Electronic structure and optical properties of B-, N-, and BN-doped black phosphorene using the first-principles

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Abstract
The structural stability, electronic structure, and optical properties of BN-doped black phosphorene systems at different concentrations were investigated using a density generalized theory approach based on the first principles. BN-doped black phosphorene was found to be more stable than B and N atom doping. With the increase of doping concentration, the stability of the structure gradually decreases, and the structure of the system with 25% doping concentration is the most stable. The intrinsic and N-doped black phosphorenes are direct bandgap semiconductors, and B and BN doping make the black phosphorene change from direct bandgap to the indirect bandgap. The total density of states is mainly contributed by the p-state electrons of the B and P atoms, and the N atoms have a role in the local density of states with little contribution to the overall one. The black phosphorene undergoes charge transfer between the B and N atoms. The amount of charge transfer increases with the increase of doping concentration. The BN-doped black phosphorene system is blue-shifted at the absorption and reflection peaks compared to the intrinsic black phosphorene system. From the dielectric constant, it is found that the doped system is shifted towards higher energy at the highest peak, leading to an increase in the intensity of the electric field generated by light, which is beneficial to increase the efficiency of photovoltaic power generation. The photoconductivity decreases and shifts toward higher energy after doping, with the most pronounced performance at BN doping concentrations of 12.5% and 25%.

Keywords First-principles · Electronic structure · Optical properties · Doping · Black phosphorene

Introduction
In 2004, Novoselov et al. [1] obtained two-dimensional graphene in the free state using a mechanical exfoliation method and prepared field-effect nanotubes on this basis. This significant discovery has aroused the interest of scholars in the research of 2D materials [2–8]. Many two-dimensional materials, such as black phosphorene, arsenene, antimonene, germanene, silicene, molybdenum disulfide, and boronene [9–15], have great applications in electronic devices, sensors, energy storage, catalysis, and composite materials [16–19]. Graphene has amazing mobility and almost zero effective mass of carriers [20] and is an ideal material to replace silicon crystals as field-effect tubes [21, 22]. However, intrinsic graphene is a “half-metal” material with a zero bandgap [23], which limits its development in the field of optoelectronics [24, 25]. Like graphene, silicene and germanene have Dirac cones at the K point [26, 27] and also possess properties such as ultra-high carrier mobility. Although they are no longer zero-bandgap structures, the bandgap opened at the Dirac point is too small and their development in the field of optoelectronics is still greatly limited. Arsenenes have good stability and wide bandgap, but their development in electronic devices is limited due to their indirect bandgap semiconductors [28]. Due to its high mobility, direct bandgap, and anisotropic mechanical and transport properties not found in other materials [29–32], black phosphorene can compensate well for the lack of performance of other two-dimensional materials.

In 2014, Xianhui Chen et al. [33] successfully produced black phosphorene for the first time using a mechanical
exfoliation method. The successful preparation of black phosphorene has attracted extensive research in the scientific community. The electronic structure and stability of black phosphorene can be tuned by doping, adsorption, strain, and defects [34–38] methods. Researchers have great interest in doping black phosphorene with N and B elements, especially the doping studies of BN or BN clusters formed by N and B. Cheng et al. [39] found that B can greatly enhance the collection of visible and infrared light by black and blue phosphorene and becomes an ideal potential material for the reduction of N2 visible light. Goulart et al. [40] found that B and N-doped black phosphorene exhibit n-type and p-type semiconductors, respectively, and the doped phosphorene with an odd number of N atoms has p-type semiconductor properties, while the even number of B and N doped phosphorene shows semiconducting properties. It can be seen that the introduction of dopants in the system can change the electronic properties of phosphorene. Doping of B, N, and BN not only in black phosphorene but also in other 2D materials can have a dramatic effect on 2D materials. Arthit et al. [41] doped BN with serrated single-walled carbon nanotubes and found that BN substitution could lead to a reduction in bandgap from 0.606 to 0.183 eV but did not affect Young’s modulus values. Fan et al. [42] applied torsional deformation and found that the bandgap of graphene was opened by BN doping. Chen et al. [43] studied CO gas adsorption using BN-doped black phosphorus and CO coupling could be promoted by applying 7% compressive strain, which in turn led to the reduction of CO dimer to CH2CH2.

