Mechanical and electronic properties of graphitic carbon nitride (g-C₃N₄) under biaxial strain

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ABSTRACT

Using the first-principles density functional theory calculations, we investigate the mechanical and electronic properties of biaxially strained graphitic carbon nitride (g-C₃N₄). The results show highly isotropic mechanical properties and large linear elasticity of g-C₃N₄. Moreover, both the Perdew-Burke-Ernzerhof (PBE) and Heyd-Scuseria-Ernzerhof (HSE06) band gaps reach the maximum values at 10% strain. The bonding properties are analyzed based on the electronic localization function (ELF). In addition, the photon transition between band gap is weak, suggesting the monolayer g-C₃N₄ is not suitable for a solar cell material. Enough biaxial strain can induce the spin splitting of g-C₃N₄, and it is found that the spin-unrestricted band gap of g-C₃N₄ can be overestimated. This work provides valuable insights for designing the new elastic electronic and spintronic devices based on two-dimensional g-C₃N₄.

1. Introduction

Graphitic carbon nitride (g-C₃N₄) is an attractive, inexpensive metal-free semiconductor with a two-dimensional (2D) structure consisting of π -conjugated graphitic planes formed via sp² hybridization of carbon and nitrogen [1,2]. G-C₃N₄ has attracted significant attention of scientists due to its unique properties, such as relatively narrow band gap, visible light harvest, natural preparation, "earth-abundant" nature, non-toxicity as well as high thermal and chemical stability [3–6]. In addition, g-C₃N₄ has a larger surface area, more reactive sites, and shorter carrier migration distance compared to bulk materials [1,2,7,8]. However, pristine g-C₃N₄ has slight absorption within a visible light region ($\lambda < 460$ nm) and a poor photocatalysis efficiency because of the fast recombination of photogenerated electron-hole pairs [9].

Therefore, most researches of g-C₃N₄ focus on its modification to improve catalytic performance, such as adsorption, inclusion, and

building heterostructures [8–10]. Both theoretical calculations and experimental demonstrations have demonstrated that all these methods are effective for improving photocatalysis efficiency in comparison with pristine g-C₃N₄ [10,11]. Notably, for many heterostructures such as graphene/g-C₃N₄ [12], g-C₃N₄/MoS₂ [13], g-C₃N₄/BiVO₄ [14,15], and g-C₃N₄/Ag₃PO₄ [16] have significantly enhanced photocatalytic performance compared to pure g-C₃N₄. In these systems, the charge rearrangement between two structures could induce the rapid separation of the built-in electric field and carrier mobility, so that the photocatalytic activity can be further enhanced. All these manners will cause significant changes of mechanical and electronic properties of materials. Strain engineering is also one powerful approach for controlling electron transport in 2D materials. Some previous studies have shown that strain can regulate the photocatalytic properties of heterostructures, including CdS/g-C₃N₄ [17], InSe/g-C₃N₄ [18], and g-C₃N₄/BiOI/EG Ref. [19]. Ruan et al. have calculated and analyzed the mechanical properties of

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Fig. 1. Top and side views of optimized g-C₃N₄ with 0% strain. The green and yellow circles represent C and N atoms, respectively, and arrows indicate the orientation of biaxial tensile strain. There are two types of C atoms (signed as C1 and C2) and three types of N atoms (signed as N1, N2, N3), and accordingly the N1–C1, C1–N2, N2–C2 and C2–N3 bonds are represented as B1, B2, B3 and B4, respectively. Contours illustrate the ELF within the unit cell, which is represented by the dashed black parallelogram. (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

pure g-C₃N₄ [20]. However, the effects of biaxial strain on pristine g-C₃N₄ are less clear. Besides, it is also unclear whether the electronic properties of pristine g-C₃N₄ is affected by the biaxial strain. These two problems have to be solved in a bid to obviously enhance the potential applications of g-C₃N₄.

