First-principles study of strain on BN-doped arsenene

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Received: 21 March 2022 / Accepted: 7 June 2022 / Published online: 17 June 2022
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Abstract
The effects of B, N, and BN doping of arsenene and different strains on the stability, electronic structure, and optical properties of BN-doped arsenene were investigated using a first-principles approach. It was found that B, N, and BN doping caused the bandgap of arsenene to shift from indirect-direct, and strong charge transfer occurred between arsenene and B, N, and BN, and the transfer between N atoms and arsenene was more intense. The binding energy of the BN-doped arsenene system is always negative at different strains and in a stable state, but the stability of the structure is gradually decreasing. The bandgap of the BN-doped arsenene system shows a trend of decreasing, then increasing, and then decreasing under different tensile and compressive deformations. The only difference is that the tensile deformation continues to increase the bandgap at 2%, while the compressive deformation decreases the bandgap. The p-state electrons of the As atom near the Fermi energy level make the main contribution to the BN-doped arsenene system, and the p-state electrons of the B atom have some contribution. Red shifting occurs at the absorption and reflection peaks for doped systems with tensile deformation of 1% to 5%, and the absorption and reflection peaks for doped systems with compressive deformation of −1% to −5%.

Keywords First principles · Electronic structure · Optical properties · BN-doped arsenene

Introduction
During the discovery of graphene in 2004 [1], two-dimensional materials (black phosphorene [2], silicene [3], germanene [4], boronene [5], arsenene [6], antimonene [7], molybdenum disulfide [8], etc.) have been developed rapidly. These two-dimensional materials have excellent properties for applications in electronics, magnetism, catalysis, and energy storage [9–17]. Since graphene, silicene, and germanene have zero bandgaps near the Fermi energy level, this greatly limits their application in electronic devices [18–20]. In 2015, Zhang et al. [21] predicted the novel two-dimensional crystalline materials arsenene and antimonene; the two-dimensional materials derived from the fifth main group elements (P, As, Sb, Bi) layered materials have greatly attracted the interest of scientists.

Arsenene is a two-dimensional VA group semiconductor material with a honeycomb structure with low thermal conductivity and similar properties to phosphorene, so the study of arsenene properties has been widely concerned by scientists in recent years [22–24]. Arsenene has a relatively wide bandgap and has high carrier mobility, structural stability, and thermodynamic stability, but its indirect bandgap makes it less desirable for practical device applications. Researchers have extensively studied arsenene through doping, stress, electric field, and adsorption and found that these factors have a modulating effect on the optoelectronic properties of arsenene, which has greatly contributed to its development in the field of optoelectronics [25–29]. Strain can effectively transform the arsenene system from indirect bandgap to direct bandgap. Xu et al. [30] studied the electronic structure and optical properties of arsenene under uniaxial strain and found that by inducing uniaxial tensile strain along with the armchair and sawtooth directions, monolayer arsenene transformed from an indirect bandgap semiconductor to a direct bandgap semiconductor, and a significant red shift was observed with an increasing strain. Cao et al. [31] studied the electronic properties of monolayer and bilayer arsenenes under
planar biaxial strain, where the band gaps of monolayer and bilayer arsenen es initially increased and then rapidly decreased under compression strain. Furthermore, monolayer arsenenes exhibited an indirect to direct bandgap transition when the compression strain reached −10%. However, at tensile strain, the bandgap of monolayer arsenene monotonically decreases with strain, while the bandgap of bilayer arsenene rapidly decreases to zero at small tensile strains. Zhang et al. [32] explored the effect of tensile strain on the magnetic properties of defective arsenic monolayers with single and double vacancies and found that unstrained defective arsenic monolayers are both inherently nonmagnetic. However, appropriate tensile strains induce ferromagnetic coupling in the single-vacancy (8%) and double-vacancy doped (7%) systems, respectively. Liu et al. [33] investigated the structural and electronic properties of substitution-doped arsenene and found that B and N doping can convert arsenene from an indirect bandgap to a direct bandgap. The N–N and B–B bonds have weaker binding energies and are more easily doped into the arsenene system than the As-B and As-N bonds. It was found that B and N doping into carbon nanotubes has a significant effect on their electronic structure. Fan et al. [34] performed torsional deformation of BN-doped graphene and found that doping has a strong modulating effect on the electronic properties of graphene. Chen et al. [35] studied the adsorption of CO gas by B and BN-doped black phosphorus and found that the application of 7% compressive strain could promote CO coupling and thus the reduction of CO dimer to CH2CH2. It can be speculated that BN co-doping also has a large effect on the properties of the arsenene system.

