV. The light loss is limited to a very narrow energy range of approximately 7.30 eV, which indicates that borophene co-doped with Al and Ga can also be used as a light storage material. The optical conductivity reaches its maximum at E = 1.78 eV and 2.52 eV, which correspond to the light irradiation with a wavelength of 698 nm (red light) and 492 nm (cyan light), respectively. The results show that the Al-Ga co-doped borophene is sensitive to cyan light and red light, so it can be used to make photosensitive devices. The results can hopefully fill the gap in the application of borophene in semiconductor photoelectric devices and provide a theoretical basis for its application.

1. Introduction

In 2004, the two-dimensional crystal material graphene was separated from graphite [1, 2]. Due to its chemical stability, good thermal conductivity, unique electrical characteristics, and good application prospect, it has attracted extensive attention from the science community and industry [3–5]. In the following years, silicene, germanene, stannene, and black phosphorene and heterostructures have received significant attention [6–9], but these two-dimensional materials easily oxidize in air and cannot stably exist, so it is difficult to apply them in electronic devices. Thus, researchers are looking for other graphene-like two-dimensional materials.

Surprisingly, boron element, which is adjacent to carbon in the periodic table and is located between metals and nonmetals, has the dual properties of metals and nonmetals, carbon-like sp² hybridized orbitals, short covalent bonds, and diversified valence states, which are beneficial to the formation of a low-dimensional allotrope of boron, such as boron nanotubes, cage structures, and plane structures. The possibility of the existence of these low-dimensional structures of boron has been a topic of intense interest to theoretical researchers. However, due to the high melting point and low vapor pressure of boron, the effective thermal evaporation temperature exceeds 2000°C, and direct thermal evaporation is very difficult. Therefore, there has been no substantial progress in the preparation of low-dimensional boron structures.

In 2015, Feng et al. [10, 11] and Mannix et al. [12] independently successfully prepared borophene, which is a two-dimensional structure of boron. They, respectively, used the molecular beam epitaxy method in an ultra-high vacuum environment to grow a two-dimensional structure of boron on the single-crystal Ag (111) substrate and obtained two types of borophene films with different structures (β_{12} phase and χ_3 phase).

Subsequently, the research on borophene has attracted extensive attention of scientific researchers. Tai et al. [13] prepared the γ -B₂₈ phase of borophene using the chemical vapor deposition method. Shi et al. [14] used molecular dynamics simulation to calculate the properties of borophene as an anode material for batteries and found that borophene had great development potential in the field of anode material application for lithium ion and sodium ion batteries. Mortazavi et al. [15] and Wang et al. [16] studied the performance of borophene in lithium storage and hydrogen storage, respectively. Compared with graphene and other two-dimensional materials, they found that borophene had more advantages in lithium ion batteries, and the hydrogen storage effect of Ca-modified borophene can reach 12.68 wt%. Gao et al. [17] and Penev et al. [18] found that β_{12} phase and χ_3 phase of borophene might exhibit obvious superconducting properties. Li et al. [19] calculated the adsorption of volatile organic compounds on borophene using density functional theory. The study found that χ_3 phase and β_{12} phase borophene could adsorb ethylene and formaldehyde, form chemical bonds, and release a large amount of energy. Lin et al. [20] analyzed the magnetic properties of χ_3 phase of borophene with vacancy defects using first-principles and concluded that only the special structures with single- and double-vacancy defects had magnetic properties. Lu et al. [21] used the Tkatchenko-Scheffler method to study the hydrogen storage performance of the Li-shrouded honeycomb borophene oxide nanosheet (h-B₃O) and showed that Li-shrouded h-B₃O is a promising reversible hydrogen storage material. Kharwar et al. [22] studied the effects of hydrogen and fluorine atomic passivation on the electronic and transport properties of zigzag borophene nanoribbons (BNRs) using the nonequilibrium Green's function technique. Akay and Maiti [23] reported the tunable electronic properties of β -borophene on a polar substrate (ZrO₂) due to an external magnetic field and optical phonons.

It is well known that the study of the electronic structure and optical properties of low-dimensional structure semiconductors is a rapidly developing research area, not only because of its high potential for device applications but also from the perspective of fundamental research [24–30]. However, there are few reports on the optical properties of borophene semiconductors. To have a broad application in the preparation of new nano-photoelectric devices, it is necessary and significant to conduct theoretical research on the photoelectric property regulation of the novel twodimensional semiconductor material borophene. Codoping can modulate the electronic structure and optical properties of the material [31, 32]. Therefore, the specific purpose of this study is to modify the electronic structure and optical properties of borophene by co-doping aluminum (Al) and gallium (Ga). Using the first-principles pseudopotential plane wave method, we calculate and analyze the geometric structure, electronic structure, and optical properties of borophene before and after co-doping. The novelty of this study is that the research results can hopefully fill the gap in the application of borophene in semiconductor photoelectric devices and provide a theoretical basis for its application.

