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Strain-engineering on mechanical and electronic properties of group IV-V two-dimensional semiconductors

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Abstract

Due to the attractive physical properties, group IV-V materials (A3B, A = C, Si, Ge and B = N, P, As) have been received much attention in recent years. In this paper, first-principles calculations have been performed to investigate the elastic and electrical properties in two-dimensional (2D) A3B materials. The in-plane stiffness, Poisson’s ratio, Young’s modulus and ultimate strength of monolayer A3Bs along armchair and zigzag direction are calculated. The band gap of monolayer C3N increases with different concentration of B and can be modified significantly by the application of strain engineering. We predicted the electron and hole mobility in the armchair (zigzag) direction, rather high and highly anisotropic. Monolayer Ge2N5 exhibits an extremely high electron mobility of 3.46 × 10^3 cm^2 V^{-1} s^{-1} along the zigzag direction. The high mobility and anisotropic characteristics endow A3Bs with many potential applications in the field of microelectronics and optoelectronic devices.

1. Introduction

Two-dimensional (2D) materials have emerged as a distinct research hotspot since the successful synthesis of graphene by mechanical exfoliation of graphite in 2004 [1–3]. In recent years, graphene has been recognized as one of the most famous 2D materials with one-atom layer thickness. The unique honeycomb structures in graphene demonstrate high stability as well as in fullerene, carbon nanotube, and accumulate three-dimensional graphite blocks [4]. Graphene also exhibits excellent mechanical properties including a reversible elastic deformation of 20% and a high Young’s modulus of 1.0 TPA [5, 6]. Besides, the physical and chemical characters of graphene can be changed along with the structural deformation [7]. Strain engineering has been widely used as an effective method to adjust the physical characteristics of 2D materials [7]. For example, the band gap of MoS2 changed from direct to indirect band gap as applying a strain greater than 1% [8–12]. The electron mobility in MoS2 can also be improved by strain engineering, which is critical to the application in adjustable photonic devices and solar cells [9, 10, 13]. Under uniaxial or biaxial strains, the anisotropy of the effective electron mass distribution and the conducting direction in black phosphorus can be switched 90° degrees [14]. Similarly, the magnetism, optical gap, and electronic properties of ReSe2 can be controlled by adjusting local strains on the nanosheet [15]. The thin-layer nature brings 2D materials the possibility of strain treatment, providing adjustable physical properties that can be used in strain sensors, scalable electrodes, solar cells, flexible FETs, and other photonic devices.

Recently, the new 2D materials formed by group IV and V elements have attracted great interest in material science. Burak et al theoretically predicted the high stability of IV-V (IV = C, Si, Ge, Sn, Pb; V = N, P, As, Sb, Bi) monolayers with hexagonal crystal structures [16]. With the method of high-pressure melt growth, Barreteau et al successfully prepared layer SiP, SiAs, GeP, and GeAs materials and demonstrated these materials all show semiconductor properties [17]. Zhang et al theoretically investigated the strain–induced conducting switch in group IV-V monolayers [18]. The band gap of monolayer C3N increases with different concentration of B doping. When the doping concentration of B is 12.5%, we found that monolayer C3N is changed from indirect
band gap to direct band gap [19], C3N and C3N3 are suitable for the formation of heterostructures and can change the electronic properties of the constituent layers. For example, MoS2/C3N and MoS2/C3N3 heterostructures both exhibit metallic features [20]. C4N3 displayed adjustable electronic performance by applying bidirectional compression strains [21]. Two-dimensional group VA-VA monolayers possess promising prospect for ultra-scaled field effect transistors [22]. The results mentioned above indicate that strain engineering has great potential for modulation of the physical properties of 2D nanomaterials.

In here, based on our previous work, we investigated the strain engineering properties of 2D group IV-V materials including C4N, C4P, C4As, Si4N, Si4P, Si4As, Ge4N, Ge4P, and Ge4As. The results indicate 2D group IV-V materials exhibit isotropic mechanical properties as well as graphene. Specially, Young’s modulus of monolayer C4N reaches a high value of 974.7 GPa. The band gaps of 2D group IV-V materials are demonstrated to change with the applied strains. Based on the deformation theory, 2D group IV-V materials all exhibit excellent conductivities of electrons and holes.

