Research paper

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Vertical strain and electric field tunable electronic properties of type-II band alignment C_2N/InSe van der Waals heterostructure

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Abstract

In this work, we construct the C_2N/InSe heterostructure and investigate its electronic properties as well as the effect of strain and electric field. Our results demonstrate that the

weak van der Waals interactions are dominated in such heterostructure. It forms the type-II band alignment and implies the spatial separation of photogenerated electron-hole pairs. The type-II band alignment can be switched to type-I one and an indirect to direct band gap transition can be achieved by applying the electric field or vertical strain. Our findings demonstrate that the C_2N/InSe heterostructure can be considered to be a good candidate for optoelectronic and nanoelectronic devices.

Key words: C_2N; InSe; vdW heterostructure; Type-II band alignment; Electric field.

1 Introduction

Fifteen years have passed since the graphene was discovered firstly in 2004 by Geim and Novoselov [1], but there are still many its extraordinary properties and applications that have not been explored thoroughly. Furthermore, the absence of a sizable band gap in graphene hinders its applications for high-performance nano- and optodevices such as field effect transistors (FETs), or logic devices. To date, many approaches have been developed to modify the graphenes' band gap. On the other hand, graphene-like two-dimensional (2D) materials with a similar structure to graphene, such as hexagonal boron nitride [2], phosphorene [3–6], transition metal dichalcogenides (TMDs) [7–9], post-transition metal chalcogenides (PTMCs) [10,11] and others [12,13] have also been received considerable interests for the scientific community due to their promising physical and chemical properties, which are acceptable for applications in next-generation nanodevices. For instance, based on 2D MoS_2 material, Radisavljevic *et al.* [7] demonstrated a FET

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with a high mobility and current on/off ratio at room temperature. Hu *et al.* [11] fabricated successfully a photodetector based on an ultrathin GaSe, showing a high responsivity and high external quantum efficiency. Among these diverse 2D materials, one of the PTMCs materials called InSe monolayer has recently been synthesized successfully and has great potential for next-generation nanodevices [10,14]. Tamalampudi et al. showed that photodetectors based on InSe material possess a high photoresponse of 12 AW^{-1}. Feng et al. [15] demonstrated that a high field effect mobility up to 1000 cm^2/Vs at the room temperature can be achieved in the InSe-based FET. Moreover, the band gap of InSe crystal can be controlled by changing the number of layers due to quantum confinement [16] or by applying strains or electric field [17].

More recently, a novel kind 2D material, called graphene-like nitrogenated holey C_2N monolayer has been synthesized successfully by Mahmood and his group [18]. To date, there are numerous theoretical and experimental studies have focused on the physical properties of C_2N monolayer, which is suitable for nanodevices [19–24]. Similarly to graphene, the C_2N monolayer shows sp^2 hybridization characters, but it is a semiconductor with a direct band gap of about 2 eV at Γ-point [18]. From first principles calculations, Guan et al. [19] showed that the electronic and optical properties of the C_2N monolayer can be tuned effectively by applying uniaxial and biaxial strains. Their results demonstrated that this material can sustain a large strain 12 % and has a small stiffness constant. Owing to these mentioned unique properties and a high on/off ratio of 10^7 in the FET [18], the C_2N monolayer can be great potential for optoelectronic and electronic devices, such as FETs.

In parallel with the efforts on single 2D materials, 2D van der Waals heterostructures by constructing different single 2D materials have been attached intensive attention and open up an opportunity for designing and creating high-performance

nananodevices. To date, there have been already numerous experimental and theoretical efforts to investigate the advantages of the 2D vdW heterostructures. Examples are graphene-based vdW heterostructures [25–37], C_2N/XSe_2 (X = Mo, W) [38], $InSe/MoS_2$ [39], and SiC/MX_2 (M = Mo, W; X = S, Se) [40,41]. These studies have demonstrated that 2D vdW heterostructures show many promising properties, which may not hold for the single-layered materials. For example, Pham et al. [42] have demonstrated that the intrinsic electronic properties of the single-layered graphene and GaSe monolayer preserves in the graphene/GaSe heterostructure owing to the weak vdW interactions, which are not enough to modify the electronic properties of the isolated graphene and GaSe monolayer. In addition, a tiny band gap was opened at the Dirac point of graphene, making it suitable for the high-performance application. Li et al. [40] showed that the SiC/MoS_2 heterostructure forms a type-II band alignment, which is required for optodevices. Moreover, by applying a biaxial strain, the type-II band alignment in the SiC/MoS_2 can also be tuned and switched to type-III band alignment, improving the electronic performance of nanodevices based on such heterostructure.

Therefore, in this letter, based on the first-principles calculations from density functional theory (DFT), we design an ultrathin $C_2N/InSe$ vdW heterostructure and investigate its electronic properties as well as the effects of vertical strain and electric field. Our results demonstrate that the $C_2N/InSe$ heterostructure forms a type-II band alignment with an indirect band gap of 1.34 eV and implies the spatial separation of photogenerated electron-hole pairs. In addition, the band gap of the heterostructure can be tuned effectively by applying vertical strain and electric field.