Numerous studies have shown that the study of the bandgap can exploit its many potential applications. Among them is the modulation of its bandgap transition: the transition between direct and indirect bandgap is of great importance for its application in nanodevices and ultraviolet laser devices involving light emission. Although there have been some studies on B- and N-doped black phosphorene, there is no more systematic study, even in terms of optical properties, on B- and N-doped black phosphorene that has not been reported. Therefore, in this paper, the effects of B-, N-, and BN-doped black phosphorene electronic structure and optical properties are investigated based on the first principles of the density generalized theory approach, and it is expected that the data results of this paper can provide some theoretical reference for the modification study of black phosphorene and provide guidance for its application in optoelectronic devices.

Model and methods

In this paper, the calculations are based on the CASTEP module [44] in the Materials-Studio software under the first principles of density generalized function theory. Both structure optimization was performed using the Broyden-Fletcher-Goldfarb-Shanno (BFGS) algorithm as well as the GGA-PBE [45] general function for B- and N-doped black phosphorene and BN-doped black phosphorene systems at different concentrations and total energy calculations. After the convergence test, the k-sampling density and the cutoff energy were set to 400 eV and 3 × 3 × 1, respectively, and the four optimized parameters 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 × 10−6 eV/atom, respectively. To avoid the influence of interlayer interaction forces, a vacuum layer with a thickness of 15 Å was set [46].

The doping concentration of BN on black phosphorene is the ratio of doped atoms to the total number of undoped P atoms before doping. In this paper, four different sizes of black phosphorus alkene supercells were used to calculate different concentrations of doping, and the black phosphorus mono cells were expanded 1/2/3 units along the base vector a and b directions to obtain 2 × 1 × 1 (8 P atoms), 2 × 2 × 1 (16 P atoms), 3 × 2 × 1 (24 P atoms), and 3 × 3 × 1 (36 P atoms) supercells, respectively. The relative stability of the black phosphorene system is determined by the formation and binding energies, which can be calculated by the following equations:

\[
E_f = E_{p+X} + E_p - E_{pure} - E_X
\]  
\[
E_b = (E_{p+X} - nE_p - mE_X)/N
\]

where \(E_f\) is the formation energy, \(E_{p+X}\) is the total energy of the doped system, \(E_p\) is the individual energy of the phosphorus atom, \(E_{pure}\) is the total energy of the black phosphorene supercell structure, and \(E_X\) is the energy of the dopant atoms (X = B, N, and BN). \(E_b\) is the binding energy, \(n\) and \(m\) are the numbers of atoms of the phosphorus atom and dopant in the supercell, and \(N\) is the total number of atoms in the doped structure.

Results and discussion

Structural stability and energy bandstructure

Figure 1 (a, b) shows the top and side views of the optimized intrinsic black phosphorene. After geometric optimization, the lattice constants \((a = 3.276 \text{ Å}, b = 4.610 \text{ Å})\) are obtained in general agreement with the experimental values [47] \((a = 3.276 \text{ Å}, b = 4.618 \text{ Å})\). The absolute value of the binding energy of a single P atom of the intrinsic black phosphore is 5.31 eV, which is not much different from 5.36 eV in the literature [48], indicating that the
model used and the calculated parameters are suitable. Figure 2 (a–d) shows the top and side views of the B- and N-doped black phosphorene. It can be seen that the structure of black phosphorene is distorted after the doping of B and N atoms, with the B and N atoms relaxing inward and the degree of distortion of the B atoms is more pronounced compared to the N atoms.

When B and N atoms are co-doped, different doping positions need to be considered. Figure 3(a) shows the schematic diagram of the BN doping positions of black phosphorene. The B atoms are denoted by P, and the positions of N atoms are denoted by P1-P3. The optimal doping positions are shown in Fig. 3(b) after full relaxation for the three models and optimization. Table 1 shows the formation and binding energies of B-, N-, and BN-doped black phosphorene, and it can be seen that BN co-doping is more stable compared to the structure of B and N atoms doped alone, and the stability of the B-, N-, and BN-doped structure is greatly improved compared to the intrinsic black phosphorene.