Most of the current studies on B- and N-doped arsenenes are based on electronic properties, and no studies on B- and N-doped arsenenes have been reported in terms of charge as well as optical properties. Therefore, we have studied B, N, and BN-doped arsenenes and the effect of strain on the stability, electronic structure, and optical properties (including absorption coefficient and reflectivity) of BN-doped arsenenes, and this study will guide the application of arsenenes in electronic devices.

Models and methods

All calculations in this paper were performed with the CASTEP [36] package based on density generalized function theory. K-point lattices and cutoff energies were set to $6 \times 6 \times 1$ and 400 eV for B, N, and BN-doped arsenene, respectively, and structural optimization was performed using the Broyden-Fletcher-Goldfarb-Shanno (BFGS) algorithm and the GGA-PBE [37] generalized function. The four parameters of the optimization, such as the maximum interatomic interaction force, the maximum atomic displacement convergence criterion, the minimum force acting on each atom, and the self-consistency accuracy, were set to 0.03 eV/Å, 0.001 Å, 0.05 GPa, and $2.0 \times 10^{-6}$ eV, respectively. A vacuum layer with a thickness of 20 Å was set [38] to avoid the effect of interlayer interaction forces.

In this paper, a $3 \times 3 \times 1$ supercell arsenene with a total of 18 atoms is used to calculate its properties. Figure 1a and b show the top and side views of the intrinsic arsenene. The deformation variables of arsenene under tensile and compressive deformation are denoted by $\varepsilon$, which we define as $\varepsilon = (m - m_0) / m_0$, where $m$ and $m_0$ represent the lattice constants of arsenene and the lattice constants of intrinsic arsenene after tensile/compression, respectively, and $\varepsilon$ is the percentage of the difference between the lattice constants of arsenene before and after deformation and the lattice constants of intrinsic arsenene. The deformation applied to the monolayer arsenene is shown in Fig. 2, where blue represents uniaxial tensile deformation and red represents uniaxial...
compressive deformation, and the coordinates of some atoms are fixed to ensure the stability of the structure. The value of Poisson’s ratio for monolayer arsenene is 0.25 [39]. We have performed calculations for BN-doped arsenene systems with and without Poisson’s ratio at different strains and found that the addition of Poisson’s ratio does not have a significant effect on the performance of the doped system. Therefore, the effect of Poisson’s ratio on the doped system is not discussed in this paper. The values of formation energy and binding energy play a decisive role in the stability of the doped system, and their values can be calculated by the following equations

\[ E_f = E_{\text{As}+X} - E_{\text{pure}} + mE_{\text{As}} - E_X \]  
\[ E_b = \frac{(E_{\text{As}+x} - nE_{\text{As}} - mE_X)}{N} \]

\( E_f \) is the formation energy, \( E_{\text{As}+X} \) is the total doping energy of the arsenene system, \( E_{\text{pure}} \) is the total energy of the intrinsic arsenene, \( E_{\text{As}} \) is the chemical potential of the arsenic atoms, and \( E_X \) is the chemical potential of the dopant atoms (\( X = \text{B, N, and BN} \)). \( E_b \) is the binding energy, \( n \) and \( m \) are the numbers of arsenic atoms and impurity atoms in the monolayer arsenene, and \( N \) is the total number of atoms in the system.