In this paper, we have investigated the mechanical and electronic and properties of biaxially strained g-C₃N₄ by using first-principles density functional theory (DFT) [21,22] calculations. The rest of the paper is organized as follows. Section 2 gives the calculation methods and optimized structures of g-C₃N₄. Section 3 describes the effects of biaxial strain on the regulation of mechanical properties and electronic structures of g-C₃N₄. Section 4 presents the conclusions.

2. Computational methods and optimized structures

First-principles calculations are performed with the Vienna *ab initio* Simulation Package (VASP) [21–24] program based on DFT using the projector augmented wave (PAW) [21,22,25] approach and the generalized gradient approximation of Perdew-Burke-Ernzerhof (GGA-PBE) form [26]. For accurate electrical calculations, the Monkhorst-Pack k-point meshes [27] of $5 \times 5 \times 1$ is used for the PBE and Heyd-Scuseria-Ernzerhof screened hybrid functional (HSE06) methods.

The total energy and force are converged to 10^{-6} eV and 0.02 eV/Å. The tensile biaxial strain is applied from 0% to 20% with an increment of 1% per step. The biaxial strain is defined as [28]:

$$\varepsilon = (a - a_0)/a_0 = (b - b_0)/b_0 \quad (1)$$

where a , b and a_0 , b_0 are the deformed (stretched or shrunk) and initial equilibrium lattice constants of the unit cell.

The optimized structure of monolayer g-C₃N₄ is shown in Fig. 1. The lattice constant for g-C₃N₄ without strain is $a = b = 7.15$ Å, which is the same with previous theoretical results [29,30]. It shows that there are six carbon atoms and eight nitrogen atoms in the unit cell of the optimized g-C₃N₄. Based on the structural symmetry, g-C₃N₄ possesses two types of C atoms (signed as C1 and C2) and three types of N atoms (signed as N1, N2, N3). Therefore, there are four types of N–C bonds, signed as the N1–C1, N2–C1, N2–C2, and N3–C2, which are represented as B1, B2, B3 and B4, respectively. To study the bonding interactions in g-C₃N₄, the electron localization function (ELF) [31] within the unit cell has been illustrated in Fig. 1. The ELF values vary between 0 and 1. It is clear that the electron localization occurs around the center of all N–C bonds of the g-C₃N₄, showing covalent bonding characters.

Fig. 2. (a) Young's modulus $E(\theta)$ and (b) Poisson's ratio $\nu(\theta)$ for g-C₃N₄.

Fig. 3. (a) Is stress-strain curve for g-C₃N₄, (b) and (c) are the bond length-strain curves, and (d) is the ELF for g-C₃N₄ under 10% strain.

3. Results and discussions

3.1. Mechanical properties

For a 2D g-C₃N₄, its elastic constants can be represented through the following equation [32]:

$$C_{ij} = \begin{pmatrix} C_{11} & C_{12} & 0 \\ C_{12} & C_{22} & 0 \\ 0 & 0 & C_{44} \end{pmatrix} \quad (2)$$

accordingly, the Young's modulus $E(\theta)$ and Poisson's ratio $\nu(\theta)$ along arbitrary in-plane of g-C₃N₄ can be calculated from the elastic constants by the following equations [32]:

$$E(\theta) = \frac{\Delta}{C_{11}s^4 + C_{12}c^4 + \left(\frac{\Delta}{C_{44}} - 2C_{12}\right)c^2s^2} \quad (3)$$

$$\nu(\theta) = -\frac{\left(C_{11} + C_{12} - \frac{\Delta}{C_{44}}\right)c^2s^2 - C_{12}(c^4 + s^4)}{C_{11}s^4 + C_{22}c^4 + \left(\frac{\Delta}{C_{44}} - 2C_{12}\right)c^2s^2} \quad (4)$$

Where $\Delta = C_{11}C_{22} - C_{12}^2$, $s = \sin \theta$ and $c = \cos \theta$, θ is the angle between the unit vectors in the xOy plane and the x-axis in Fig. 2. The calculated elastic constants (C_{ij}) are $C_{11} = 198.197$, $C_{12} = 45.736$, $C_{22} = 197.454$ and $C_{44} = 75.863$ respectively. It is obvious that the monolayer g-C₃N₄ is isotropic and has a high Young's modulus (Figs. 2a and 187 N/m). The Poisson ratio is constant in the angle θ (Figs. 2b and 0.23), which further verifies the planar isotropy the monolayer g-C₃N₄.