2 Computational model and methods

In this letter, we perform the structural optimization and calculate the electronic properties of systems using the DFT method within the projector augmented wave (PAW) pseudopotentials [43], which is implemented in the Quantum Espresso open-source simulation package [44]. To better describe the exchange-correlation energy in the considered materials, the generalized gradient approximation (GGA) [45] by choosing the Perdew-Burke-Ernzerhof (PBE) [46] parametrization was adopt for all calculations. Moreover, in this work, in order to expand the wave functions, we use a plane-wave basic set with the kinetic cut-off energy of 510 eV. In all calculations, the convergence of the total energy was set to less than 10^{-5} eV. A Gaussian smearing with a smearing width of $\sigma = 0.001$ eV is applied. In addition, it should be noted that the traditional DFT methods are unable to describe correctly the vdW interactions, existing in layered 2D vdW heterostructures. Thus, to solve this issue, we chose to opt the DFT-D2 scheme proposed by Grimme [47]. In order to confirm that the DFT-D2 method is sufficient to describe the vdW heterostructures, we also performed the Tkatchenko-Scheffler DFT-TS method [48] for comparison. A large vacuum thickness of 25 Å was applied to avoid any interactions between two neighbor layers.

3 Results and discussion

The lattice parameters of single-layered C_2N and InSe are optimized and illustrated in Fig. 1(a) and Fig. 1(b), respectively. The obtained lattice parameters of C_2N and InSe monolayers are 8.33 Å and 4.06 Å, respectively. These values are inconsistent with the previous experimental and theoretical reports [18,20,49]. Therefore, to construct the C_2N/InSe heterostructure with a small lattice mismatch,

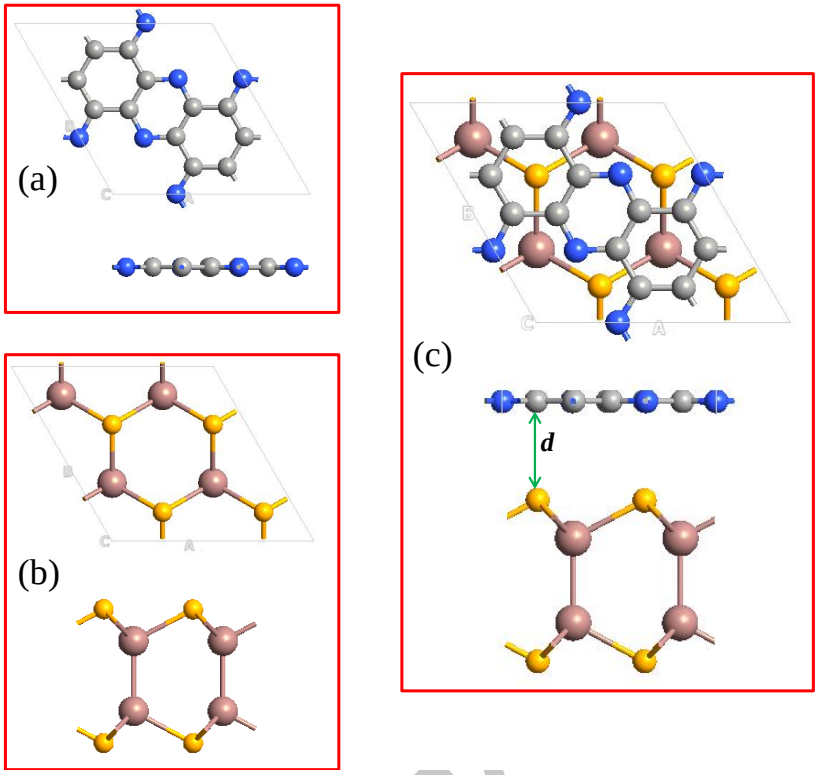

Fig. 1. Top view and side view of the optimized atomic structure of single layered C_2N (a), InSe (b) monolayers and their C_2N/InSe heterostructure (c), respectively.

we use a (2×2) supercell of InSe monolayer and a unit cell of C_2N monolayer. The lattice mismatch between the C_2N and InSe monolayer is small of 2.5 %. The atomic structure of the C_2N/InSe heterostructure is displayed in Fig. 1(c). After geometric optimization, the obtained interlayer distance between the C_2N and InSe monolayers in the heterostructure is 3.325 Å, calculated by DFT-D2 method and 3.471 Å, calculated by DFT-TS method. This distance indicates that the bonding between the C_2N and InSe monolayers in heterostructure is mainly characterized by the physical mechanism. Moreover, this distance is the same as that in other heterostructures, dominated by the weak vdW interactions, such as C_2N/Sb [50], borophene/C_2N [51]. All these findings illustrate that in the C_2N/InSe heterostructure, the weak vdW interactions are dominated between the C_2N and InSe monolayers. Additionally, to establish the stability of the heterostructure, we further calcu-

late its binding energy (E_b) as follows: $E_b = E_H - E_{C_2N} - E_{InSe}$, where E_H, E_{C_2N} and E_{InSe} are the total energies of heterostructure, isolated C_2N, and InSe monolayers, respectively. Our obtained binding energy of the C_2N/InSe heterostructure is -0.71 eV and -0.98 eV, respectively, calculated by DFT-D2 and DFT-TS methods. The negative value of the binding energy indicates that the formed heterostructure is stable structure. It can be seen that the DFT-TS method tends to yield large interlayer distance and binding energy than the DFT-D2 method does. However, we find that the values of the interlayer distance as well as the binding energy of the C_2N/InSe heterostructure obtained from DFT-D2 and DFT-TS methods are very similar, indicating that the DFT-D2 and the Tkatchenko-Scheffler DFT-TS methods yield very good estimate of the interlayer spacing and the binding energy in the C_2N/InSe vdW heterostructure. Thus, in the following, we investigate the electronic properties of the C_2N/InSe heterostructure by using only DFT-D2 method.