The doping concentration affects the electrical and optical properties of the black phosphorene, among others. To investigate these properties, four different doping models were optimized and calculated, as shown in Fig. 4. Table 2 shows the formation energy, binding energy, and bond length of BN-doped black phosphorene. Combined with Fig. 4 and Table 2, it can be concluded that the stability of the structure gradually increases with the increase of the doping concentration, and the structure of the system with a doping concentration of 25% is the most stable. The B-N bond length, B-P bond length, and N-P bond length all fluctuate in a small range, and the P-P bond length varies more, which indicates that the doping concentration has a greater effect on the bonding between homologous atoms.

Figure 5 shows the energy band structure of intrinsic black phosphorene, which is a direct bandgap semiconductor.
with a bandgap value of 0.905 eV, which is in agreement with the previous results [34, 49, 50]. Figure 6(a) shows the energy band structure of B-doped black phosphorene, where B-doping can reduce the bandgap value and a direct–indirect bandgap transition occurs. Figure 6(b) shows the energy band structure of N-doped black phosphorene, where the bandgap decreases after N doping and remains as a direct bandgap semiconductor. From the density of states, it can be seen that in the energy range of $-2$–$2$ eV, the total peak density of states is mainly contributed by the p-orbital, and the s-orbital contributes to part of the density of states, and the maximum peak density of states occurs at the energy value of $-1.1$ eV for intrinsic black phosphorene and at the energy values of $-1.43$ eV and $-1.54$ eV for B and N doping, respectively. The B-doping results in an impurity energy level within 0–1 eV compared to the intrinsic (N-doped)

Table 1 Formation energy ($E_f$) and binding energy ($E_b$) of B-, N-, and BN-doped black phosphorene

| Doping type | B   | N   | BN  |
|-------------|-----|-----|-----|
| $E_f$/eV    | $-0.539$ | $-2.287$ | $-3.225$ |
| $E_b$/eV    | $-5.468$ | $-5.517$ | $-5.543$ |

Fig. 4 Optimized model of BN-doped black phosphorene at different concentrations: a 25%; b 12.5%; c 8.33%; d 5.56%

Table 2 Formation energy ($E_f$), binding energy ($E_b$), and bond length of BN-doped black phosphorene at different concentrations

| Doping degree/% | $E_f$/eV | $E_b$/eV | $d_{N, S}$/Å | $d_{B, P3}$/Å | $d_{B, P2}$/Å | $d_{N, P3}$/Å | $d_{N, P4}$/Å | $d_{P1, P5}$/Å |
|----------------|----------|----------|-------------|-------------|-------------|-------------|-------------|-------------|
| 5.56           | $-3.225$ | $-5.543$ | 1.498       | 1.987       | 1.871       | 1.792       | 1.769       | 2.222       |
| 8.33           | $-3.248$ | $-5.588$ | 1.498       | 1.983       | 1.873       | 1.791       | 1.768       | 2.226       |
| 12.5           | $-3.138$ | $-5.647$ | 1.496       | 2.012       | 1.872       | 1.796       | 1.789       | 2.203       |
| 25             | $-3.258$ | $-5.848$ | 1.498       | 2.005       | 1.886       | -           | 1.767       | 2.287       |
black phosphorene, which not only changes the bandgap from direct to indirect but also decreases the bandgap.

**Effect of different doping concentrations on BN-doped black phosphorene**

Figure 7 shows the energy band structures of BN-doped black phosphorene at different doping concentrations. All systems are indirect bandgap semiconductors, and the change of doping concentration does not affect the bandgap type. However, with the increase of doping concentration, the bandgap shows a trend of decreasing, increasing, and then decreasing. The bandgap reaches a minimum value of 0.697 eV at a doping concentration of 8.33% and a maximum value of 1.012 eV at a doping concentration of 12.5%, which indicates that the change of doping concentration can modulate the bandgap of black phosphorene.