Fig. 3a shows the stress-strain curve of g-C₃N₄ under biaxial strain from 0% to 20%. It is found that the stress-strain curve presents almost linear growth with the biaxial strain increasing from 0% to 10%,

showing large linear elasticity, which is similar to other 2D materials, like graphene, MoS₂ and borophene [33,34], whose deformation are mostly produced by bond stretching. We note that in the porous structure of g-C₃N₄, the first deformation is mainly implemented from the structural deflection rather than the bond stretching, which can induce better malleability compared with the complete 2D materials like graphene, borophene et al. [34,35]. And the maximum stress is about 59.27 N/m at 10% strain. Because of its porous structure, during the initial stretch, the deformation is mostly due to the structural deflection instead of the bond stretch. Then the stress decreases nonlinearly with the increasing strain, indicating higher brittleness of g-C₃N₄ under biaxial tensile strain.

To further investigate the strain-induced mechanism of g-C₃N₄, we show the bond length-strain curves in Fig. 3b and c, where we consider four different N-C bonds marked in Fig. 1. It is found that the B1, B2, and B3 bonds increase first and then decreases lowly with the increasing biaxial tensile strain, which reduces the stress in Fig. 3a. However, the B4 bond will always increase with strain, and its stretch is more significant than the B1, B2, and B3 bonds, since the stress of g-C₃N₄ is concentrated around the tip of pores. This result is similar to the nanoporous graphene [36,37]. In Fig. 3d, we show the ELF contour of g-C₃N₄ at 10% strain, and we found that the B4 bond suddenly breaks at 10% strain. But the ELF values around B1, B2, and B3 bonds are all 0.85, suggesting the complete covalent bonding of these bonds under stretching tension. Besides, the phonon spectrum for the g-C₃N₄ under large strain is investigated and shown in supporting information Figs. S1a-S1b. Here, the g-C₃N₄ under 10% and 17% strains are taken as example. We can see obvious imaginary frequency modes under large strain, exhibiting the g-C₃N₄ is dynamically unstable to the lattice distortion, which is similar to the results of other materials under large strain [38].

Fig. 4. PBE and HSE06 calculated band gap-strain curves for g-C₃N₄.

3.2. Electronic properties

Fig. 4 shows the band gap-strain curves calculated by the PBE and HSE06 methods. At the same strain, the HSE06 band gaps for the single layer g-C₃N₄ are found to be higher than the PBE values. Generally, the HSE06 band gaps are closer to the experimental values [39] compared to the PBE results. This is because HSE06 corrects the underestimation of band gap by partially removing the self interaction. Previous studies have shown that the hybrid-functional HSE06 method shows significant improvement of band gap of 2D materials [40–43]. Moreover, both PBE and HSE06 methods have shown the same variation trends of gap-strain curves. For example, both of their band gaps are increasing with the increasing strain, and the maximum of band gap is at 10% strain.

Therefore, it is challenging to predict the band gap accurately. The PBE and HSE06 calculated band structures of g-C₃N₄ are shown in Fig. 5a–c and Fig. 5g–i, respectively. It is clear that g-C₃N₄ is an indirect band gap semiconductor at 0% strain (Fig. 5a and g), and PBE method shows semiconductor-metal transitions under 17% strains, respectively (Fig. 5c). Previous studies [40,42–45] on other 2D honeycomb materials have proven that the band gap calculated by DFT obeys similar strain-dependency, suggesting that the electronic properties can be effectively regulated by changing strain, and g-C₃N₄ is so flexible that may have potential applications in flexible devices. In addition, we have also calculated the PBE high transition probabilities between the upper most valence band (VB) and the lowest conduction band (CB) of g-C₃N₄, which are shown by the squares of the dipole transition matrix elements [46], P^2 , at k points in Fig. 5d–f. For the strain of 0% and 17% (Fig. 5d and f), we can see that the dipole matrix elements are zero between CB and VB edges at all k points, indicating that there is no photon transition between CB and VB edges. However, at strain of 10% (Fig. 5e), the calculated dipole transition matrix element increases as the k point change from Γ to M point. Hence, the single layer g-C₃N₄ shows weak photon transition between band gap, that is to say, the biaxial tensile strain could not make the pure g-C₃N₄ to be an ideal material for thin-film solar cell applications.