We next explore in detail the electronic properties of the C_2N/InSe heterostructure as compared with those of the isolated C_2N and InSe monolayers. The band structures of the isolated C_2N, InSe monolayers and the heterostructure are displayed in Fig. 2(a-c), respectively. One can see from Fig. 2(a) that the monolayer C_2N is a direct semiconductor. The calculated band gap of the monolayer C_2N is 1.66 eV, forming between the conduction band minimum (CBM) and valence band maximum (VBM) at the Dirac Γ point of the Brillouin zone. These results are in good agreement with the available reports [18,21]. Whereas, monolayer InSe is an indirect semiconductor with the CBM at the Γ point and the VBM at the Γ-M path. Our calculated band gap of the monolayer InSe is 1.54 eV, which is in good agreement with other calculations [52,53]. The band structure of the C_2N/InSe heterostructure is illustrated in Fig. 2(c). It can be found that the C_2N/InSe heterostructure is a semiconductor with an indirect band gap of 1.34 eV, which is smaller than that of both C_2N and InSe monolayers. It indicates that electrons can be excited

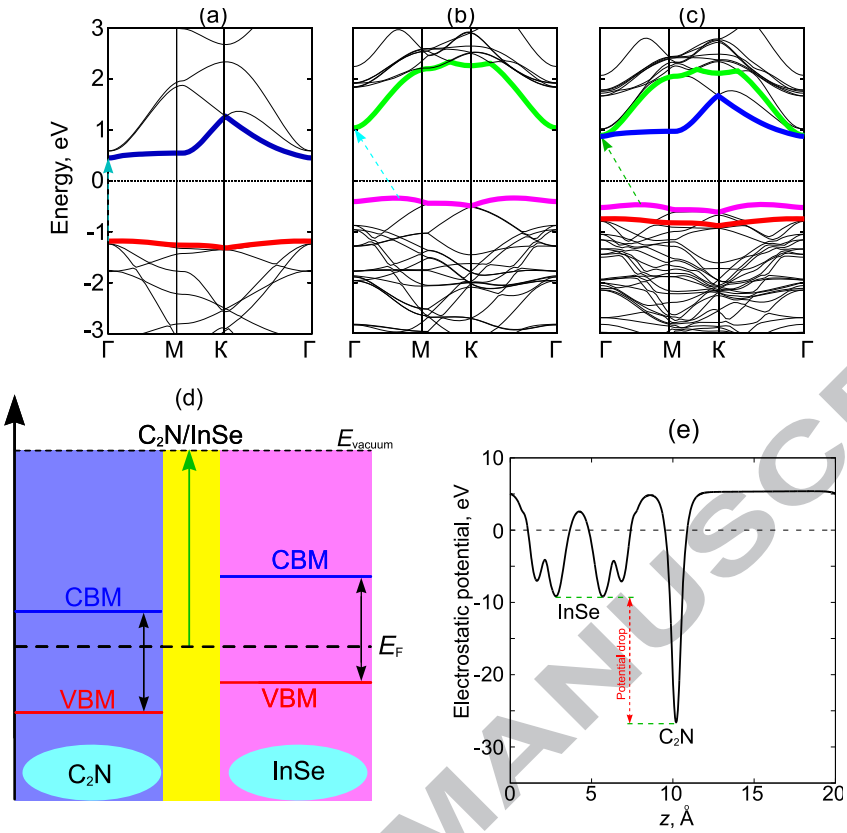

Fig. 2. Band structures of the single-layered C_2N (a), InSe (b) and C_2N/InSe heterostructure (c). The Fermi level is set to be zero. Red and blue lines stand for the VBM and CBM of the C_2N, whereas violet and green stand for the VBM and CBM of the InSe in the heterostructure. Schematic representation of the type–II band alignment (d) and the electrostatic potential (e) of the C_2N/InSe heterostructure.

easily from the VBM to CBM in the heterostructure when a visible light irradiation is applied. In addition, it can be seen that the band structure of the heterostructure is well kept upon contact owing to their vdW bonding. Furthermore, by analyzing the band structure of the heterostructure, one can find that its CBM at M point comes from the C_2N monolayer, whereas its VBM at $M-\Gamma$ path comes from the InSe monolayer. It indicates that the C_2N/InSe heterostructure forms a type–II band alignment with the electrons and holes in the InSe and C_2N monolayers.

In Fig. 2(d) we present the band alignment of the C_2N/InSe heterostructure to

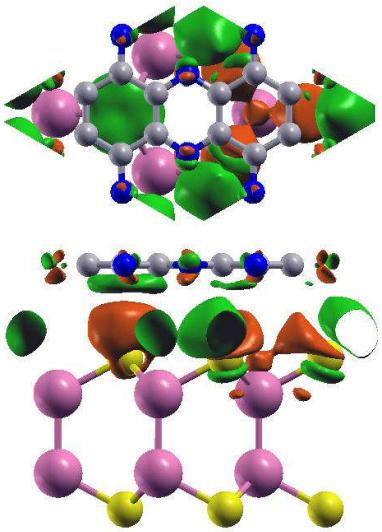

Fig. 3. (a) Top view and (b) side view of the charge density difference in the C_2N/InSe heterostructure. The red and green color isosurfaces correspond to the accumulation and depletion of electrons.

understand deeply its carrier separation. It is clear that the CBM and VBM of the C_2N part in the heterostructure are lower than those of the InSe part. It confirms an observation of type-II band alignment in the C_2N/InSe heterostructure and implies the spatial separation of photogenerated electron-hole pairs. Fig. 2(d) shows the electrostatic potential of the C_2N/InSe heterostructure. One can observe that the C_2N monolayer has a deeper potential than that of the InSe monolayer, resulting in a strong electrostatic potential at the interface. A large potential drop between the C_2N and InSe monolayers in the heterostructure leads to the charge transfer from the C_2N to the InSe monolayers due to a built-in electric field, which can reduce the recombination of photogenerated electron-hole pairs.