2. Computational method

In this work, all the calculations are performed based on the density functional theory (DFT) as implemented in CASTEP code [23]. Exchange-correlation potentials are described using the generalized gradient approximation (GGA) and Perdew-Burke-Ernzerhof (PBE) function. The classic BFGS algorithm [23] is used for the geometric optimization, and the ultrasoft pseudopotentials [24] is used to describe the interactions between electrons. The energy cutoff for plane-wave expansion is set to 500 eV, and the energy tolerance is less than 5.0 × 10−6 eV/atom. The residual atomic forces difference is less than 0.01 eV Å. A Monkhorst-Pack k-point mesh of 7 × 7 × 1 has been selected for the geometry optimization, structural stability, electronic and strain engineering calculations. The simulation models are constructed by 3 × 3 × 1 supercells with a 20 Å vacuum slab to avoid interlayer interactions.

The mechanical properties of group IV-V 2D materials can be calculated as follows. The in-plane stiffness $C$ of 2D systems is calculated by formula (1):

$$ C = \left( \frac{1}{S_0} \right) \left( \frac{\partial^2 E_i}{\partial \xi_i^2} \right) $$

where $S_0$ is the equilibrium area, $E_i$ is the strain energy (the energy difference between the equilibrium and the strained structure), $\xi_i$ indicates uniaxial strains along $i$ direction ($i = x$ or $y; x$ and $y$ indicate zigzag and armchair directions of A,B, respectively.). The strain energy $E_i$ can be fitted by the formula (2):[25]

$$ E_i = a_1 \xi_{xx}^2 + a_2 \xi_{yy}^2 + a_3 \xi_{xx} \xi_{yy} + a_4 \xi_{xy}^2 $$

where $\xi_{xx}$ and $\xi_{yy}$ are strains along the zigzag direction and armchair direction, respectively. The in-plane stiffness can be calculated as formula (3):[26]

$$ C_x = \left( \frac{1}{S_0} \right) \left( \frac{2a_2 - a_1^2}{2a_4} \right), \quad C_y = \left( \frac{1}{S_0} \right) \left( \frac{2a_2 - a_1^2}{2a_4} \right) $$

where $C_x$ and $C_y$ represent the in-plane stiffness along zigzag and armchair directions, respectively. Poisson’s ratio and Shear modulus can be calculated according formula (4):[25]

$$ \nu_{xy} = a_5 / 2a_2, \quad \nu_{yx} = a_5 / 2a_2, \quad G_{xy} = 2a_4 / A_0 d_0 $$

The elastic stiffness constants can be calculated using the formula (5):[25]

$$ C_{ij} = \left( \frac{1}{A_0 d_0} \right) \left( \frac{\partial E_i}{\partial \xi_j} \right) (i, j = xx, yy, xy) $$

$A_0$ is the equilibrium area of the 2D material, $d_0$ is the effective thickness of the system.

The Young’s modulus $Y(\theta)$ and Poisson’s ratio $\nu(\theta)$ along the in-plane $\theta$ can be expressed as follows:[27, 28]

$$ Y(\theta) = \frac{C_{11} C_{22} - C_{12}^2}{C_{11} \sin^4 \theta + C_{22} \cos^4 \theta + M \cos^2 \theta \sin^2 \theta} $$

$$ \nu(\theta) = \frac{C_{12} (\cos^4 \theta + \sin^4 \theta) - N \cos^2 \theta \sin^2 \theta}{C_{11} \sin^4 \theta + C_{22} \cos^4 \theta + M \cos^2 \theta \sin^2 \theta} $$

where $M = (C_{11} C_{22} - C_{12}^2) / C_{66} - 2C_{22}, \quad N = C_{11} + C_{22} - (C_{11} C_{22} - C_{12}^2) / C_{66}$.

The electron carrier mobility $\mu$ at the band extremes (CBM and VBM) was estimated according to the formula (7):[29, 30]

$$ \mu_{2D} = \frac{2 e h C_{2D}}{(3 k_B T |m^*|^2 E_1)} $$

where $m^*$ ($m^*_x$ or $m^*_y$) is the effective mass along the transport direction, $h$ is the reduced Plank constant, $k_B$ is the Boltzmann constant. $T$ indicates the temperature, $C_{2D}$ is the elastic modulus of a uniformly deformed crystal is used to simulate the lattice distortion activated by strain. $E_1$ is the deformation potential (DP) constant.
3. Results and discussion