We further simulate the spin electronic properties of the biaxial strained g-C₃N₄ using PBE spin-unrestricted and spin-restricted calculations upon the singlet ground state. Here, we take the g-C₃N₄ at 0%, 10% and 17% strain for example. First of all, for the spin-unrestricted calculation, the magnetic moment of g-C₃N₄ is calculated to be 0 at 0% and 10% strain. This is mainly because both C and N atoms do not have highly localized d electrons. However, the magnetic moment is 0.213 μ_B at 17% biaxial strain, indicating that enough biaxial strain can induce spin-splitting. For spin-restricted calculations upon 0% and 10% strained systems, we artificially set the total magnetic moment as 2 μ_B , realizing the spin inversion of one electron, that is to say, the lowest triple state. We plot the spin-unrestricted and spin-restricted spin

Fig. 5. (a)–(c) and (d)–(f) are PBE calculated band structures and transition matrix elements for g-C₃N₄ under strain of 0%, 10% and 17%. (g)–(i) are HSE06 calculated band structures for g-C₃N₄ under strain of 0%, 10% and 17%. The Fermi energy is set at zero energy and indicated by the red dashed line. (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

densities of g-C₃N₄ in the supporting information Figs. S2a–S2d, at 0% and 10% strain, showing the D6h symmetry, mainly because the biaxial deformation is subjected to the equibiaxial case. This is really different from these uniaxial and shear deformations [40,42,43,47], which can induce symmetry-breaking. The projected density of states (PDOS) of g-C₃N₄ without strain in Fig. S3 shows that, when the system is excited from the ground state to the lowest triple state, the electron located on p_y state of N atom transfers to p_z state of C atom. In addition, we show the spin band structures of g-C₃N₄ in Figs. S4a–S4d. It is obvious that the band gap of spin-unrestricted system is higher than that of the corresponding spin-restricted, showing that the spin-unrestricted calculation can yield overestimated band gaps. Compared with previous studies upon g-C₃N₄ [39,48], the biaxial strained pure g-C₃N₄ demonstrates more interesting potential applications in elastic spintronic devices and new 2D magnets.

4. Conclusions

In summary, we perform first-principles calculations based on DFT to study the mechanical and electronic properties of g-C₃N₄ under biaxial strain range from 0% to 20%. Through research, we found that g-C₃N₄ shows highly isotropic mechanical properties, and the Young's modulus is estimated to be 187 N/m. Under the same strain, the HSE06 band gap energies are higher than PBE values. PBE calculated band structures show semiconductor-metal transitions under 17% strain. Moreover, at 10% strain, the B4 bond breaks and both the stress and band gap of g-C₃N₄ reach the maximum values. The g-C₃N₄ under biaxial strain has a weak photon transition between its band gap. When the biaxial strain increases to 17%, there is spin splitting, and the magnetic moment is 0.213 μ_B . Both the spin-unrestricted and spin-restricted spin densities of g-C₃N₄ show D6h symmetry because of the deformation is applied by the equibiaxial strain. Besides, the spin-unrestricted calculation can yield overestimated band gap of g-C₃N₄. This work presents a simple and promising approach for developing high-efficiency g-C₃N₄ based elastic electronic and spintronic devices.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.vacuum.2020.109358>.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

References

- [1] D. Yuan, W. Huang, X. Chen, Z. Li, J. Ding, L. Wang, H. Wan, W.L. Dai, G. Guan, Introduction of in-plane π -conjugated heterojunction via rGO modulation: a promising approach to enhance photoexcited charge separation and transfer of g-