Furthermore, in order to have a deeper understanding for the vdW interaction between the C_2N and the InSe monolayers in the heterostructure, we further calculate the charge density difference of the C_2N/InSe heterostructure, as shown in Fig. 3. The charge density difference of the heterostructure can be visualized as $\Delta\rho = \rho_{C_2N/InSe} - \rho_{C_2N} - \rho_{InSe}$, where $\rho_{C_2N/InSe}$, ρ_{C_2N}, and ρ_{InSe} are, respec-

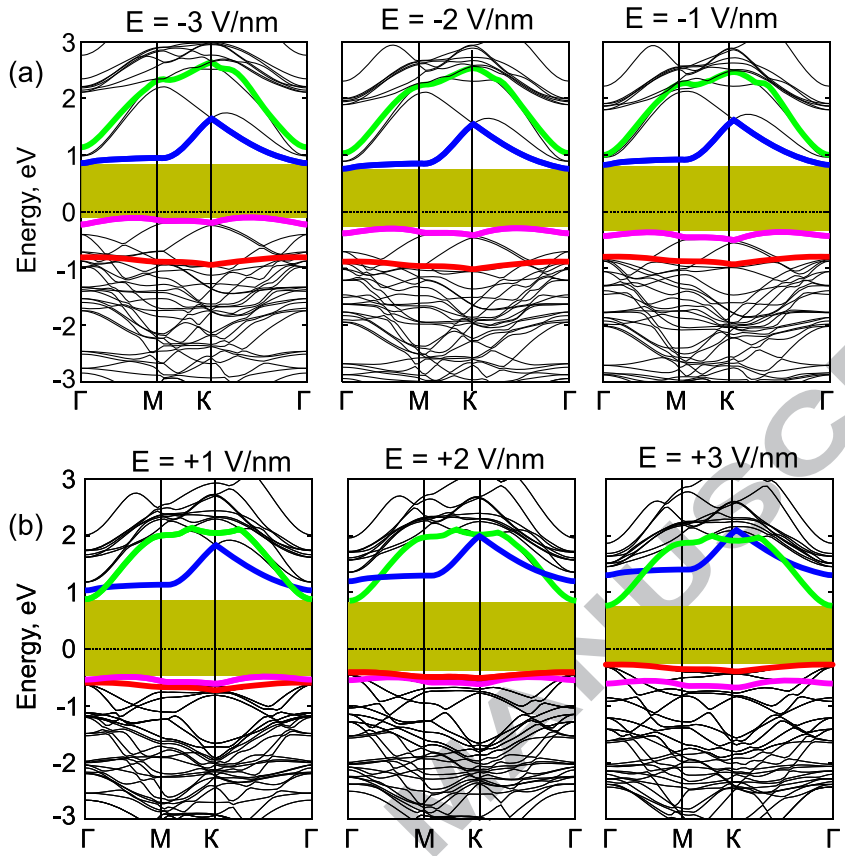

Fig. 4. Band structures of the C_2N/InSe heterostructure under negative (a) and positive (b) electric field. The Fermi level is set to be zero.

tively, the charge energies of the C_2N/InSe heterostructure, the C_2N and the InSe monolayers. It is obvious that the charges are redistributed in the region between the C_2N and InSe monolayer, forming the vdW gap. In addition, we find that the charges are more accumulated in the topmost Se layer of the InSe monolayer, and depleted in the C_2 layer. The Bader charge analysis indicates that the charge of only $0.018e$ is transferred from the C_2N layer to the InSe one. It also demonstrates the weak vdW interactions in the heterostructure.

We further investigate whether the electronic properties of the C_2N/InSe heterostructure can be controlled by applying the electric field or by changing the interlayer distance. Here, we first consider the effect of the electric field on the electronic properties of the heterostructure. The electric field is applied perpendic-

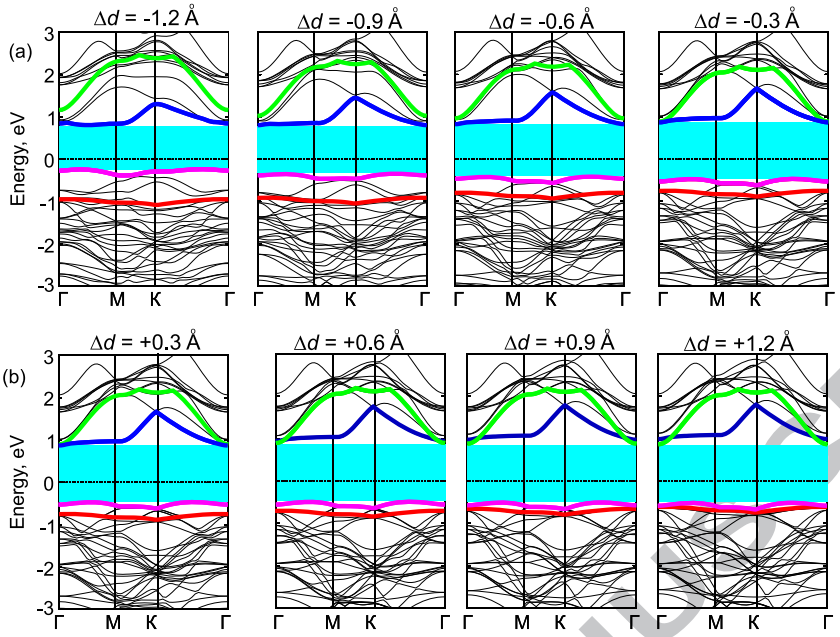

Fig. 5. Band structures of the C_2N/InSe heterostructure under compressive (a) and tensile (b) out-of-plane strains. The Fermi level is set to be zero.