Results and discussion

Stability and energy band structure of different doping systems

The optimization process used the BFGS algorithm to optimize the 3 × 3 × 1 supercell arsenene structure. After geometry optimization, the lattice constant \( (a = b = 3.59 \text{ Å}) \), As-As bond length \( (d = 2.50 \text{ Å}) \), and fold height \( (h = 1.38 \text{ Å}) \) were obtained, which are not much different from the results of previous studies [33, 40, 41]. Figure 3 shows the top and side views of the optimized B- and N-doped arsenenes. As shown in Table 1, the As-B bond length after B doping optimization is 2.04 Å and the As-As bond length is 2.48 Å. The As-N bond length after N doping optimization is 1.98 Å, and the As-As bond length is 2.52 Å, which is consistent with the bond length obtained from the literature [33]. Compared with the intrinsic arsenene, the lattice constants of B, N, and BN doping all decrease, and the As-As bond lengths of B and BN doping decrease, while the As-As bond lengths of N doping increase. Internal distortion and inward relaxation of B and N atoms can be observed in the arsenene layer, and the degree of B-atom distortion is more pronounced.

### Table 1

| Doping type | \( a = b \) (Å) | As-As (Å) | As-X (Å) | \( E_f \) (eV) | \( E_b \) (eV) | Charge (e) | As (e) Maximum | As (e) Minimum |
|-------------|----------------|-----------|----------|----------------|----------------|------------|----------------|---------------|
| Pure        | 3.59           | 2.50      | -        | -              | -4.76          | 0          | 0              | 0             |
| B           | 3.55           | 2.48      | 2.04     | -0.60          | -4.79          | -0.42      | 0.13           | -0.06         |
| N           | 3.51           | 2.52      | 1.98     | -1.90          | -4.86          | -0.84      | 0.29           | -0.01         |
| BN          | 3.46           | 2.49      | 2.00(As-N)| -3.92          | -4.97          | 0.03 (B)   | 0.34           | -0.04         |

Fig. 3 Optimized models: a, c top and side views of B-doped arsenene; b, d top and side views of N-doped arsenene
compared to that of N atoms, which indicates a stronger interaction between B and As atoms.

Since the arsenene monolayer is a diagonal hexagonal structure, we considered six possible BN co-doped conformations, as shown in Fig. 4(a), with the doping positions of N(B) atoms denoted by P and B(N) atoms denoted by P1-P3, and carried out sufficient relaxation for these six BN-doped arsenene systems. Figure 4b and c show the top and side views of the most stable conformation after optimization. It can be seen that the same distortion occurs inside the arsenene layer after BN co-doping, which makes the N atoms relax inward and the B atoms relax outward. Table 1 shows the formation and binding energies of B, N, and BN doping. It can be seen that the formation and binding energies obtained for all three doped arsenene systems are negative, indicating that all three doped structures are stable, with the BN co-doping having the smallest formation and binding energies and the most stable structure obtained.

Table 1 shows the charge transfer between arsenene and B and N atoms in the different doped structures. Negative values indicate electron gain and positive values indicate electron loss. There is no charge transfer in intrinsic arsenene, and the charge transfer becomes drastic after doping. Combining Table 1 and Fig. 6, it can be concluded that when the B atom is doped 0.42e electrons

![BN co-doping model](image)

**Fig. 4** BN co-doping model: a N atoms are represented by P and B atoms are represented by P1–P3; b top view of BN co-doping; c side view of BN co-doping

![Energy band structures](image)

**Fig. 5** Energy band structures: a intrinsic arsenene; b B-doped arsenene; c N-doped arsenene; d BN co-doped arsenene

with a bandgap size of 1.587 eV, which is consistent with the previous results [41–43].

Figure 5b and c show the energy band structures of B- and N-doped arsenenes, and it can be found that the doping of B and N atoms leads to an indirect to direct bandgap transition in the arsenene system, which is consistent with the results obtained in the literature [33, 44]. Figure 5d shows the energy band diagram of the BN co-doped arsenene system, and it is found that the co-doping also enables the indirect-direct bandgap transition of the arsenene system and the co-doped structure is more stable, which also makes the application of arsenene in optoelectronic devices further developed.