- C₃N₄, Appl. Surf. Sci. 48 (2019) 658–667, <https://doi.org/10.1016/j.apsusc.2019.05.303>.
- [2] S. Bellamkonda, R. Shanmugam, R.R. Gangavarapu, Extending the π -electron conjugation in 2D planar graphitic carbon nitride: efficient charge separation for overall water splitting, J. Mater. Chem. A 7 (2019) 3757–3771, <https://doi.org/10.1039/C8TA10580D>.
- [3] F. Li, X. Gu, K. Zhang, T.T. Nguyen, M. Guo, Fabrication of freestanding NFC/g-C₃N₄ composite film as supercapacitor electrode via vacuum-induced self-assembly, Vacuum 160 (2019) 54–59, <https://doi.org/10.1016/j.vacuum.2018.10.005>.
- [4] M. Gao, R. Tong, H. Huang, Y. Kang, Q. Luo, Y. Huang, P.K. Chu, Activation of graphitic carbon nitride by surface discharge plasma treatment for enhanced photocatalysis, Vacuum 159 (2019) 235–238, <https://doi.org/10.1016/j.vacuum.2018.10.038>.
- [5] P. Arora, A.P. Singh, B.R. Mehta, S. Basu, Metal doped tubular carbon nitride (tC₃N₄) based hematite photoanode for enhanced photoelectrochemical performance, Vacuum 146 (2017) 570–577, <https://doi.org/10.1016/j.vacuum.2017.07.010>.
- [6] G. Liao, Y. Gong, L. Zhang, H. Gao, G.J. Yang, B. Fang, Semiconductor polymeric graphitic carbon nitride photocatalysts: the “holy grail” for the photocatalytic hydrogen evolution reaction under visible light, Energy Environ. Sci. 12 (2019) 2080–2147, <https://doi.org/10.1039/C9EE00717B>.
- [7] H. Miao, G. Zhang, X. Hu, J. Mu, T. Han, J. Fan, C. Zhu, L. Song, J. Bai, X. Hou, A novel strategy to prepare 2D g-C₃N₄ nanosheets and their photoelectrochemical properties, J. Alloy. Compd. 690 (2017) 669–676, <https://doi.org/10.1016/j.jallcom.2016.08.184>.
- [8] D. Zhou, C. Qiu, Study on the effect of Co doping concentration on optical properties of g-C₃N₄, Chem. Phys. Lett. 728 (2019) 70–73, <https://doi.org/10.1016/j.cplett.2019.04.060>.
- [9] J. Wang, Q. Lu, S. Zhao, Two-dimensional g-C₃N₄/ α -GaAlO₄Ga₂O₂ p-n heterostructure with improved visible-light-driven photocatalytic property, Appl. Surf. Sci. 470 (2019) 150–160, <https://doi.org/10.1016/j.apsusc.2018.11.139>.
- [10] B. Zhu, S. Wageh, A.A. Al-Ghamdi, S. Yang, Z. Tian, J. Yu, Adsorption of CO₂, O₂, NO and CO on s-triazine-based g-C₃N₄ surface, Catal. Today 335 (2019) 117–127, <https://doi.org/10.1016/j.cattod.2018.09.038>.
- [11] X. Hao, J. Zhou, Z. Cui, Y. Wang, Y. Wang, Z. Zou, Zn-vacancy mediated electron-hole separation in ZnS/g-C₃N₄ heterojunction for efficient visible-light photocatalytic hydrogen production, Appl. Catal. B Environ. 229 (2018) 41–51, <https://doi.org/10.1016/j.apcatb.2018.02.006>.
- [12] H.Z. Wu, S. Bandaru, J. Liu, L.L. Li, Z. Wang, Adsorption of H₂O, H₂, O₂, CO, NO, and CO₂ on graphene/g-C₃N₄ nanocomposite investigated by density functional theory, Appl. Surf. Sci. 430 (2018) 125–136, <https://doi.org/10.1016/j.apsusc.2017.06.073>.
- [13] X. Shi, M. Fujitsuka, S. Kim, T. Majima, Faster electron injection and more active sites for efficient photocatalytic H₂ evolution in g-C₃N₄/MoS₂ hybrid, Small 14 (2018) 1703277, <https://doi.org/10.1002/smll.201703277>.