ularly to the heterostructure surface. The positive electric field points from the C_2N layer to the InSe monolayer in the heterostructure. In Fig. 4, we show the band structures of the C_2N/InSe heterostructure under a different electric field. It can be seen that by applying the negative electric field the CBM at the Γ point and the VBM at the Γ-M path of the InSe monolayer move upward, whereas the CBM and the VBM of the C_2N monolayer at the Γ point move downward. The band gap of the heterostructure, therefore, reduces with increasing the strength of the negative electric field. It is obvious that the VBM of the C_2N is slightly higher than that of the InSe, but the CBM of the InSe is also higher than that of the C_2N. It indicates that the C_2N/InSe heterostructure still keeps the type-II band alignment when the negative electric field is applied. As is illustrated in Fig. 4(d-f), we find that by applying the positive electric field, the CBM at the Γ point and the VBM at the Γ-M path of the InSe move downward, while the CBM and the VBM at the Γ point of the C_2N move upward. When the strength of the positive electric field is less than

$+1$ V/nm, the CBM of the InSe is slightly lower than that of the C_2N, whereas the VBM of the InSe is higher than that of the C_2N. The C_2N/InSe heterostructure, in this case, forms the type-I band alignment. Thus, when the strength of the positive electric field is less than $+1$ V/nm, a transition of the band alignment from the type-II to the type-I is observed in the C_2N/InSe heterostructure. When the strength of the positive electric field increases and exceeds $+2$ V/nm, the VBM at the Γ point of the C_2N moves upward and becomes higher than at Γ-M path of the InSe. The C_2N/InSe heterostructure, in this case, switches from the type-I to the type-II band alignment. In addition, we find that the band gap of the C_2N/InSe heterostructure is switched from indirect to direct when the positive electric field is larger than $+2$ V/nm.

We now consider the impact of the vertical strain by changing the interlayer distance between the C_2N and InSe monolayers in the heterostructure. The change in the interlayer distance is defined as $\Delta d = d_0 - d$, where d_0 and d are the strained and equilibrium interlayer distances, respectively. It should be noted that the interlayer distance in vdW heterostructures could be controlled effectively in experiments by applying pressure with a scanning tunnelling microscopy tip [54], or by inserting dielectric BN layers into the vdW heterostructure [55], or by vacuum thermal annealing [56]. For instance, Tongay *et al.* [56] demonstrated that the interlayer distance in TMDs heterostructure could be tuned from noncoupling to strong coupling by applying vacuum thermal annealing. On the other hand, Fang *et al.* [55] showed that the interlayer distance in TMDs heterostructures could be increased by the insertion of the BN dielectric layer. These findings indicate that the interlayer distance in the C_2N/InSe heterostructure can also be controlled by similar experimental approaches. The band structures of the C_2N/InSe heterostructure under different compressive and tensile vertical strains are displayed in Fig. 5. One can observe from Fig. 5(a-c) that by applying the compressive vertical strain, i.e

$\Delta d < 0$, the CBM and VBM of the InSe monolayer slightly shift upward, whereas the CBM and VBM of the C_2N shift downward. It leads to a decrease in a band gap of the heterostructure. However, it can be seen that by decreasing the interlayer distance, there is no occurrence of a transition of the type-II band alignment. The C_2N/InSe heterostructure still keeps the type-II band alignment. By applying the tensile strain, i.e $\Delta d > 0$ as shown in Fig. 5(d-f), we can observe that the CBM at the Γ point and the VBM at the $\Gamma - M$ path of the InSe monolayer move downward, whereas the CBM and VBM at the Γ point of the C_2N monolayer move upward. When Δd is larger than $+0.6$ Å, the CBM at the Γ point of the InSe monolayer is slightly lower than that of the C_2N at the same point, whereas the VBM at the $\Gamma - M$ path of the InSe is higher than that of the C_2N at the Γ point, resulting in a transition from the type-II to type-I band alignment. Thus, we can see that that changing the interlayer distance between the C_2N and InSe monolayers in the C_2N/InSe heterostructure could lead to a transition from the type-II to the type-I band alignment. All these findings demonstrate that the C_2N/InSe heterostructure can be considered to be a good candidate for applications in optoelectronic and nanoelectronic devices.

4 Conclusion

In summary, in this work, we have comprehensively investigated the electronic properties of the C_2N/InSe heterostructure using DFT method. Due to the weak vdW interactions, the electronic properties of single-layered C_2N and InSe monolayer are found to be well preserved in their heterostructure. At the equilibrium interlayer distance of 3.325 Å and without a presence of electric field, the C_2N/InSe heterostructure possesses a type-II band alignment with an indirect band gap of 1.34 eV. Furthermore, the transition from type-II to type-I band alignment

and indirect to direct band gap can be achieved in such heterostructure by applying the electric field or by changing the interlayer distance. Our findings demonstrate that the C_2N/InSe heterostructure can be considered to be a good candidate for applications in optoelectronic and nanoelectronic devices.