2. Calculation Model and Method

2.1. Calculation Model. The model used for the calculation is α -sheet borophene, which is a single layer of boron with a planar structure composed of a mixture of triangular lattices and hexagonal holes. The characteristic is that all boron atoms are in the same plane. The lattice constants are a = 0.5050 nm, b = 0.5050 nm, and c = 3 nm [33]. The borophene model is a $3 \times 2 \times 1$ supercell that contains 48 boron (B) atoms, as shown in Figure 1(a). According to the symmetry analysis, three models of Al and Ga co-doped borophene are listed: Al-Ga codoped I, Al-Ga co-doped II, and Al-Ga co-doped III, as shown in Figures 1(b)–1(d). In Al-Ga co-doped I, Al and Ga replace two B atoms on the mid-vertical line of the center line of the two hexagonal holes, as shown in Figure 1(b). In Al-Ga codoped II, Al and Ga are located on the two vertices of a large triangle that contains a hexagonal hole, as shown in Figure 1(c). In Al-Ga co-doped III, Al and Ga are located on two vertices of a large parallelogram containing hexagonal holes, as shown in Figure 1(d).

2.2. Calculation Method. Calculations were performed using the first-principles method based on the density functional theory. The geometric structure, energy, band structure, Mulliken population analysis, and optical properties of Al and Ga co-doped two-dimensional material borophene were obtained using the CASTEP software package [34]. The ultra-soft pseudo-potential (USPP) [35] was used to handle the interaction between ionic cores and electrons, and the Perdew-Burke-Ernzerhof (PBE) functional [36] of the generalized gradient approximation (GGA) was used to handle the exchange-correlation energy between electrons. We set the plane wave truncation energy to 240 eV and the energy convergence accuracy to $1.0 \times 10^{-6} \text{ eV/atom}$. We selected B 2s²2p¹, Al 3s²3p¹, and Ga 3d¹⁰4s²4p¹ as valence electrons, and other orbital electrons were the core electrons for the calculation. The K-point path was set as Γ (0, 0, $0) \longrightarrow K (-0.333, 0.667, 0) \longrightarrow F (0, 0.5, 0) \longrightarrow \Gamma (0, 0, 0).$ The $6 \times 6 \times 1$ Monkhorst and Pack [37] symmetric special Kpoint method was adopted for the Brillouin region integration, and the FFT grid parameter was set to $72 \times 48 \times 135$. Since the band gap calculated by GGA is relatively low and Wu et al. [33] calculated the band gap of α -sheet borophene using hybrid PBE0 to be 1.40 eV, we set the Scissors to correct the electronic structure and optical properties, and Scissors = 1.37 eV.



FIGURE 1: Model of borophene: (a) undoped; (b-d) Al-Ga co-doped.

In order to ensure the stability of the co-doped structure, we have calculated the binding energy of the co-doped system. The binding energy E_b [38] can be calculated as follows:

$$E_b = \frac{\left[E_T - n_B E(P) - E(AI) - E(Ga)\right]}{n},$$
 (1)

where E_T is the total energy of the doping system, n_B is the number of B atoms in the system, E (B) is the total energy of a single isolated B atom, E (Al) is the total energy of a single isolated doped atom Al, E (Ga) is the total energy of a single isolated doped atom Ga, and 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 the novel two-dimensional material borophene co-doped with Al and Ga. D_{X-B} (X = Al,

Ga) is the average bond length between atom X and the surrounding B atom, D_{B-B} is the average bond length between a B atom and a surrounding B atom, and E_b is the binding energy of the system.

In Table 1, after the C-axis was fixed and the structure was optimized, the errors of lattice constants *a* and *b* between the calculation model and Wu et al. [33] did not exceed 0.2% and 0.4%, respectively. The average value of $D_{\rm B}_{\rm B}$ in the calculation model is 0.1693 nm, and the error is less than 1.4% compared with Yang et al. [39] (0.167 nm). Thus, the calculation model adopted in this paper is reliable.