The unit cell of monolayer A₃B contains six group IV atoms and three group V atoms. In here, we studied the properties of nine 2D A₃B compounds including C₃N, C₃P, C₃As, Si₃N, Si₃P, Si₃As, Ge₃N, Ge₃P, and Ge₃As. Each group-V element atom binds to three groups-IV element atoms forming a hexagonal ring, as shown in figure 1. Similar to the graphene sheet, C₃N is a honeycombed structure composed of six carbon and two

![Figure 1. Top view of monolayer C₃N structure in which the grey and blue spheres indicate carbon and nitrogen atoms.](image)

![Figure 2. Energy-varying surface of (a) C₃N, (b) C₃P, (c) C₃As, (d) Si₃N, (e) Si₃P, (f) Si₃As, (g) Ge₃N, (h) Ge₃P and (i) Ge₃As in terms of zigzag strains εₓ and armchair strains εᵧ.](image)
To calculate the elastic properties, we construct a rectangular unit cell with a size of 8.4 Å. $\varepsilon_{xy}$ is the shear strain. $E$ is the in-plane stiffness of C$_3$N is 382 N m$^{-1}$, which is consistent with previous reports [31, 32]. The calculated in-plane stiffness of graphene using the same method is 342.5 N m$^{-1}$, which is consistent with the value (340 N m$^{-1}$) reported in previous work [33], which demonstrates that our method for the calculation of in-plane stiffness and the obtained results are reasonable and reliable, respectively. Noted that, the calculated in-plane stiffness of C$_3$N shows an extraordinary in-plane stiffness (382 N m$^{-1}$) than is even higher than graphene (342.5 N m$^{-1}$), MoS$_2$ (180 N m$^{-1}$) [34], and h-BN (267 N m$^{-1}$) [35], suggesting that C$_3$N monolayer has better resistance to in-plane deformation. There are two different types of bonds in each structure, type-I was formed between the elements of the group-V and group-IV, and type-II formed between the elements of the group-IV and group-IV. The values are shown in Figure S3. When the type-II bond lengths of these structures are equal, the in-plane stiffness decreases with the increase of type-I bond lengths. For example, the in-plane stiffness of C$_3$N, C$_3$P and C$_3$As follows the rule: C$_3$N > C$_3$P > C$_3$As. However, the rule is not available as the bond lengths of type-II is not equal. The electronegativity of the element is another factor affecting the in-plane stiffness of A$_3$B$_n$. This remains to be confirmed by further research.

### Table 1. Coefficient of elastic stiffness ($C_{11}$, $C_{22}$, $C_{12}$, $C_{06}$), in-plane stiffness ($C_{11}$, $C_{22}$; N/m) and Poisson’s ratio ($\nu_{xy}$, $\nu_{yx}$) of monolayer A$_3$B$_n$.

|        | $C_{11}$ | $C_{22}$ | $C_{12}$ | $C_{06}$ | $C_{11}$ | $C_{22}$ | $\nu_{xy}$ | $\nu_{yx}$ |
|--------|----------|----------|----------|----------|----------|----------|------------|------------|
| graphene | 1091     | 1091     | 191.6    | 449.6    | 342.5    | 341.5    | 0.18       | 0.18       |
| C$_3$N | 985.4    | 983.6    | 102.8    | 441.3    | 381.3    | 382.0    | 0.10       | 0.10       |
| C$_3$P | 768.2    | 767.2    | 139.3    | 314.5    | 233.5    | 233.8    | 0.18       | 0.18       |
| C$_3$As | 727.4    | 724.7    | 138.0    | 294.7    | 205.6    | 206.4    | 0.19       | 0.19       |
| Si$_3$N | 562.4    | 559.1    | 139.5    | 211.4    | 106.3    | 106.9    | 0.25       | 0.25       |
| Si$_3$P | 473.2    | 474.7    | 108.3    | 182.4    | 75.5     | 75.3     | 0.23       | 0.23       |
| Si$_3$As | 460.2   | 458.2    | 104.3    | 177.9    | 70.1     | 70.4     | 0.23       | 0.23       |
| Ge$_3$N | 429.5    | 429.6    | 113.9    | 157.8    | 72.9     | 72.9     | 0.27       | 0.27       |
| Ge$_3$P | 377.7    | 375.1    | 84.6     | 146.6    | 55.3     | 55.7     | 0.23       | 0.22       |
| Ge$_3$As | 369.5   | 367.3    | 85.8     | 141.9    | 52.1     | 52.4     | 0.23       | 0.23       |

Figure 3. Orientation dependent (a) Young’s modulus (GPa) and (b) Poisson’s ratio of monolayer A$_3$B compared with graphene and phosphorene.
To have an in-depth knowledge of the mechanical properties, the Young’s modulus and Poisson’s ratio in different directions were also calculated, as shown in figure 3. The Young’s modulus and Poisson’s ratio of the A3B are equal in all directions and higher than that of the already synthesized phosphorene. We can conclude that they are symmetrical isotropic materials as well as graphene. However, most of the A3Bs show lower Young’s modulus compared to graphene except for C3N. The Young’s modulus of C3N is very close to graphene, suggesting that C3N is as stiff as graphene.

