



Article Stacking-Mediated Type-I/Type-II Transition in Two-Dimensional MoTe₂/PtS₂ Heterostructure: A First-Principles Simulation

Kai Ren^{1,*,†}, Zhengyang Zhu^{2,†}, Ke Wang³, Wenyi Huo¹ and Zhen Cui⁴

- School of Mechanical and Electronic Engineering, Nanjing Forestry University, Nanjing 211189, China; wyhuo@njfu.edu.cn
- ² School of Mechanical Engineering, Wanjiang University of Technology, Maanshan 243031, China; zhengyang_zhu@126.com
- ³ School of Automation, Xi'an University of Posts and Telecommunications, Xi'an 710121, China; kewang@xupt.edu.cn
- ⁴ School of Automation and Information Engineering, Xi'an University of Technology, Xi'an 710048, China; zcui@xaut.edu.cn
- * Correspondence: kairen@njfu.edu.cn
- + These authors contributed equally to this work.

Abstract: Recently, a two-dimensional (2D) heterostructure has been widely investigated as a photocatalyst to decompose water using the extraordinary type-II band structure. In this work, the $MoTe_2/PtS_2$ van der Waals heterostructure (vdWH) is constructed with different stacking structures. Based on density functional calculations, the stacking-dependent electronic characteristic is explored, so that the $MoTe_2/PtS_2$ vdWH possesses type-I and type-II band structures for the light-emitting device and photocatalyst, respectively, with decent stacking configurations. The band alignment of the $MoTe_2/PtS_2$ vdWH is also addressed to obtain suitable band edge positions for water-splitting at pH 0. Furthermore, the potential drop is investigated, resulting from charge transfer between the $MoTe_2$ and PtS_2 , which is another critical promotion to prevent the recombination of the photogenerated charges. Additionally, the $MoTe_2/PtS_2$ vdWH also demonstrates a novel and excellent optical absorption capacity in the visible wavelength range. Our work suggests a theoretical guide to designing and tuning the 2D heterostructure using photocatalytic and photovoltaic devices.

Keywords: MoTe₂/PtS₂; heterostructure; stacking-dependent; photocatalyst

1. Introduction

Hydrogen (H₂) is regarded as an important energy source to alleviate environmental pollution and energy shortage, because the combustion productions are almost water. Comparing the bulk photocatalysts, its use of two-dimensional (2D) materials as a photocatalyst to decompose the water is advantageous characteristic [1–3]. Since the graphene was proposed to have novel performances [4], tremendous efforts were made to develop other 2D materials [5–8]. 2D semiconductors show a broad specific surface area [9], suggesting extraordinary electronic [10,11], thermal [12,13] and optical [14,15] performances. Especially, the large surface area can provide more active sites in the photocatalytic process, which also contributes to the photoexcited carrier motion [16]. Furthermore, some 2D materials have been proved to be potential photocatalysts [17–20].

At the same time, when the single semiconductor is used as a photocatalyst to decompose water, the photogenerated charges move to the surface of the 2D materials. Even if the larger specific surface area of the 2D materials provides a shorter path, the rapid recombination between the photogenerated electrons and holes also hinders photocatalytic efficiency. Thus, the 2D heterostructure constructed by two different semiconductors is adopted to separate the photogenerated electrons and holes using an extraordinary type-II



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Copyright: © 2022 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (https:// creativecommons.org/licenses/by/ 4.0/). band structure. More importantly, some strategies are further conducted to modulate the novel properties of the heterostructure, such as external electric field [21], external strain [22] and imperfection [23]. When the 2D heterostructure is constructed, there are possible stacking configurations. These stacking structures possess a similar binding energy (E_b) but different properties. For example, the charge transfer of the MoS₂/WS₂ heterostructure is strongly dependent on the interlayer stacking configurations using optical, two-color, ultrafast pump—probe spectroscopy [24]. The valence band-splitting is remarkable. It is induced in a multilayer heterostructure based on transition-metal dichalcogenide (TMD) using stacking engineering in spintronics [25]. Additionally, the different stacking styles of the WSe₂/WS₂ heterostructure can be prepared by vapor growth, which also affects the optical properties [26]. These results suggest that the stacking configurations of the heterostructure have a promising impact on the electronic and optical performances of the 2D heterostructure when used as a photocatalyst.

Recently, a novel transition metal dichalcogenides (TMDs) material, 2D MoTe₂, was prepared with a chemical vapor deposition synthesis method using promising nanoelectronics [27]. MoTe₂ also possesses excellent electronic [28], carrier transport [29] and thermoelectric [30] properties. Another TMDs, 2D PtS₂ was also investigated as a heterostructure, such as $PtS_2/InSe$ [31], HfS_2/PtS_2 [32] and $PtS_2/arsenene$ [33], which are potential photocatalysts for water-splitting. The synthesized MoTe₂ and PtS_2 provide the possibility of preparing the MoTe₂/PtS₂ heterostructure using potential photocatalytic, photovoltaic, and optical devices. The stacking tuning of the electronic performances of the 2D materials is also a popular method. Therefore, in this report, we aim to study these novel TMDs materials, using first-principles simulations, to explore the response of the structural, electronic and optical performances to the stacking configuration of the MoTe₂/PtS₂ heterostructure as a latent further nano-device, which could provide theoretical guidance for the design of the 2D heterostructure.