To further explain the reason for the bandgap variation, a study of the density of states is necessary, as shown in Fig. 8. The doped system valence band energy is distributed from $-20$ to $0$ eV and the conduction band energy is distributed in the region of $0$ to $12$ eV. At energy values of $-18.06$ to $-17.43$ eV, the contribution of the total density of states comes mainly from the s-state electrons of the N atom, the s- and p-state electrons of the B atom make partial contributions, and the s- and p-state electrons of the P atom and the p-state electrons of the N atom contribute very weakly. At energy values of $-15$ to $-6.97$ eV, the main contribution to the total density of states comes from the s-state electron contribution of the P atom. The s- and p-states of the B atom, the p-state of the N atom, and the p-state electron of the P atom make some contributions to this part, while the s-state electron of the N atom does not contribute. At energy values of $-6.97$ to $0$ eV, the main contribution to the total density of states comes from the electronic contribution of the p-state of the P atom, the p-state of the B atom, and the p-state of the N atom, and the s-state electrons of the P atom make partial contributions to this part, and the s-state of the B atom and the s-state of the N atom make essentially no contribution. In the conduction band part, the total density of states is mainly contributed by the p-state electrons of the P and B atoms, the s-state electrons contribute very weakly, and the s- and p-states of the N atom contribute essentially nothing. Overall, the N atom contributes very weakly to the total density of states and only contributes to the local density of states. Near the Fermi energy level, the p-states of the...
B and P atoms play a dominant role in the overall density of states, and the N atoms do not contribute, which explains the fact that the black phosphorene behaves as an indirect bandgap semiconductor after BN co-doping.

To express the properties of B-, N-, and BN-doped black phosphorene more graphically, we plotted the differential charge densities of B-doped, N-doped, and BN-doped black phosphorene at different concentrations. The differential charge density is defined as:

\[
\delta \rho = \rho_{\text{pure}+X} - (\rho_X + \rho_{\text{pure}})
\]  

(3) where \(\rho_{\text{pure}+X}\) is the total charge density of the doped black phosphorene, \(\rho_X\) is the charge density of the doped atoms (X=B, N, and BN), and \(\rho_{\text{pure}}\) is the charge density of the intrinsic black phosphorene. The number of Mulliken charge populations of B, N, and P atoms in the doped system is listed in Tables 3 and 4. The overlapping populations of B-P, N-P, and P-P bond lengths in the doped system are listed in Tables 5 and 6, and the charge densities of the doped system are shown in Figs. 9 and 10. Combining the graphs, it can be concluded that the charges are redistributed after B, N, and BN doping, where the red and blue colors indicate the accumulation and reduction of charges. Charge transfer occurs between B and N atoms and black phosphorene. In the single doping, the maximum overlapping B-P and N-P bond lengths are 1.02\(\text{e}\) and 0.41\(\text{e}\), respectively, which indicates the formation of covalent bonds between B and P atoms and N and P atoms. The P atoms in black phosphorene are covalently bonded to each other, but the N atom makes the minimum P-P bond \(-0.18\text{e}\) so that ionic bonds are formed between them. When B doped black phosphorene,
there is a 0.39e charge transfer to B atom on the surface of black phosphorene, and B becomes a negatively charged ion. When N is doped with black phosphorene, 1.01e charge is transferred to N atoms on the surface of black phosphorene, and N atoms become negatively charged ions, and N atoms get more electrons compared with B. When BN is co-doped, the B-N bonds are around 0.80e for all four different doping concentrations, which indicates that covalent bonds are formed between B and N atoms, and the change of doping

| Mulliken population | B(N) | P |
|---------------------|------|---|
| Maximum value       | Minimum value |
| B doping            | −0.39 | 0.12 | −0.01 |
| N-doped             | −1.01 | 0.39 | −0.02 |

| Overlapping population | B(N)-P | P-P |
|------------------------|--------|-----|
| Maximum value          | Minimum value |
| Maximum value          | Minimum value |
| B doping                | 1.02   | 0.74 | 0.54 | 0.40 |
| N-doped                | 0.41   | 0.31 | 0.50 | −0.18 |

**Table 3** Mulliken charge population numbers of B, N, and P atoms in B(N)-doped black phosphorene structures

**Table 4** Mulliken charge population numbers of B, N, and P atoms at different doping concentrations

**Table 5** Overlapping population of B(N)-P and P-P bond lengths in B(N)-doped black phosphorene structures

**Fig. 8** Density of states of BN-doped black phosphorene at different concentrations: a 5.56%; b 8.33%; c 12.5%; d 25%
concentration does not affect the type of bonding. The maximum B-P and N-P bond lengths for different doping concentrations are around 0.90e and 0.40e, respectively, which indicates that covalent bonds are formed between B and P atoms and N and P atoms. When the doping concentration is 5.56% and 8.33%, the B atom loses 0.04e electrons, and the N atom gains 0.92e electrons. When the doping concentration is 12.5% and 25%, the B atom loses 0.05e electrons, and the N atom gains 0.91e electrons. With the increase of doping concentration, the amount of charge transfer increases. After BN co-doping, covalent bonds are formed between B and N atoms, B(N) atoms, and black phosphorene, in which the strong electron transfer makes the electronic properties of black phosphorene change, which intensifies the charge transfer of P atoms themselves and makes the type of bonding between some P atoms change. It can be found that the overlapping B-P bond lengths are twice as long as the overlapping N-P bond lengths. Therefore, the impurity energy levels appearing near the Fermi energy level may be formed by the violent interaction between B and P atoms.