The stress-strain curve is obtained from the simulated uniaxial tensile test, as shown in figure 4. The stress-strain curve initially exhibits a linear relationship, then a nonlinear response up to the ultimate tensile strength in which the maximum load bearing of the sheet is reached. After reaching the ultimate tensile strength point, if the strain continues to increase, the stress value suddenly drops, which indicates that the specimen has been destroyed due to the bond fracture. As mentioned in previous work [5, 36–41], the mechanical failure during the tension can be ascribed to elastic or phononic instability. Considering the calculation cost, we herein estimated the elastic constants of e.g., C3N monolayer under its critical strain. The obtained elastic constans are $C_{11}=1274.8 \, \text{N/m}$, $C_{22}=463.08 \, \text{N/m}$, $C_{12}=43.8 \, \text{N/m}^{-1}$, and $C_{66}=49.8 \, \text{N/m}^{-1}$, fully satisfying the mechanical stability criteria [42, 43], which demonstrates that C3N monolayer can still satisfy elastic stability under the critical strain. Based on this, we inferred that the failure of e.g., C3N monolayer under the critical strain origins from phononic instability. In the A3B family, Young’s modulus is positively related to the ultimate strength. We also found that the ultimate strength of A3B is anisotropic due to the different distribution of the different types of bonds that make up the A3B structure. The ultimate tensile strength of single layer C3Ni n armchair(zigzag) direction is 35.2 GPa (32.7 GPa), which is slightly lower than that of graphene 36.7 GPa (40.4 GPa) [44], but higher than that of phosphorene 8GPa (18GPa) [25]. The electronic properties of monolayer C3N honeycomb structures subjected to uniaxial and biaxial compression and tensile strains were investigated, as can be seen in table 2. When uniaxial tensile strain is applied, the band gap of C3N increases with an increasing strain in the armchair direction while decreases with an increasing strain in the zigzag direction. With applying a 10% strain at the armchair and zigzag direction separately, the corresponding band gap will rise to a value of 1.28 eV or fall to 0.62 eV, respectively. It is also found that the decrease rate in the zigzag direction is greater than that in the armchair direction, indicating that the band gap of C3N is more sensitive to the deformation in the zigzag direction with an uniaxial tensile strain is applied. When a uniaxial compression strain is applied, the band gap of C3N decreases with an increasing strain at the armchair and zigzag direction. When the biaxial compressive

| Strain | −0.1 | −0.08 | −0.06 | −0.04 | −0.02 | 0 | 0.02 | 0.04 | 0.06 | 0.08 | 0.1 |
|--------|------|-------|-------|-------|-------|---|------|------|------|------|-----|
| GGA Arm | 1.17 | 1.04  | 0.02  | 0.15  | 0.26  | 0.33| 0.34 | 0.35  | 0.37  | 0.37 | 0.30|
| Zig  | 0.27 | 0.37  | 0.20  | 0.26  | 0.31  | 0.27| 0.21 | 0.15  | 0.09  | 0.04 | 
| Bial  | 1.85 | 1.80  | 0.63  | 0.78  | 0.91  | 0.99| 1.00 | 1.00  | 1.02  | 0.95 | 
| HSE06 Arm | 0.59 | 0.59  | 0.76  | 0.79  | 0.90  | 1.00| 1.03 | 1.07  | 1.13  | 1.20 | 1.28|
| Zig  | 0.79 | 0.98  | 0.82  | 0.90  | 0.96  | 0.93| 0.86 | 0.79  | 0.73  | 0.62 | 

Figure 4. Stress-strain relation along the (a) zigzag and (b) armchair direction. The strain is defined as $(l - l_0)/l_0$, where $l_0$ is the equilibrium lattice and $l$ stand for the strained one.

Table 2. Band gap of monolayer C3N under uniaxial strain along the armchair (Arm) and zigzag (Zig) directions, as well as biaxial (Bial) strain.
strain reaches 10%, the band gap of C₃N will increase to 1.85 eV, much larger than the change value along the engineering.