We analyzed the charge transfer in these structures using Mulliken. Table 1 shows the charge transfer between arsenene and B and N atoms in the different doped structures. Negative values indicate electron gain and positive values indicate electron loss. There is no charge transfer in intrinsic arsenene, and the charge transfer becomes drastic after doping. Combining Table 1 and Fig. 6, it can be concluded that when the B atom is doped 0.42e electrons
Fig. 6 Charge transfer arsenene model: a B doping; b N doping; c BN co-doping

Table 2 Binding energy ($E_b$) and band gap values ($E_g$) of BN co-doped arsenene at different strains

| Strain | $E_b$ (eV) | $E_g$ (eV) |
|--------|------------|------------|
| −5%    | −4.886     | 0.644      |
| −4%    | −4.912     | 0.703      |
| −3%    | −4.938     | 0.662      |
| −2%    | −4.957     | 0.673      |
| −1%    | −4.970     | 0.680      |
| 0      | −4.975     | 0.694      |
| 1%     | −4.967     | 0.674      |
| 2%     | −4.945     | 0.681      |
| 3%     | −4.908     | 0.655      |
| 4%     | −4.845     | 0.711      |
| 5%     | −4.758     | 0.669      |

Fig. 7 a–e Energy band structure for tensile deformation of 1%, 2%, 3%, 4%, and 5%
are gained, and when the N atom is doped 0.84e electrons are gained, the charge transfer after N atom doping is more drastic compared to the B atom. When BN is co-doped, the B atom loses 0.03e electrons, and the N atom gains 0.78e electrons. Also, in the co-doped system, the charge transfer between the N atom and the arsenene is more drastic compared to the B atom.

Effect of tensile and compression deformation on the energy band structure of BN co-doped arsenene

To investigate the structural stability of BN-doped arsenene, the binding energy of the BN-doped arsenene system under tensile and compressive deformation was calculated from −5% to 5%. As shown in Table 2, the binding energy of the doped system is always negative at different strains and in a stable state, but the stability of the structure is gradually decreasing, and it can be found that the absolute value of the binding energy of compressive deformation is significantly larger than that of tensile deformation. This indicates that the compressive deformation is more stable compared with the tensile deformation.

The energy band structure of the BN-doped arsenene system at different tensile and compressive deformation is shown in Figs. 7 and 8, the bandgap values are listed in Table 2, and the changes of both band gaps are shown in Fig. 9. As shown in Fig. 7 and Table 2, the bandgap of the doped system changes more obviously with the increase of tensile deformation, which indicates that the tensile deformation

Fig. 8 a e Energy band structure for compression deformation of −1%, −2%, −3%, −4%, and −5%
deformation has a greater influence on the doped system. The bandgap reaches a maximum value of 0.711 eV at a tensile deformation of 4%. As shown in Fig. 8 and Table 2, the bandgap shows a trend of decreasing, then increasing, and then decreasing with increasing compressive deformation. The bandgap increases from 0.662 eV at −3% strain to 0.703 eV at −4% strain, reaching the bandgap maximum.

In general, the deformation does not lead to a transition from direct to indirect in the system within the range we studied. As shown in Fig. 9, there is almost a close trend for both tensile and compressive deformation, where the bandgap first decreases to 3% strain, then increases at 4%, and then decreases again at 5%. The only difference is that the tensile deformation continues to increase the bandgap.
at 2%, while the compressive deformation decreases the bandgap.

**Effect of tensile and compression deformation on the density of states of BN co-doped arsenene**

Figure 10a shows the density of states diagram of intrinsic arsenene, which is mainly contributed by the s-state and p-state electrons together. At the energy value of $-5$ to 4 eV, the total density of states is mainly contributed by the p-state electrons of As atom, and the s-state contribution is relatively small. The highest peak occurs at an energy value of $-0.4$ eV. At the Fermi energy level, the p-state electrons play a major role and the s-state electrons do not contribute. Figure 10b shows the density of states plot for the BN co-doped arsenene system. Compared with the intrinsic arsenene, the density of states at the Fermi energy level is mainly contributed by the p-state of the As atom, with some contribution from the p-state of the B atom, a very weak contribution from the p-state electrons of the N atom and the s-state electrons of the As atom, and essentially no contribution from the s-state electrons of the B and N atoms. The maximum peak of the density of states occurs at an energy value of $-0.97$ eV.