Figure 1 shows that the novel two-dimensional material borophene has a two-dimensional planar structure, but the structure is distorted after the Al and Ga co-doping. In Table 1, the bond length D_{X-B} significantly changes because the atomic covalent radius of the replaced atom varies. For example, the covalent radii of B, Al, and Ga are 0.084 nm, 0.121 nm, and 0.122 nm, respectively. Since the impurity atom X has a larger covalent radius than B, the bond length

TABLE 1: Structural parameters and binding energy of borophene.

Sample	a (Å)	b (Å)	$D_{\mathrm{Al-B}}$ (Å)	$D_{\text{Ga-B}}$ (Å)	$D_{\mathrm{B-B}}$ (Å)	E_b (eV)
Borophene (reference [33])	5.050	5.050	_	_	1.670	_
Borophene	5.060	5.070	_	_	1.693	-5.267
Al-Ga co-doped I	5.207	5.155	2.024	2.039	1.707	-6.060
Al-Ga co-doped II	5.193	5.191	1.889	1.902	1.713	-5.994
Al-Ga co-doped III	5.194	5.187	1.896	1.914	1.707	-6.000

 D_{X-B} is larger than D_{B-B} without doping. Compared with Al-Ga co-doped II and Al-Ga co-doped III, in Al-Ga co-doped I, Al and Ga atoms have formed bonds with a bond length of 2.378 Å, and the two B atoms (such as B1 and B6) that bond together with Al and Ga no longer form bonds, so the hexagonal holes in the model almost become pentagonal holes, as shown in Figure 1(b). Through the calculation of the distance between Al and Ga and analysis of the bonding situation after co-doping, combined with Figure 1 and Table 1, it can be seen that Al-Ga co-doped I has the most obvious distortion.

According to the binding energy of the borophene system in Table 1, after the Al and Ga co-doping, the binding energy E_b of the systems is negative and lower than that of the undoped system, which indicates that the structures of the three co-doped systems are stable, and Al-Ga co-doped I has the lowest binding energy among the three co-doped systems. Therefore, the following calculation and analysis of various properties of Al and Ga co-doped borophene system are based on Al-Ga co-doped I.

3.2. Band Structure. Figure 2 shows the band structure of the novel two-dimensional material borophene co-doped with Al and Ga.

Figure 2(a) shows that borophene is an indirect bandgap semiconductor, the valence band top was obtained at a point between Γ and K, the conduction band bottom was obtained at a point between F and Γ , and the band gap Eg is 1.409 eV, which is consistent with the calculated value of 1.40 eV by Wu et al. [33]. Thus, the calculation method and accuracy in this paper are reliable. The co-doping of Al and Ga affects the band structure of borophene. In Figure 2(b), after co-doping, the position of the top of the valence has remained the same, but the bottom of the conduction band has moved down by 0.033 eV, which resulted in a narrower indirect band gap: Eg = 1.376 eV. Due to the defects introduced by impurities, such as the increase of cell size of borophene (such as a and b in Table 1), some band tail states are formed near the bottom of the conduction band. The appearance of the band tail states causes the band gap to shrink. Thus, borophene codoped with Al and Ga can be used to prepare new nanophotoelectric devices.

3.3. Mulliken Population Analysis. Table 2 shows the Mulliken population analysis of B atoms around the co-doped atoms.

Table 2 shows that the charge transfer between B-B atoms in the borophene system is only 0.01 e without doping, which indicates that the B-B bond is mainly

covalent. When Al and Ga were co-doped, the charge transfer between Al-B and Ga-B atoms significantly increased, which indicates that the ionic property of Al-B and Ga-B bond was enhanced, the covalent strength weakened, and the chemical bond exhibited a certain directionality. Table 3 shows the properties of chemical bonds in the borophene co-doped system in the population analysis.

In Table 3, after Al and Ga had been co-doped, the corresponding population of Al-B and Ga-B bonds was lower than that of B-B bonds without doping, which is 0.54. The decrease in population indicates that the ionic bond strength of chemical bond increases and the covalent bond strength weakens in the co-doped system. The population of Al-Ga band was 0.39, which indicates that Al and Ga atoms formed bonds, as shown in Figure 1(b). This Mulliken population analysis shows that the introduction of two impurities can diversify the properties of chemical bonds between atoms in the borophene co-doped system.