- [14] J. Zhang, F. Ren, M. Deng, Y. Wang, Enhanced visible-light photocatalytic activity of a g-C₃N₄/BiVO₄ nanocomposite: a first-principles study, Phys. Chem. Phys. 17 (2015) 10218–10226, <https://doi.org/10.1039/C4CP06089J>.
- [15] J. Zhang, M. Deng, Y. Yan, T. Xiao, W. Ren, P. Zhang, Tunable type-II BiVO₄/g-C₃N₄ Nanoheterostructures for photocatalysis applications, Phys. Rev. Appl. 11 (2019), 044052, <https://doi.org/10.1103/PhysRevApplied.11.044052>.
- [16] X. Miao, X. Yue, Z. Ji, X. Shen, H. Zhou, M. Liu, K. Xu, J. Zhu, G. Zhu, L. Kong, S. A. Shah, Nitrogen-doped carbon dots decorated on g-C₃N₄/Ag₃PO₄ photocatalyst with improved visible light photocatalytic activity and mechanism insight, Appl. Catal. B Environ. 227 (2018) 459–469, <https://doi.org/10.1016/j.apcatb.2018.01.057>.
- [17] G. Wang, F. Zhou, B. Yuan, S. Xiao, A. Kuang, M. Zhong, S. Dang, X. Long, W. Zhang, Strain-tunable visible-light-responsive photocatalytic properties of two-dimensional CdS/g-C₃N₄: a hybrid density functional study, Nanomaterials 9 (2019) 244, <https://doi.org/10.3390/nano9020244>.
- [18] H.C. Zhang, J.H. Zhang, W.X. Zhang, T.T. Li, Type-II InSe/g-C₃N₄ heterostructure as a high-efficiency oxygen evolution reaction catalyst for photoelectrochemical water splitting, J. Phys. Chem. Lett. 10 (2019) 3122–3128, <https://doi.org/10.1021/acs.jpclett.9b00909>.
- [19] P.J. Mafa, A.T. Kuvarega, B.B. Mamba, B. Ntsendwana, Photoelectrocatalytic degradation of sulfamethoxazole on g-C₃N₄/BiOI/EG p-n heterojunction photoanode under visible light irradiation, Appl. Surf. Sci. 483 (2019) 506–520, <https://doi.org/10.1016/j.apsusc.2019.03.281>.
- [20] L. Ruan, Y. Zhu, L. Qiu, Y. Lu, Mechanical properties of doped g-C₃N₄-a first-principle study, Vacuum 106 (2014) 79–85, <https://doi.org/10.1016/j.vacuum.2014.02.015>.
- [21] G. Kresse, J. Hafner, Ab initio molecular dynamics for liquid metals, Phys. Rev. B 47 (1993) 558–561, <https://doi.org/10.1103/PhysRevB.47.558>.
- [22] G. Kresse, J. Furthmüller, Efficient iterative schemes for ab initio total-energy calculations using a plane-wave basis set, Phys. Rev. B 54 (1996) 11169–11186, <https://doi.org/10.1103/PhysRevB.54.11169>.
- [23] G. Kresse, J. Hafner, Ab initio molecular-dynamics simulation of the liquid-metal-amorphous-semiconductor transition in germanium, Phys. Rev. B 49 (1994) 14251–14269, <https://doi.org/10.1103/PhysRevB.49.14251>.
- [24] G. Kresse, J. Furthmüller, Efficiency of ab-initio total energy calculations for metals and semiconductors using a plane-wave basis set, Comput. Mater. Sci. 6 (1996) 15–50, [https://doi.org/10.1016/0927-0256\(96\)00008-0](https://doi.org/10.1016/0927-0256(96)00008-0).
- [25] G. Kresse, D. Joubert, From ultrasoft pseudopotentials to the projector augmented-wave method, Phys. Rev. B 59 (1999) 1758–1775, <https://doi.org/10.1103/PhysRevB.59.1758>.