Figures 11a–e and 12a–e show the density of state plots under different tensile and compressive deformations. It can be found that the density of states under different tensile and compressive deformations does not change much the shape of the BN-doped arsenene system compared to the one without applied deformation. In the energy values of $-5.5$ to $-3.6$ eV, the p-state of the N atom makes the main contribution, the p-state electrons of As and B atoms also contribute to the region, and the s-state electrons of the B atom make a partial contribution to the region, and the s-state electrons of As and N atom contribute less. At energies of $-3.6$ to 0 eV, the p-state electrons of the As atom make the main contribution, and the p-state electrons of the B and N atoms also make some contribution to this region. In the energy range of 0–3.5 eV, the p-states of As and B atoms make the largest contribution to the total density of states, the p-state electrons of N atoms also make some contribution, the s-states of As atoms make a local contribution, and the s-states of N and B atoms make a small contribution. From the density of states analysis, it is concluded that the N atom is more strongly interacting with the As atom compared to the B atom, making the variation of the peak density of states more pronounced. Figures 11f and 12f show the variation of the total density of states for different tensile and compressive deformations. It can be seen that the maximum peak of the total density of states occurs at the energy value of $-1.03$ eV for strains of 1%, 3%, and 4% and at the energy values of $-0.99$ eV and $-1.05$ eV for strains of 2% and 5%, respectively. When the strain was $-1\%, -2\%, -3\%, -4\%$, and $-5\%$, the maximum density of states occurred at
energy values of $-0.98 \text{ eV}$, $-1.01 \text{ eV}$, $-0.96 \text{ eV}$, $-0.98 \text{ eV}$, and $-1.04 \text{ eV}$, respectively.

**Effect of tensile and compression deformation on the optical properties of BN co-doped arsenene**

Figure 13a and b show the absorption coefficients of the BN-doped arsenical system for different tensile and compressive deformations. From Fig. 13a, it can be seen that the doped systems have only one absorption peak at different tensile deformations. The absorption coefficients for all doped systems are 0.820, 0.697, 0.692, 0.771, 0.525, and 0.605 (cm$^{-1}$) in the order of doping concentration from 0 to 5% at an energy value of 0.01 eV. It can be found that the tensile deformation reduces the absorption of light by arsenene in different degrees, with the smallest absorption coefficient at

![Absorption coefficient and reflectance of BN-doped arsenene under different strains: a absorption coefficient under tensile deformation; b absorption coefficient under compressive deformation; c reflectance under tensile deformation; d reflectance under compressive deformation](image)

**Table 3** Energy and eigenvalues corresponding to the maximum absorption peak (reflection peak) of BN-doped arsenene system at different strains: $E_1$ ($E_2$) is the absorption (reflection) energy value at different strains, and A (R) is the maximum value at the absorption peak (reflection peak) at different strains

| Strain | $E_1$ (eV) | $E_2$ (eV) | $A$ (cm$^{-1}$) | $R$ |
|--------|------------|------------|----------------|-----|
| −5%    | 4.320      | 5.544      | 104219.35      | 0.418 |
| −4%    | 4.296      | 5.662      | 103232.73      | 0.417 |
| −3%    | 4.302      | 5.678      | 104583.26      | 0.419 |
| −2%    | 4.293      | 5.543      | 101956.92      | 0.407 |
| −1%    | 4.331      | 5.565      | 103280.31      | 0.413 |
| 0      | 4.291      | 5.523      | 103484.05      | 0.414 |
| 1%     | 4.302      | 5.568      | 99896.73       | 0.399 |
| 2%     | 4.294      | 5.579      | 99171.68       | 0.397 |
| 3%     | 4.301      | 5.538      | 97643.64       | 0.389 |
| 4%     | 4.293      | 5.531      | 99239.75       | 0.395 |
| 5%     | 4.292      | 5.525      | 95847.08       | 0.380 |

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4% strain and the largest absorption coefficient at 0%. From Fig. 13b, it can be obtained that the doped system has only one absorption peak at different compressive deformations. The absorption coefficients of the doped system at energy values of 0.01 eV are 0.820, 0.767, 1.163, 1.160, 0.819, and 1.419 (cm⁻¹) according to the doping concentration from 0 to −5% in that order. The strain of −2%, −3%, and −5% improved the absorption of light by arsenene. The absorption coefficient is the largest at a strain of −5% and the smallest at −1%. Combining Fig. 13a–b and Table 3, we can see that the doped system with a tensile (compressive) deformation of 0% (−3%) at the absorption peak absorbs the best, and the 5% (−2%) doped system absorbs the least. Compared with the 0% doping system, the doping system with 1% to 5% tensile deformation has a redshift at the absorption peak, and the doping system with −1% to −5% compressive deformation also has a redshift at the absorption peak. The redshift of the absorption peak may be due to the change in bandgap caused by the structural deformation due to the continuous tensile deformation.