Effect of different doping concentrations on the optical properties of BN-doped black phosphorene

As shown in Fig. 11(a), all doped systems have only one absorption peak, and the wavelengths are 229 nm, 228 nm, 221 nm, 222 nm, and 185 nm, respectively, from small to large according to the doping concentration. The system with 25% doping concentration starts to absorb the light at 49 nm first, and the system with 0% doping concentration absorbs the light at 64 nm at the latest. As the doping concentration increases, the absorption of light by black phosphorene increases. Similarly, the system with a 25% doping concentration is the first to stop absorbing light at 7386 nm, and the system with a 5.56% doping concentration is the last to stop absorbing light at about 7944 nm. Figure 11(b) shows the magnified view of the absorption peak, which shows that the system with 12.5% doping concentration has the best absorption effect at the absorption peak, and the system with 5.56% doping concentration has the worst absorption effect at the absorption peak. The absorption effect at the peak is the worst. Compared with the doping concentration of 0, the rest of the doped systems have different degrees of blue shift, among which the doping concentration of 12.5% has the most obvious blue shift, which corresponds to its minimum wavelength and maximum bandgap.

Figure 11(c) shows the reflectance of the doped systems. It can be obtained that all systems have only one reflection peak, which is 191 nm, 197 nm, 166 nm, 145 nm, and 129 nm in order of doping concentration from small to large. The system with 0 doping concentration is the last to reflect light at 62 nm. When the wavelength
is greater than 1000 nm, all the systems tend to stabilize, and the system with 25% doping concentration reflects the light best, while the systems with 0 and 5.56% doping concentration reflect the light the least. Figure 11(d) shows the magnified view of the reflection peak, and it can be seen that the system with 12.5% doping concentration has the best reflection effect at the reflection peak, and the system with 5.56% doping concentration has the worst reflection effect at the reflection peak. Compared with the system with a doping concentration of 0, the remaining doped system has a blue shift.

**Dielectric function and conductivity of B-, N-, and BN-doped black phosphorene**

The complex dielectric function is a common indicator for studying optical properties, and the information on the energy band structure of solids and various other optical information can be obtained from the dielectric function, and the expression of the complex dielectric function is:

\[
\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)
\]

where \(\omega\) is the frequency of the incident photon; \(\varepsilon_1(\omega)\) and \(\varepsilon_2(\omega)\) are the real and imaginary parts of the complex dielectric function, respectively; and the rate of decrease of the real part of the dielectric function curve determines the height of the peak of the imaginary part, which corresponds to the absorption condition of light. Figure 12 shows the complex dielectric function of B-, N-, and BN-doped black phosphorene. From Fig. 12(a), we can get the dielectric function of intrinsic black phosphene as 3.65, and the dielectric function after B and N doping are 3.31 and 3.56, respectively. When BN is co-doped, the dielectric function is 3.12, 3.34, 3.67, and 4.34 in order of the doping concentration. We can find that when B, N, and BN doping concentrations are 5.56 and 8.33, all decrease. The dielectric function of black phosphorene is significantly increased only when the BN doping concentration is 12.5 and 25. Compared with the intrinsic black phosphorene, the doping system shifts to the high-energy direction at the highest peak, resulting in an increase in the electric field intensity generated by light, which is more conducive to improving the efficiency of photovoltaic power generation. Among them, the shift is most obvious when the BN doping concentration is 12.5 and 25. From Fig. 12(b), it can be seen that all systems have two peaks, the photon energy is between 0 and 10 eV, and the imaginary part of the dielectric function is not zero, indicating that electrons are jumped in this interval.