- [26] J.P. Perdew, K. Burke, M. Ernzerhof, Generalized gradient approximation made simple, *Phys. Rev. Lett.* 77 (1996) 3865–3868, <https://doi.org/10.1103/PhysRevLett.77.3865>.
- [27] H.J. Monkhorst, J.D. Pack, Special points for Brillouin-zone integrations, *Phys. Rev. B* 13 (1976) 5188–5192, <https://doi.org/10.1103/PhysRevB.13.5188>.
- [28] L. Sun, Q.X. Li, H. Ren, H.B. Su, Q.W. Shi, J.L. Yang, Strain effect on electronic structures of graphene nanoribbons: a first principles study, *J. Chem. Phys.* 129 (2008), 074704, <https://doi.org/10.1063/1.2958285>.
- [29] B. Zhu, J. Zhang, C. Jiang, B. Cheng, J. Yu, First principle investigation of halogen-doped monolayer g-C₃N₄ photocatalyst, *Appl. Catal. B Environ.* 207 (2017) 27–34, <https://doi.org/10.1016/j.apcatb.2017.02.020>.
- [30] J. Cui, S. Liang, X. Wang, J. Zhang, First principle modeling of oxygen-doped monolayer graphitic carbon nitride, *Mater. Chem. Phys.* 161 (2015) 194–200, <https://doi.org/10.1016/j.matchemphys.2015.05.036>.
- [31] B. Silvi, A. Savin, Classification of chemical-bonds based on topological analysis of electron localization functions, *Nature* 371 (1994) 683–686, <https://doi.org/10.1038/371683a0>.
- [32] E. Cadelano, P.L. Palla, S. Giordano, L. Colombo, Elastic properties of hydrogenated graphene, *Phys. Rev. B* 82 (2010) 235414, <https://doi.org/10.1103/PhysRevB.82.235414>.
- [33] S. Biccai, C.S. Boland, D.P. O'Driscoll, A. Harvey, C. Gabbett, D.R. O'Suilleabhain, A.J. Griffin, Z. Li, R.J. Young, J.N. Coleman, Negative gauge factor piezoresistive composites based on polymers filled with MoS₂ nanosheets, *ACS Nano* 13 (2019) 6845–6855, <https://doi.org/10.1021/acsnano.9b01613>.
- [34] H. Zhong, K. Huang, G. Yu, S. Yuan, Electronic and mechanical properties of few-layer borophene, *Phys. Rev. B* 98 (2018), 054104, <https://doi.org/10.1103/PhysRevB.98.054104>.
- [35] Y. Zeng, C.L. Lo, S. Zhang, Z. Chen, A. Marconnet, Dynamically tunable thermal transport in polycrystalline graphene by strain engineering, *Carbon* 158 (2020) 63–68, <https://doi.org/10.1016/j.carbon.2019.11.060>.
- [36] B. Mortazavi, M.E. Madjet, M. Shahrokhi, S. Ahzi, X. Zhuang, T. Rabczuk, Nanoporous graphene: a 2D semiconductor with anisotropic mechanical, optical and thermal conduction properties, *Carbon* 147 (2019) 377–384, <https://doi.org/10.1016/j.carbon.2019.03.018>.
- [37] A.A. Anastasi, K. Ritos, G. Cassar, M.K. Borg, Mechanical properties of pristine and nanoporous graphene, *Mol. Simulat.* 42 (2016) 1502–1511, <https://doi.org/10.1080/08927022.2016.1209753>.
- [38] Y.W. Luo, J.H. Hu, Y. Jia, Novel porous aluminum nitride monolayer: a first-principles study, *J. Phys. Condens. Matter* 32 (2020) 225301, <https://doi.org/10.1088/1361-648X/ab73a0>.