Acknowledgements

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References

[1] K. S. Novoselov, A. K. Geim, S. V. Morozov, D. Jiang, Y. Zhang, S. V. Dubonos, I. V. Grigorieva, A. A. Firsov, Electric field effect in atomically thin carbon films, Science 306 (5696) (2004) 666–669.

[2] N. Alem, R. Erni, C. Kisielowski, M. D. Rossell, W. Gannett, A. Zettl, Atomically thin hexagonal boron nitride probed by ultrahigh-resolution transmission electron microscopy, Phys. Rev. B 80 (15) (2009) 155425.

[3] L. Li, J. Kim, C. Jin, G. J. Ye, D. Y. Qiu, H. Felipe, Z. Shi, L. Chen, Z. Zhang, F. Yang, K. Watanabe, T. Taniguchi, W. Ren, S. G. Louie, X. H. Chen, Y. Zhang, F. Wang, Direct observation of the layer-dependent electronic structure in phosphorene, Nat. Nanotechnol. 12 (1) (2017) 21.

[4] Y. Jing, X. Zhang, Z. Zhou, Phosphorene: what can we know from computations?, Wiley Interdiscip. Rev. Comput. Mol. Sci. 6 (1) (2016) 5–19.

[5] A. Carvalho, M. Wang, X. Zhu, A. S. Rodin, H. Su, A. H. C. Neto, Phosphorene: from theory to applications, Nat. Rev. Mater. 1 (11) (2016) 16061.

[6] M. Sun, S. Wang, J. Yu, W. Tang, Hydrogenated and halogenated blue phosphorene as dirac materials: A first principles study, Appl. Surf. Sci. 392 (2017) 46–50.

[7] B. Radisavljevic, A. Radenovic, J. Brivio, i. V. Giacometti, A. Kis, Single-layer MoS_2 transistors, Nat. Nanotechnol. 6 (3) (2011) 147.

[8] Q. H. Wang, K. Kalantar-Zadeh, A. Kis, J. N. Coleman, M. S. Strano, Electronics and optoelectronics of two-dimensional transition metal dichalcogenides, Nat. Nanotechnol. 7 (11) (2012) 699.

[9] S. Z. Butler, S. M. Hollen, L. Cao, Y. Cui, J. A. Gupta, H. R. Gutiérrez, T. F. Heinz, S. S. Hong, J. Huang, A. F. Ismach, J.-H. Ezekiel, K. Masaru, V. V. Plashnitsa, R. D. Robinson, R. S. Ruoff, S. Salahuddin, J. Shan, L. Shi, M. G. Spencer, M. Terrones, W. Windl, J. E. Goldberger, Progress, challenges, and opportunities in two-dimensional materials beyond graphene, ACS Nano 7 (4) (2013) 2898–2926.

[10] W. Huang, L. Gan, H. Li, Y. Ma, T. Zhai, 2d layered group III-A metal chalcogenides: synthesis, properties and applications in electronics and optoelectronics, CrystEngComm 18 (22) (2016) 3968–3984.

[11] P. Hu, Z. Wen, L. Wang, P. Tan, K. Xiao, Synthesis of few-layer gase nanosheets for high performance photodetectors, ACS Nano 6 (7) (2012) 5988–5994.

[12] M. Sun, Q. Ren, S. Wang, J. Yu, W. Tang, Electronic properties of janus silicene: new direct band gap semiconductors, J. Phys. D: Appl. Phys. 49 (44) (2016) 445305.

[13] W. Tang, M. Sun, J. Yu, J.-P. Chou, Magnetism in non-metal atoms adsorbed graphene-like gallium nitride monolayers, Appl. Surf. Sci. 427 (2018) 609–612.

[14] S. R. Tamalampudi, Y.-Y. Lu, R. Kumar U, R. Sankar, C.-D. Liao, K. Moorthy B, C.-H. Cheng, F. C. Chou, Y.-T. Chen, High performance and bendable few-layered inse photodetectors with broad spectral response, Nano Lett. 14 (5) (2014) 2800–2806.

[15] W. Feng, W. Zheng, W. Cao, P. Hu, Back gated multilayer inse transistors with

enhanced carrier mobilities via the suppression of carrier scattering from a dielectric interface, Adv. Mater. 26 (38) (2014) 6587–6593.

[16] S. Magorrian, V. Zólyomi, V. Fal'ko, Electronic and optical properties of two-dimensional inse from a dft-parametrized tight-binding model, Phys. Rev. B 94 (24) (2016) 245431.

[17] D. Q. Khoa, D. T. Nguyen, C. V. Nguyen, V. T. T. Vi, H. V. Phuc, L. T. T. Phuong, B. D. Hoi, N. N. Hieu, Modulation of electronic properties of monolayer inse through strain and external electric field, Chem. Phys. 516 (2019) 213 – 217.

[18] J. Mahmood, E. K. Lee, M. Jung, D. Shin, I.-Y. Jeon, S.-M. Jung, H.-J. Choi, J.-M. Seo, S.-Y. Bae, S.-D. Sohn, N. Park, J. H. Oh, H.-J. Shin, J.-B. Baek, Nitrogenated holey two-dimensional structures, Nat. Commun. 6 (2015) 6486.

[19] S. Guan, Y. Cheng, C. Liu, J. Han, Y. Lu, S. A. Yang, Y. Yao, Effects of strain on electronic and optic properties of holey two-dimensional C_2N crystals, Appl. Phys. Lett. 107 (23) (2015) 231904.