The band gaps of single-, double-, three- and four-layer C₃N are 1.00 eV, 0.93 eV, 0.81 eV, and 0.75 eV, respectively, which is consistent with the reported results in the literature. The mobility of C₃As is calculated based on deformation potential (DP) theory [50]. As shown in Figure S4, the deformation potential is derived from the linear fitting of the respective energies of the conduction-band maximum and the valence-band minimum [51].

### Table 3. Band structures for bulk and different layers of A₃Bₙ calculated with GGA and HSE06 method.

| A₃Bₙ | Ge₃N | Ge₃P | C₃N | C₃P | C₃As | Si₃N | Si₃P | Si₃As |
|------|------|------|-----|-----|------|------|------|------|
|      | GGA  | GGA  | HSE06 | HSE06 | HSE06 | HSE06 | HSE06 | HSE06 |
| Bulk | 0.23 | 1.24 | 1.87 | 0    | 0.01 | 0.58 | 0    | 0.30 | 0.49 |
| 1-layer | 0.35 | 0.62 | 1.42 | 0    | 0.28 | 0.56 | 0.46 | 0.25 | 0.50 |
| 2-layers | 1.00 | 0.18 | 2.08 | 0.33 | 0.52 | 0.93 | 0.93 | 0.49 | 0.97 |
| 3-layers | 0.32 | 0.26 | 1.18 | 0    | 0.91 | 0.52 | 0.57 | 0.23 | 0.73 |
| 4-layers | 0.93 | 0.77 | 1.84 | 0.36 | 0.84 | 1.28 | 1.00 | 0.53 | 1.20 |

### Table 4. The stiffness C₂D, DP constant E₁, effective mass m⁺, and mobility carrier μ₂D of monolayer structure along with the armchair and zigzag directions.

| Direction | C₂D (N/m) | E₁ (eV) | m⁺ (m₀) | μ₂D (cm²V⁻¹s⁻¹) |
|-----------|-----------|---------|---------|------------------|
| Arm       | 381.6     | −7.6    | −7.4    | 0.6              | 0.9              | 0.6 | 0.3 | 47554.7 |
| C₃N       | 381.3     | −4.3    | −7.4    | 0.3              | 0.4              | 35620.0 | 508.0 |
| Arm       | 233.8     | −2.8    | −5.6    | 0.7              | 1.1              | 9797.7 | 87.6 |
| C₃P       | 233.5     | −2.7    | −5.1    | 0.4              | 0.5              | 2803.9 | 483.4 |
| Arm       | 206.4     | −2.8    | −2.1    | 0.7              | 1.0              | 807.0 | 620.7 |
| C₃As      | 205.6     | −1.5    | −2.1    | 0.4              | 0.5              | 8480.2 | 2711.9 |
| Arm       | 106.4     | −3.2    | −1.8    | 0.5              | 0.8              | 236.8 | 734.2 |
| Si₃N      | 106.3     | −1.8    | −2.7    | 0.3              | 0.5              | 6230.3 | 1867.6 |
| Arm       | 75.3      | −2.1    | −4.1    | 0.7              | 1.0              | 485.0 | 70.1 |
| Si₃P      | 75.5      | −7.9    | −4.2    | 0.4              | 0.5              | 107.9 | 215.0 |
| Arm       | 70.4      | −3.0    | −2.7    | 0.4              | 1.0              | 601.0 | 157.6 |
| Si₃As     | 70.1      | −2.8    | −2.1    | 0.3              | 0.5              | 1679.7 | 895.5 |
| Arm       | 72.9      | −0.5    | −1.3    | 0.3              | 0.5              | 4735.4 | 2433.7 |
| Ge₃N      | 72.9      | −0.2    | −1.2    | 0.3              | 0.4              | 346296.4 | 4705.8 |
| Arm       | 55.7      | −2.7    | −1.9    | 0.6              | 1.0              | 272.6 | 235.8 |
| Ge₃P      | 55.3      | −2.4    | −1.0    | 0.4              | 0.6              | 952.8 | 2811.7 |
| Arm       | 52.4      | −3.4    | −3.7    | 0.5              | 1.1              | 218.9 | 47.9 |
| Ge₃As     | 52.1      | −3.5    | −2.6    | 0.4              | 0.6              | 338.4 | 350.1 |