The photoconductivity effect is a phenomenon in which the conductivity of a system to an electric charge is greatly
Fig. 11  Optical properties of BN-doped black phosphorene at 0%, 5.56%, 8.33%, 12.5%, and 25% concentrations

Fig. 12  Dielectric function of B-, N-, and BN-doped black phosphorene: a real part; b imaginary part
enhanced by the action of light, and photoconductivity is mainly related to the density and mobility of carriers. Figure 13 shows the photoconductivity of B-, N-, and BN-doped black phosphorene. From Fig. 13(a), it can be obtained that the photoconductivity of both intrinsic and doped black phosphorene increases with the increase of photon energy in the low-energy region from 0 to 5 eV. The peak photoconductivity of BN-doped 25 reaches 2.36 fs$^{-1}$ at a photon energy of 6.1 eV. It can be seen that the peak photoconductivity of B-, N-, and BN-doped 5.56 decreases slightly and moves toward higher energy, while the photoconductivity of BN-doped 8.33, 12.5, and 25 increases significantly and moves toward higher energy. From Fig. 13(b), it can be seen that the photoconductivity decreases and shifts toward higher energies after doping in the low-energy region from 0 to 6.6 eV of photon energy and increases and shifts toward higher energies when it is greater than 6.6 eV.

Conclusions

The effects of electronic structure and optical properties of B- and N-doped black phosphorene and BN-doped black phosphorene at different concentrations were investigated based on a density generalized theory first-principles approach. BN-doped black phosphorene was found to be more stable than B and N atom doping. With the increase of doping concentration, the stability of the structure gradually decreases, and the structure of the system with 25% doping concentration is the most stable. From the electronic structure, B atom doping is the direct bandgap, and N atom and BN doping can change the black phosphorene from the direct bandgap to the indirect bandgap. With the increase of doping concentration, the bandgap shows a trend of decreasing, increasing, and then decreasing. The doping of BN changes the energy band structure of black phosphorene, and impurity energy levels appear in the conduction band. The p-states of B and P atoms play a dominant role in the overall density of states, and N atoms play a role in the local density of states. According to Mulliken’s analysis, charge transfer occurs between black phosphorene and B and N atoms. The amount of charge transfer increases with the increase of doping concentration. In terms of absorption coefficient and reflectance, the doped system is blue-shifted at the absorption and reflection peaks compared to the intrinsic black phosphorene. In terms of dielectric constant, the doped system is shifted toward higher energy at the highest peak, leading to an increase in the intensity of the electric field generated by light, which is beneficial to improving the efficiency of photovoltaic power generation. The photoconductivity decreases and shifts toward higher energy after doping, with the most pronounced shift at BN doping concentrations of 12.5 and 25.

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

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Data availability Data sharing does not apply to this article as no data sets 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.