- [39] X. Wang, K. Maeda, A. Thomas, K. Takanabe, G. Xin, J.M. Carlsson, K. Domen, M. Antonietti, A metal-free polymeric photocatalyst for hydrogen production from water under visible light, *Nat. Mater.* 8 (2009) 76–80, <https://doi.org/10.1038/NMAT2317>.
- [40] T.V. Vu, N.V. Hieu, H.V. Phuc, N.N. Hieu, H.D. Bui, M. Idrees, B. Amin, C. V. Nguyen, Graphene/WSeTe van der Waals heterostructure: controllable electronic properties and Schottky barrier via interlayer coupling and electric field, *Appl. Surf. Sci.* 507 (2020) 145036, <https://doi.org/10.1016/j.apsusc.2019.145036>.
- [41] H.U. Din, M. Idrees, A. Albar, M. Shafiq, I. Ahmad, C.V. Nguyen, B. Amin, Rashba spin splitting and photocatalytic properties of GeC-MSse ($M = \text{Mo}, \text{W}$) van derWaals heterostructures, *Phys. Rev. B* 100 (2019) 165425, <https://doi.org/10.1103/PhysRevB.100.165425>.
- [42] K.D. Pham, N.N. Hieu, H.V. Phuc, I.A. Fedorov, C.A. Duque, B. Amin, C.V. Nguyen, Layered graphene/GaS van der Waals heterostructure: controlling the electronic properties and Schottky barrier by vertical strain, *Appl. Phys. Lett.* 113 (2018) 171605, <https://doi.org/10.1063/1.5055616>.
- [43] D.D. Vo, T.V. Vu, N.V. Hieu, N.N. Hieu, H.V. Phuc, N.T.T. Binh, L.T.T. Phuong, M. Idrees, B. Amin, C.V. Nguyen, Band alignment and optical features in Janus-MoSeTe/X(OH)₂ ($X = \text{Ca}, \text{Mg}$) van der Waals heterostructures, *Phys. Chem. Chem. Phys.* 21 (2019) 25849–25858, <https://doi.org/10.1039/C9CP06019G>.
- [44] W. Guo, X. Ge, S. Sun, Y. Xie, X. Ye, The strain effect on the electronic properties of the MoSse/WSe van der Waals heterostructure: a first-principles study, *Phys. Chem. Chem. Phys.* 22 (2020) 4946–4956, <https://doi.org/10.1039/D0CP00403K>.
- [45] L.H. Qu, J. Yu, Y.L. Mu, X.L. Fu, C.G. Zhong, Y. Min, P.X. Zhou, J.M. Zhang, Y. Q. Zou, T.S. Lu, Strain tunable structural, mechanical and electronic properties of monolayer tin dioxides and dichalcogenides SnX₂ ($X = \text{O}, \text{S}, \text{Se}, \text{Te}$), *Mater. Res. Bull.* 119 (2019) 110533, <https://doi.org/10.1016/j.materresbull.2019.110533>.
- [46] A.E. Maughan, A.M. Ganose, M.M. Bordelon, E.M. Miller, D.O. Scanlon, J. R. Neilson, Defect tolerance to intolerance in the vacancy-ordered double perovskite semiconductors Cs₂SnI₆ and Cs₂TeI₆, *J. Am. Chem. Soc.* 138 (2016) 8453–8464, <https://doi.org/10.1021/jacs.6b03207>.
- [47] L.H. Qu, J.M. Zhang, K.W. Xu, V. Ji, Armchair graphene nanoribbons under shear strain, *Physica E* 60 (2014) 156–159, <https://doi.org/10.1016/j.physe.2014.02.021>.
- [48] D. Huang, Z. Li, G. Zeng, C. Zhou, W. Xue, X. Gong, X. Yan, S. Chen, W. Wang, M. Cheng, Megamerger in photocatalytic field: 2D g-C₃N₄ nanosheets serve as support of 0 D nanomaterials for improving photocatalytic performance, *Appl. Catal. B Environ.* 240 (2019) 153–173, <https://doi.org/10.1016/j.apcatb.2018.08.071>.