3.4. Optical Properties. To explore the effect of co-doping on the optical properties of borophene, we further calculated the optical properties. According to the optical properties of a semiconductor, the dielectric function, which acts as a bridge between the micro-physical process of the interband transition and the electronic structure, can reflect the band structure and other spectral information. In the linear response range, the complex dielectric function is given by

$$\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega), \tag{2}$$

where $\varepsilon_1(\omega)$ is the real part of the complex dielectric function and $\varepsilon_2(\omega)$ is the imaginary part of the complex dielectric function. According to Kramers–Kronig dispersion relationships and the definition of the direct transition probability, the real part $\varepsilon_1(\omega)$, imaginary part $\varepsilon_2(\omega)$, absorption coefficient, reflection coefficient, refractive index, extinction coefficient, loss function, and photoconductivity can be derived [40].

3.4.1. Complex Dielectric Function. Figure 3 shows the curves of the real part $\varepsilon_1(\omega)$ and imaginary part $\varepsilon_2(\omega)$ of the dielectric function $\varepsilon(\omega)$ as functions of energy.

Figure 3(a) shows that the static dielectric constant ε_1 (0) of borophene increased from 5.08 to 7.01 after the Al and Ga co-doping. ε_1 (ω) had the dielectric peak at E = 1.42 eV, which is blue-shifted, and the peak increased compared with the undoped case. This peak is mainly contributed by the inter-band transition of B 2p and a small amount of Al 3p and Ga 4p state electrons. The blue shift of the peak is due to



FIGURE 2: Band structure of borophene. (a) Undoped. (b) Al-Ga co-doped.

TABLE 2: Mulliken population analysis of B atoms around the co-doped atoms.

Sample	Atom	\$	p	d	Total	Charge/e
Borophene	В	0.63	2.38	0	3.01	-0.01
	В	0.69	2.31	0	2.99	0.01
Al-Ga co-doped	Al	0.30	0.55	0	0.85	2.15
	B1	0.94	2.40	0	3.35	-0.35
	B2	0.83	2.69	0	3.52	-0.52
	B3	0.87	2.44	0	3.30	-0.30
	B4	0.87	2.46	0	3.33	-0.33
	B5	0.83	2.70	0	3.53	-0.53
	B6	0.94	2.40	0	3.34	-0.34
	Ga	0.55	0.88	9.98	11.41	1.59
	B1	0.94	2.40	0	3.35	-0.35
	B6	0.94	2.40	0	3.34	-0.34
	B7	0.78	2.60	0	3.38	-0.38
	B8	0.82	2.36	0	3.18	-0.18
	B9	0.82	2.39	0	3.21	-0.21
	B10	0.78	2.60	0	3.38	-0.38

the narrowing of the optical absorption end. When E < 1.64 eV, the borophene co-doped with Al and Ga had a larger $\varepsilon_1(\omega)$ than undoped borophene, which indicates that the ability of borophene to store electromagnetic energy is enhanced after co-doping.

The imaginary part $\varepsilon_2(\omega)$ describes that as light propagates through the material, part of the energy will be absorbed by the material and converted into other forms of energy. Figure 3(b) shows that although the peak of $\varepsilon_2(\omega)$ decreased, when E < 2.08 eV, borophene co-doped with Al and Ga had a larger $\varepsilon_2(\omega)$ than undoped borophene, which indicates that the visible light absorption ability of

TABLE 3: Mulliken population analysis of the bands around the co-doped atoms.

Sample	Band	Population
Borophene	B-B	0.54
	Al-B1	0.24
	Al-B2	0.01
	Al-B3	0.17
	Al-B4	0.17
	Al-B5	0.02
	Al-B6	0.24
Al-Ga co-doped	Ga-B1	0.34
	Ga-B6	0.34
	Ga-B7	0.06
	Ga-B8	0.25
	Ga-B9	0.25
	Ga-B10	0.06
	Al-Ga	0.39

borophene is enhanced after co-doping. Thus, co-doping can modulate the dielectric properties of borophene materials.

3.4.2. Absorption Coefficient and Reflection Coefficient. Figure 4 shows the absorption coefficient of the novel twodimensional material borophene co-doped with Al and Ga. When E < 2.08 eV, the absorption of visible light by codoped borophene was significantly enhanced, since additional Al 3p and Ga 4p state electrons were introduced near the Fermi level. Simultaneously, the peak value of absorption decreased, and the optical absorption end of borophene moved toward the lower energy direction, which is consistent with the imaginary part ε_2 (ω) in Section 3.4.1.



FIGURE 3: Dielectric function of Al-Ga co-doped borophene. (a) $\varepsilon_1(\omega)$. (b) $\varepsilon_2(\omega)$.