References

1. Novoselov KS et al (2004) Electric field effect in atomically thin carbon films. Science 306:666–669. https://doi.org/10.1126/science.1102896
2. Shen P-C et al (2018) CVD technology for 2-D materials. IEEE Trans Electron Devices 65:4040–4052. https://doi.org/10.1109/TED.2018.2866390
3. Fatima U et al (2021) Two-dimensional materials and synthesis, energy storage, utilization, and conversion applications of two dimensional MXene materials. Int J Energy Res 45:9878–9894. https://doi.org/10.1002/er.6595
4. Wu Z, Ni Z (2017) Spectroscopic investigation of defects in two-dimensional materials. Nanophotonics 6:1219–1237. https://doi.org/10.1515/nanoph-2016-0151
5. Dong S, Xia Y, Huang R, Zhao J (2020) Modulating mechanical anisotropy of two-dimensional materials by controlling their defects. Carbon 158:77–88. https://doi.org/10.1016/j.carbon.2019.11.085
6. Ma Y, Li B, Yang S (2018) Ultrathin two-dimensional metallic nanomaterials. Mater Chem Front 2:456–467. https://doi.org/10.1039/c7qm00548b
7. Burch KS, Mandrus D, Park J-G (2018) Magnetism in two-dimensional van der Waals materials. Nature 563:47–52. https://doi.org/10.1038/s41586-018-0631-z
8. Du W et al (2020) Nanolasers based on 2D materials. Laser Photonics Rev 14. https://doi.org/10.1002/lpor.202000271
9. Ren X et al (2017) Properties, preparation and application of black phosphorus/phosphorene for energy storage: a review. J Mater Sci 52:10364–10386. https://doi.org/10.1007/s10853-017-1194-3
10. Osipa DA, Cisternas E, Duque CA, Correa JD (2018) Electronic structure and STM images simulation of defects on hBN/ black-phosphorene heterostructures: a theoretical study. Surf Sci 669:95–102. https://doi.org/10.1016/j.susc.2017.11.015
11. Xu W et al (2017) Electronic and optical properties of arsenene under uniaxial strain. IEEE J Sel Top Quantum Electron 23. https://doi.org/10.1109/jstQE.2016.2593106
12. Ares P et al (2021) Few-layer antimonene electrical properties. Appl Mater Today 24. https://doi.org/10.1016/j.apmt.2021.101132
13. Kaloni TP, Schreckenbach G, Freund MS, Schwingenschlögl U (2016) Current developments in silicene and germanene. Phys Status Solidi Rapid Res Lett 10:133–142. https://doi.org/10.1002/pssr.201510338
14. Shiri M, Madani A, Shaaban N (2021) Optical properties of molybdenum disulfide based photonic crystal. Opt Quantum Electron 53. https://doi.org/10.1007/s11082-020-02729-3
15. Wang Z-Q, Lu T-Y, Wang H-Q, Feng YP, Zheng J-C (2019) Review of borophene and its potential applications. Front Phys 14. https://doi.org/10.1007/s11467-019-0884-5
16. Lee HS et al (2012) MoS2 nanosheet phototransistors with thickness-modulated optical energy gap. Nano Lett 12:3695–3700. https://doi.org/10.1021/nl301485q
17. Zhao J, Chen Z (2015) Carbon-doped boron nitride nanosheet: an efficient metal-free electrolator for the oxygen reduction reaction. J Phys Chem C 119:26348–26354. https://doi.org/10.1021/acs.jpcc.5b09037
18. Feng L, Liu Y, Zhao J (2015) Fe- and co-P-4-embedded graphene as electrolators for the oxygen reduction reaction: theoretical insights. Phys Chem Chem Phys 17:30687–30694. https://doi.org/10.1039/c5cp0551b
19. Yang Q et al (2016) First-principles study of sulfur dioxide sensor based on Phosphorenes. IEEE Electron Device Lett 37:660–662. https://doi.org/10.1109/LED.2016.2543243
20. Wu YH, Yu T, Shen ZX (2010) Two-dimensional carbon nanostructures: fundamental properties, synthesis, characterization, and potential applications. J Appl Phys 108. https://doi.org/10.1063/1.3460809
21. Balandin AA et al (2008) Superior thermal conductivity of single-layer graphene. Nano Lett 8:902–907. https://doi.org/10.1021/nl0731872
22. Castro Neto AH, Guinea F, Peres NMR, Novoselov KS, Geim AK (2009) The electronic properties of graphene. Rev Mod Phys 81:109–162. https://doi.org/10.1103/RevModPhys.81.109
23. Weiss NO et al (2012) Graphene: an emerging electronic material. Adv Mater 24:5782–5825. https://doi.org/10.1002/adma.201201482
24. Peng L, Zhu Y, Li H, Yu G (2016) Chemically integrated inorganic–Graphene two-dimensional hybrid materials for flexible energy storage devices. Small 12:6183–6199. https://doi.org/10.1002/smll.201602109
25. Schwierz F (2010) Graphene transistors. Nat Nanotechnol 5:487–496. https://doi.org/10.1038/nnano.2010.89
26. Chen L et al (2012) Evidence for Dirac fermions in a honeycomb lattice based on silicon. Phys Rev Lett 109. https://doi.org/10.1103/PhysRevLett.109.056804