[20] R. Zhang, B. Li, J. Yang, Effects of stacking order, layer number and external electric field on electronic structures of few-layer C_2N-h2D, Nanoscale 7 (33) (2015) 14062–14070.

[21] H. V. Phuc, V. V. Tuan, N. N. Hieu, V. V. Ilyasov, I. A. Fedorov, B. D. Hoi, L. T. T. Phuong, N. V. Hieu, E. Feddi, C. V. Nguyen, Tuning the electronic and optical properties of two-dimensional graphene-like C_2N nanosheet by strain engineering, J. Electron. Mater. 47 (2018) 4594–4603.

[22] R. Longuinhos, J. Ribeiro-Soares, Stable holey two-dimensional C_2N structures with tunable electronic structure, Phys. Rev. B 97 (19) (2018) 195119.

[23] H. Yu, X. Jiang, M. Cai, J. Feng, X. Chen, X. Yang, Y. Liu, Electronic and magnetic properties of zigzag C_2N-h2D nanoribbons: Edge and width effects, Chem. Phys. Lett. 685 (2017) 363–370.

[24] A. Hashmi, M. U. Farooq, I. Khan, J. Son, J. Hong, Ultra-high capacity hydrogen storage in a li decorated two-dimensional C_2N layer, J. Mater. Chem. A 5 (6) (2017) 2821–2828.

[25] M. Sun, J.-P. Chou, J. Yu, W. Tang, Effects of structural imperfection on the electronic properties of graphene/WSe_2 heterostructures, J. Mater. Chem. C 5 (39) (2017) 10383–10390.

[26] N. N. Hieu, H. V. Phuc, V. V. Ilyasov, N. D. Chien, N. A. Poklonski, N. V. Hieu, C. V. Nguyen, First-principles study of the structural and electronic properties of graphene/MoS_2 interfaces, J. Appl. Phys. 122 (10) (2017) 104301.

[27] Y. Sata, R. Moriya, S. Morikawa, N. Yabuki, S. Masubuchi, T. Machida, Electric field modulation of schottky barrier height in graphene/$MoSe_2$ van der Waals heterointerface, Appl. Phys. Lett. 107 (2) (2015) 023109.

[28] K. D. Pham, N. N. Hieu, H. V. Phuc, I. Fedorov, C. 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 (17) (2018) 171605.

[29] D. Pierucci, H. Henck, J. Avila, A. Balan, C. H. Naylor, G. Patriarche, Y. J. Dappe, M. G. Silly, F. Sirotti, A. C. Johnson, M. C. Asensio, A. Ouerghi, Band alignment and minigaps in monolayer MoS_2-graphene van der Waals heterostructures, Nano Lett. 16 (7) (2016) 4054–4061.

[30] M. Sun, Q. Ren, Y. Zhao, J.-P. Chou, J. Yu, W. Tang, Electronic and magnetic properties of 4d series transition metal substituted graphene: a first-principles study, Carbon 120 (2017) 265–273.

[31] M. Sun, J. Chou, J. Yu, W. Tang, Electronic properties of blue phosphorene/graphene and blue phosphorene/graphene-like gallium nitride heterostructures, Phys. Chem. Chem. Phys. 19 (26) (2017) 17324–17330.

[32] Y. Cai, G. Zhang, Y.-W. Zhang, Electronic properties of phosphorene/graphene and phosphorene/hexagonal boron nitride heterostructures, J. Phys. Chem. C 119 (24) (2015) 13929–13936.

[33] W. Kim, C. Li, F. A. Chaves, D. Jiménez, R. D. Rodriguez, J. Susoma, M. A. Fenner, H. Lipsanen, J. Riikonen, Tunable graphene–GaSe dual heterojunction device, Adv. Mater. 28 (9) (2016) 1845–1852.

[34] C. Si, Z. Lin, J. Zhou, Z. Sun, Controllable schottky barrier in GaSe/graphene heterostructure: the role of interface dipole, 2D Mater. 4 (1) (2016) 015027.

[35] Z. Ben Aziza, H. Henck, D. Pierucci, M. G. Silly, E. Lhuillier, G. Patriarche, F. Sirotti, M. Eddrief, A. Ouerghi, van der waals epitaxy of GaSe/graphene heterostructure: electronic and interfacial properties, ACS Nano 10 (10) (2016) 9679–9686.

[36] Z. B. Aziza, D. Pierucci, H. Henck, M. G. Silly, C. David, M. Yoon, F. Sirotti, K. Xiao, M. Eddrief, J.-C. Girard, et al., Tunable quasiparticle band gap in few-layer GaSe/graphene van der Waals heterostructures, Phys. Rev. B 96 (3) (2017) 035407.

[37] H. V. Phuc, V. V. Ilyasov, N. N. Hieu, B. Amin, C. V. Nguyen, Van der waals graphene/g-GaSe heterostructure: Tuning the electronic properties and schottky barrier by interlayer coupling, biaxial strain, and electric gating, J. Alloys Compd. 750 (2018) 765–773.

[38] Z. Zheng, X. Wang, W. Mi, Electric field tunable electronic structure in two dimensional van der Waals g-C_2N/XSe_2 (X= Mo, W) heterostructures, Carbon 117 (2017) 393–398.

[39] X. Chen, Z.-Z. Lin, M. Ju, Controllable band alignment transition in InSe–MoS_2 Van der Waals heterostructure, Phys. Status Solidi Rapid Res. Lett. 12 (7) (2018) 1800102.