We further studied the electron structure of multi-layer A₃Bₓ, as shown in table 3. Shi et al. found that the double-layer C₃N structure formed by AE accumulation is more stable [45]. In this paper, only the multi-layer A₃B energy band properties of the AEA stacking sequence are studied. In AE stacking pattern, e.g., C₃N bilayer (Figure S2), the top-layer atom moves about √3/2 times C-N bond length along the zigzag direction. The order of band gap in single layer A₃B is: C₃As > C₃N > Ge₃As > Si₃As > Ge₃P > Si₃P > Ge₃N > Si₃N > C₃P. Compared with MoS₂ (1.8 eV) [46] and phosphorene (1.88 eV) [47], monolayer A₃Bₙ possesses a slightly small band gap. The calculated band gaps of single-, double-, three- and four-layer C₃N are 1.00 eV, 0.93 eV, 0.81 eV, and 0.75 eV, respectively, which is consistent with the reported results in the literature [48]. For the bulk C₃N, the band-gap value further decreases to 0.45 eV. The results show that the band gap of C₃N and C₃As decreases with the increase of the number of layers monotonously. The similar results were also found on MoS₂ [49]. Besides, the relationship between layer number and the calculated band-gap values of C₃P and Si₃N exhibits a similar pattern compared with that of C₃N. However, in the case of Si₃As, Si₃P, Ge₃P and Ge₃N, the band-gap values do not show any patterns with the layer number. The reason for this difference remains to be elucidated.

A critical feature in 2D materials is the carrier mobility at the band extremes (CBM and VBM). Mobility determines the electrical conductivity of a semiconductor material. The mobility of A₃B is calculated based on deformation potential (DP) theory [50]. As shown in Figure S4, the deformation potential is derived from the linear fitting of the respective energies of the conduction-band maximum and the valence-band minimum [51].
The deformation potential, effective mass and carrier mobility are calculated in table 4. Among A3Bs, C3As, Si3N and Ge3N show a high mobility along the zigzag (armchair) direction. Ge3N shows the highest electron mobility along zigzag up to $3.46 \times 10^5 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$, which is far greater than that in the MoS2 ($200 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$) [52]. The major reason for the high electron mobility is the small DP constant ($-0.2$) along the zigzag direction. The conducting rates between zigzag and armchair directions in C3As, Si3N and Ge3N are 10.5:1, 26.4:1 and 7.3:1, respectively, indicating a typically anisotropic characteristics. As report in phosphorene, the ratio of the conductivities along the armchair and zigzag directions is 1.8 [53]. The anisotropic features of C3As, Si3N and Ge3N are more significant than that in phosphorene. We found that the hole mobility in A3Bs is also anisotropic. The ratio of the conductivities along zigzag and armchair directions in C3As, Ge3N and Ge3P are 4.4:1, 1.9:1 and 11.9:1, respectively. The monolayer Ge3N has a super high mobility up to $4.7 \times 10^5 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$ for the holes along the zigzag direction. However, it’s two orders of magnitude lower than the electron mobility. It was suggested that the DP constant is also a reason that influences the hole’s mobility. The excellent electrical conductivity makes monolayer A3B have a broad application in electrode materials and microelectronics.

A3B has a broad application prospect in many fields, such as high-speed field-effect transistors, energy storage and optoelectronic devices. In particular, the ultrahigh in-plane stiffness of C3N monolayer suggests that C3N has an application prospect in structural superlubricity, because high in-plane stiffness of layered materials can minimize the in-plane deformation of layered materials and hence preserve the incommensurate state during sliding [54–56].

4. Conclusions

In summary, the mechanical and electronic properties of group IV-V materials A3B have been systematically studied. The elastic constants of two-dimensional monolayer A3B are calculated by using the strain energy method. The in-plane stiffness of A3B family decreases with the increase of relative molecular mass. A3B have isotropic elastic parameters such as the Young’s modulus and Poisson’s ratio. The ultimate strength of A3B was also calculated. Monolayer C3N has the highest ultimate strength and Young’s modulus. The band gap of C3N can be modified significantly by strain engineering. It is also found that the band gap of C3N is more sensitive to zigzag deformation when the uniaxial tensile strain is applied. Besides, electrons and holes in the A3B show anisotropic and high mobility, which can be ascribed to the anisotropic effective-masses and deformation-potential constants. These findings will help to the future applications of the 2D group IV-V materials, such as high-speed field-effect transistors, energy storage, optoelectronic devices and structural superlubricity.

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Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

Conflicts of interest

The authors declare no competing financial interest.

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