27. Behera H, Mukhopadhyay G (2011) 55th Symposium on DAE solid state physics (SSPS), pp 823–824
28. Kamal C, Ezawa MA (2015) Two-dimensional buckled and puckered honeycomb arsenic systems. Phys Rev B 91. https://doi.org/10.1103/PhysRevB.91.085423
29. Yu Y et al (2020) Synthesis and electrical properties of single crystalline black phosphorus nanoribbons. Crystengcomm 22:3824–3830. https://doi.org/10.1039/d0ce00390e
30. Galluzzi M, Zhang Y, Yu X-F (2020) Mechanical properties and applications of 2D black phosphorus. J Appl Phys 128. https://doi.org/10.1063/5.0034983
31. Li XJ, Yu JH, Luo K, Wu ZH, Yang W (2018) Tuning the electrical and optical anisotropy of a monolayer black phosphorus magnetic superlattice. Nanotechnology 29. https://doi.org/10.1088/1361-6528/aaaaf0
32. Li T et al (2017) High field transport of high performance black phosphorus transistors. Appl Phys Lett 110. https://doi.org/10.1063/1.4982033
33. Li L et al (2014) Black phosphorus field-effect transistors. Nat Nanotechnol 9:372–377. https://doi.org/10.1038/nnano.2014.35
34. He J, Liu G, Wei L (2021) Effect of O adsorption on the electronic structure and optical properties of black phosphorene. Mol Phys. https://doi.org/10.1080/00268976.2021.2000858
35. Yu WY et al (2015) Anomalous doping effect in black phosphorene using first-principles calculations. Phys Chem Chem Phys 17:16351–16358. https://doi.org/10.1039/c5cp01732g
36. Luo Y et al (2018) Adsorption of transition metals on black Phosphorene: a first-principles study. Nanoscale Res Lett 13. https://doi.org/10.1186/s11671-018-2696-x
37. Yarmohammadi M, Mortezaei M, Tien TS, Phuong LTT (2020) Linear interband optical refraction and absorption in strained black phosphorene. J Phys Condens Matter 32. https://doi.org/10.1088/1361-648X/abaad0
38. Rezaee AE, Kashi MA, Baktash A (2018) Stone-Wales like defects formation, stability and reactivity in black phosphorene. Materials Science and Engineering B-Advanced Functional Solid-State Materials 236:208–216. https://doi.org/10.1016/j.mseb.2018.11.008
39. Cheng Y, Song Y, Zhang Y (2019) The doping and oxidation of 2D black and blue phosphorene: a new photocatalyst for nitrogen reduction driven by visible light. Phys Chem Chem Phys 21:24449–24457. https://doi.org/10.1039/c9cp04647j
40. Goulart L, Fernandes LdS, dos Santos CL, Rossato J (2019) Electronic and structural properties of black phosphorene doped with Si, B and N. Phys Lett A 383. https://doi.org/10.1016/j.physleta.2019.125945
41. Vongachariya A, Parasuk V (2015) Stabilities and mechanical and electronic properties on BN doped zigzag single-wall carbon nanotubes. Solid State Commun 223:28–31. https://doi.org/10.1016/j.ssc.2015.09.006
42. Fan D, Liu G, Wei L (2018) Electronic theoretical study on the influence of torsional deformation on the electronic structure and optical properties of BN-doped graphene. Mod Phys Lett B 32. https://doi.org/10.1142/s0217984918501798
43. Chen Z, Liu X, Zhao J, Jiao Y, Yin L (2020) Strain effect on the catalytic activities of B- and B/N-doped black phosphorene for electrochemical conversion of CO to valuable chemicals. J Mater Chem A 8:11986–11995. https://doi.org/10.1039/d0ta03991h
44. Segall MD et al (2002) First-principles simulation: ideas, illustrations and the CASTEP code. J Phys Condens Matter 14:2717–2744. https://doi.org/10.1088/0953-8984/14/11/301
45. Perdew JP, Burke K, Ernzerhof M (1998) Comment on “generalized gradient approximation made simple” - reply. Phys Rev Lett 80:891–891. https://doi.org/10.1103/PhysRevLett.80.891
46. Payne MC, Teter MP, Allan DC, Arias TA, Joannopoulos JD (1992) Iterative minimization techniques for ab initio total-energy calculations: molecular dynamics and conjugate gradients. Rev Mod Phys. https://doi.org/10.1103/revmodphys.64.1045
47. Mu G-Y, Liu G-L, Zhang G-Y (2020) Bending deformation regulates the electronic and optical properties of black phosphorene. Int J Mod Phys B 34. https://doi.org/10.1142/s021797922050191x
48. Du YL (2010) New anode materials for lithium-ion batteries, Jiangxi Normal University
49. Mu GY, Liu GL, Zhang GY (2020) Bending deformation regulates the electronic and optical properties of black phosphorene. Int J Mod Phys B 34. https://doi.org/10.1142/s021797922050191x
50. He J-L, Liu G-L, Li X-Y (2021) Effect of twisting deformation on electronic structure and optical properties of gold-doped black phosphorene. Acta Phys Sin 70. https://doi.org/10.7498/aps.70.20210795

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