[40] S. Li, M. Sun, J.-P. Chou, J. Wei, H. Xing, A. Hu, First-principles calculations of the electronic properties of SiC-based bilayer and trilayer heterostructures, Phys. Chem. Chem. Phys. 20 (2018) 24726–24734.

[41] H. U. Din, M. Idrees, G. Rehman, C. V. Nguyen, L.-Y. Gan, I. Ahmad, M. Maqbool, B. Amin, Electronic structure, optical and photocatalytic performance of $SiCMX_2$ (M = Mo, W and X = S, Se) van der Waals heterostructures, Phys. Chem. Chem. Phys. 20 (2018) 24168–24175.

[42] H. V. Phuc, N. N. Hieu, B. D. Hoi, C. V. Nguyen, Interlayer coupling and electric field tunable electronic properties and schottky barrier in graphene/bilayer-GaSe van der Waals heterostructure, Phys. Chem. Chem. Phys. 20 (2018) 17899.

[43] P. E. Blöchl, Projector augmented-wave method, Phys. Rev. B 50 (24) (1994) 17953.

[44] P. Giannozzi, S. Baroni, N. Bonini, M. Calandra, R. Car, C. Cavazzoni, D. Ceresoli, G. L. Chiarotti, M. Cococcioni, I. Dabo, A. D. Corso, S. de Gironcoli, S. Fabris, G. Fratesi, R. Gebauer, U. Gerstmann, C. Gougoussis, A. Kokalj, M. Lazzeri, L. Martin-Samos, N. Marzari, F. Mauri, R. Mazzarello, S. Paolini, A. Pasquarello, L. Paulatto, C. Sbraccia, S. Scandolo, G. Sclauzero, A. P. Seitsonen, A. Smogunov, P. Umari, R. M. Wentzcovitch, Quantum espresso: a modular and open-source software project for quantum simulations of materials, J. Phys.: Condens. Matter 21 (2009) 395502–395520.

[45] J. P. Perdew, K. Burke, M. Ernzerhof, Generalized gradient approximation made simple, Phys. Rev. Lett. 77 (18) (1996) 3865.

[46] J. P. Perdew, K. Burke, M. Ernzerhof, Perdew, burke, and ernzerhof reply, Phys. Rev. Lett. 80 (1998) 891–891.

[47] S. Grimme, Semiempirical GGA-type density functional constructed with a long-range dispersion correction, J. Comput. Chem. 27 (2006) 1787–1799.

[48] A. Tkatchenko, M. Scheffler, Accurate molecular van der waals interactions from ground-state electron density and free-atom reference data, Phys. Rev. Lett. 102 (7) (2009) 073005.

[49] L. Debbichi, O. Eriksson, S. Lebègue, Two-dimensional indium selenides compounds: An ab initio study, J. Phys. Chem. Lett. 6 (15) (2015) 3098–3103.

[50] X. Wang, R. Quhe, W. Cui, Y. Zhi, Y. Huang, Y. An, X. Dai, Y. Tang, W. Chen, Z. Wu, W. Tang, Electric field effects on the electronic and optical properties in C_2N/Sb van der Waals heterostructure, Carbon 129 (2018) 738 – 744.

[51] J. Jiang, X. Wang, Y. Song, W. Mi, Tunable schottky barrier and electronic properties in borophene/g-C_2N van der Waals heterostructures, Appl. Surf. Sci. 440 (2018) 42 – 46.

[52] T. Hu, J. Zhou, J. Dong, Strain induced new phase and indirect–direct band gap transition of monolayer inse, Phys. Chem. Chem. Phys. 19 (32) (2017) 21722–21728.

[53] G. Mudd, M. Molas, X. Chen, V. Zólyomi, K. Nogajewski, Z. R. Kudrynskyi, Z. D. Kovalyuk, G. Yusa, O. Makarovsky, L. Eaves, M. Potemski, V. I. Falko, A. Patan, The direct-to-indirect band gap crossover in two-dimensional van der waals indium selenide crystals, Sci. Rep. 6 (2016) 39619.

[54] M. Yankowitz, K. Watanabe, T. Taniguchi, P. San-Jose, B. J. LeRoy, Pressure-induced commensurate stacking of graphene on boron nitride, Nat. Commun. 7 (2016) 13168.

[55] H. Fang, C. Battaglia, C. Carraro, S. Nemsak, B. Ozdol, J. S. Kang, H. A. Bechtel, S. B. Desai, F. Kronast, A. A. Unal, et al., Strong interlayer coupling in van der waals heterostructures built from single-layer chalcogenides, Proc. Natl. Acad. Sci. U. S. A. 111 (17) (2014) 6198–6202.

[56] S. Tongay, W. Fan, J. Kang, J. Park, U. Koldemir, J. Suh, D. S. Narang, K. Liu, J. Ji, J. Li, et al., Tuning interlayer coupling in large-area heterostructures with CVD-grown MoS_2 and WS_2 monolayers, Nano Lett. 14 (6) (2014) 3185–3190.

HIGHLIGHTS

- Electronic properties of the C_2N/InSe heterostructure have investigated for the first time.
- The C_2N/InSe heterostructure possesses a type-II band alignment with an indirect band gap of 1.34 eV.
- The transition from type-II to type-I band alignment and indirect to direct band gap can be achieved by applying the electric field or strain.
- The C_2N/InSe heterostructure can be considered to be a good candidate for optoelectronic and nanoelectronic devices.

Graphical Abstract