Figure 13c and d show the reflectance of BN-doped arsenene systems under different tensile and compressive deformations. From Fig. 13c, it can be obtained that at 0.01 eV, all doped systems start to reflect light, and the reflectance is 0.106, 0.102, 0.101, 0.100, 0.097, and 0.094 according to the doping concentration from 0 to 5%. We find that the reflectance decreases gradually with the increase of tensile deformation. The tensile deformation decreases the reflectivity of the doped system, but the overall range of decrease is not large. From Fig. 13d, it can be obtained that all doped systems start to reflect light at 0.01 eV and the reflectance is 0.106, 0.107, 0.110, 0.113, 0.110 and 0.113 according to the doping concentration from 0 to −5% in order. It can be seen that the reflection of light by the doped system is promoted as the compressive deformation decreases. Combining Fig. 13c–d and Table 3, we can see that the doped system with a tensile (compressive) deformation of 0% (−3% and −5%) at the reflection peak reflects the best and the 5% (−2%) doped system reflects the least. Compared with the 0% doping system, the doping system with a tensile deformation of 1% to 5% has a redshift at the reflection peak, and the doping system with a compressive deformation of −1% to −5% also has a redshift at the reflection peak.

Conclusion

The effects of B, N, and BN-doped arsenenes and strain on the optoelectronic properties of BN-doped arsenene were investigated by the method based on the first principle of density generalized theory. The binding energy of the BN-doped arsenene system was always negative at different strains and in a stable state, but the stability of the structure was gradually decreased, and the structural stability of compressive deformation was always higher than that of tensile deformation. The energy band structure shows that the intrinsic arsenene is an indirect bandgap semiconductor and B, N, and BN doping are all able to convert the indirect bandgap to a direct bandgap, with a strong charge transfer between the arsenene and B, N, and BN and an even more intense transfer between the N atom and the arsenene. The tensile and compressive deformations almost all have a close trend, where the bandgap first decreases to 3% strain, then increases at 4%, and then decreases again at 5%. The only difference is that the tensile deformation continues to increase the bandgap at 2%, while the compressive deformation decreases the bandgap. At the Fermi energy level, the total density of states of the BN-doped arsenene system is dominated by the electronic action of the p-state of the As atom, with some contribution from the p-state of the B atom. From the optical properties, it can be seen that the doped system with tensile deformation of 1% to 5% is redshifted at the absorption and reflection peaks, and the doped system with compressive deformation of −1% to −5% is redshifted at the absorption and reflection peaks. The doping system with tensile deformation of 0% has the best effect on absorption and reflection, and the doping system with tensile deformation of 5% has the worst effect on absorption and reflection. The doped system with compression deformation of −3% and −5% has the best absorption and reflection effect, and the doped system with compression deformation of −2% has the worst absorption and reflection effect.

Author contribution Jianlin He: investigation, methodology, validation, writing-original draft, writing-review and editing. Guili Liu: software, data curation, formal analysis, funding acquisition, investigation, methodology, project administration, resources, software, supervision. Xinyue Li: writing-review and editing. Guoying Zhang: writing-review and editing.

Funding This work was supported by the National Natural Science Foundation of China (grant number 51371049), the Natural Science Foundation of Liaoning Province (grant number 20102173), the Educational Department of Liaoning Province (grant number LZGD2019003), and the Educational Department of Liaoning Province (grant number LJGD2019012).

Data availability Data sharing does not apply to this article as no datasets were generated or analyzed during the current study.

Code availability Code availability does not apply to this article as no codes were used during the current study.

Declarations

Conflict of interest The authors declare no competing interests.
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