Figure 5 shows the reflection coefficient. The peak of the reflectivity could decrease from 71% to 61% at E = 2.94 eV, which corresponds to violet light with a wavelength of 420 nm. Although the reflectance of borophene is reduced by co-doping, it continues to exhibit metallic reflection characteristics. The reason is that in Figure 3(a), when 2.40 eV < E < 7.08 eV, then ε_1 (ω) < 0, which indicates that light cannot propagate in borophene, so it exhibits metallic reflection characteristics.

3.4.3. Refractive Index and Extinction Coefficient. The refractive index and extinction coefficient are physical quantities that characterize the optical properties of materials. Figure 6 shows that the static refractive index n_0 can be increased from 2.25 to 2.65 by co-doping. It has potential application prospects for optical devices with certain requirements of the refractive index. When E < 1.47 eV, the refractive index n increased with the increase in incident photon frequency, which shows normal dispersion. When 1.47 eV < E < 3.14 eV, the refractive index *n* decreased with the increase in incident photon frequency, which shows anomalous dispersion.

The extinction coefficient represents the absorption capacity of the material. In Figure 7, the extinction coefficient shows strong band edge absorption at the low-energy range: the absorption edge is 0.85 eV, which corresponds to the transition of electrons at the bottom of the conduction band. Meanwhile, a comparison of Figures 6 and 7 shows that for 2.40 eV < E < 7.08 eV, k > n, which indicates that light cannot propagate in borophene in this energy range. This finding is consistent with the results of the previous discussion of the reflection coefficient.

3.4.4. Loss Function and Optical Conductivity. Figure 8 shows the loss function. The peak of the loss function significantly increased after co-doping. Moreover, the light loss was limited to a very narrow energy range of approximately













7.30 eV, which indicates that borophene co-doped with Al and Ga can also be used as a light storage material.

The optical conductivity of a semiconductor refers to the change in its conductivity upon light irradiation. Figure 9 shows the real part of the optical conductivity. Compared to undoped borophene, the peak of the optical conductivity significantly decreased for doped borophene. The optical conductivity reached its maximum at E = 1.78 eV and 2.52 eV, which correspond to the irradiation with wavelengths of 698 nm (red light) and 492 nm (cyan light), respectively. The results show that Al-Ga co-doped borophene is sensitive to cyan light and red light, so it can be used to make photosensitive devices.

4. Conclusions

The first-principles method based on density functional theory is used to analyze the geometric structure, band structure, Mulliken population, and optical properties of the novel two-dimensional material borophene co-doped with Al and Ga. After the structure optimization, the errors of the lattice constants a and b between the calculated and theoretical values are less than 0.2% and 0.4%, respectively. After co-doping, the structure of borophene was clearly distorted, since Al and Ga atoms formed bonds with a bond length of 2.378 Å, and the two B atoms (such as B1 and B6) that bonded together with Al and Ga no longer formed bonds.

The band gap width narrowed after co-doping, and the band gap was Eg = 1.376 eV, which decreased by 0.033 eV. Mulliken population analysis shows that an obvious charge transfer occurred between Al-B and Ga-B atoms, and the decrease in population number indicates that the ionic bond strength of chemical bond increases and the covalent bond strength weakens in the co-doped system. The analysis of optical properties shows that the co-doping of Al and Ga can enhance the electromagnetic energy storage capacity and visible light absorption ability. Simultaneously, the peak absorption value decreased, and the optical absorption end of borophene moved toward the lower energy direction, which is consistent with the imaginary part $\varepsilon_2(\omega)$. Although the reflectance of borophene is reduced by co-doping, e.g., the reflectivity peak decreased from 71% to 61% at E = 2.94 eV, it continues to exhibit metallic reflection characteristics. The static refractive index n_0 can be increased from 2.25 to 2.65 by co-doping. This mechanism has potential application prospects for optical devices with certain requirements of the refractive index. The extinction coefficient showed a strong band edge absorption in the lowenergy range, with an absorption edge of 0.85 eV. The light loss was also limited to a very narrow energy range of approximately 7.30 eV, which indicates that borophene codoped with Al and Ga can also be used as a light storage material. The optical conductivity reaches its maximum at E = 1.78 eV and 2.52 eV, which corresponds to irradiation with wavelengths of 698 nm (red light) and 492 nm (cyan light), respectively. The results show that the Al-Ga codoped borophene is sensitive to cyan light and red light, so it can be used to make photosensitive devices. These results indicate that the electronic structure and optical properties of the novel two-dimensional material borophene can be modulated by Al and Ga co-doping according to actual requirements.

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 regarding the publication of this article.

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