2. Computing Method

Using the Vienna ab initio simulation package, the first-principles simulations were employed using the density functional theory [34,35]. The core electrons were considered using the projector augmented wave potentials (PAW) [36], which were explored using the Perdew–Burke–Ernzerhof (PBE) functional together with the generalized gradient approximation (GGA) [37]. In all calculations, the Grimme was conducted using a DFT-D3 method to describe the weak dispersion forces [38]. The Heyd–Scuseria–Ernzerhof (HSE06) hybrid functional was utilized [39]. Energy cut-off was set at 550 eV; Monkhorst– Pack *k*-point grids were15 × 15 × 1. The vacuum space was selected to be 25 Å to hold back the forces between the nearby slabs. The convergence force in the simulations was $0.01 \text{ eV}\cdot\text{Å}^{-1}$; at the same time, the energy converged to 0.01 meV. The binding energy (*E*_b) of the MoTe₂/PtS₂ heterostructure was decided by:

$$E_{\rm b} = E_{\rm MoTe2/PtS2} - E_{\rm MoTe2} - E_{\rm PtS2},\tag{1}$$

where the $E_{MoTe2/PtS2}$, E_{MoTe2} and E_{PtS2} are the total energy of the MoTe₂/PtS₂ heterostructure, pristine MoTe₂ and PtS₂ monolayers, respectively. The charge density difference ($\Delta \rho$) was calculated by:

$$\Delta \rho = \rho_{\rm MoTe2/PtS2} - \rho_{\rm MoTe2} - \rho_{\rm PtS2},\tag{2}$$

where the $\rho_{MoTe2/PtS2}$, ρ_{MoTe2} and ρ_{PtS2} are total charge density of the MoTe₂/PtS₂ heterostructure, pristine MoTe₂ and PtS₂ monolayers, respectively. The optical absorption property of the monolayered was obtained as follows:

$$\alpha(\omega) = \frac{\sqrt{2}\omega}{c} \left\{ \left[\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega) \right]^{1/2} - \varepsilon_1(\omega) \right\}^{1/2}$$
(3)

where the angular frequency, absorption coefficient and speed of light are used by ω , α and c, respectively. $\varepsilon_1(\omega)$ and $\varepsilon_2(\omega)$ were used as real and imaginary elements in the dielectric constant.

3. Results and Discussion

Before constructing the $MoTe_2/PtS_2$ heterostructure, the structure of $MoTe_2$ and PtS_2 monolayers were optimized by the 3.529 Å and 3.564 Å, respectively. The obtained band energy of the $MoTe_2$ and PtS_2 monolayers are exhibited in Figure S1 in the Supporting Information, with bandgaps of 1.22 eV and 2.60 eV, respectively. Then, the $MoTe_2/PtS_2$ heterostructure was formed by six different representative structures, shown in Figure S2, named from P1 to P6. For example, the P1 configuration was formed by putting the Mo atoms and the Te atoms on top of the Pt atoms and the upper S atoms. P2 was built so that the Mo atoms are on top of the Pt atoms, while the Te atoms were located on top of the lower S atoms. The following investigations are all based on these six configurations.

The binding energy of these $MoTe_2/PtS_2$ heterostructures is summarized in Table 1, which suggests the van der Waals interactions in these interfaces [40]. The bond lengths of Mo–Te and Pt–S are almost small changes compared with those in pristine $MoTe_2$ (2.74 Å) and PtS_2 (2.40 Å) monolayers, which further demonstrates the $MoTe_2/PtS_2$ vdW heterostructures (vdWH). In addition, the interface across the interface of these $MoTe_2/PtS_2$ vdWH is also calculated by Table 1.

Table 1. The obtained binding energy (E_b , eV), bond length (B, Å), the interface across the interface (H, Å), the bandgap (E_g , eV), the charge transfer ($\Delta \rho$, electron) and potential drop (ΔV , eV) in the optimized MoTe₂/PtS₂ heterostructure constructed with different stacking styles.

		E _b	B _{Mo-Te}	L _{Pt-S}	H	$E_{\mathbf{g}}$	Δho	ΔV
P1	Type-II	-17.08	2.73	2.40	3.79	1.27	0.047	4.416
P2	Type-II	-26.39	2.73	2.39	2.85	1.20	0.051	4.578
P3	Type-II	-17.40	2.73	2.40	3.77	0.95	0.017	4.417
P4	Type-I	-25.98	2.73	2.40	3.10	1.35	0.033	4.584
P5	Type-I	-26.39	2.73	2.40	3.06	1.31	0.035	4.558
P6	Type-II	-28.10	2.73	2.39	2.87	1.44	0.047	4.672

The projected band energy of the $MoTe_2/PtS_2$ vdWH with different stacking configurations is calculated in Figure 1. One can see that P1-, P2-, P3- and P6-MoTe₂/PtS₂ vdWHs possess a type-II band structure, with the conduction-band minimum (CBM) resulting from PtS₂ and the valence-band maximum (VBM) from MoTe₂. While the P4- and P5-MoTe₂/PtS₂ vdWHs have a type-I band alignment by the CBM and VBM located at the MoTe₂ monolayer. Furthermore, the bandgap obtained with these MoTe₂/PtS₂ vdWHs is explained in Table 1. P3-MoTe₂/PtS₂ vdWH has a narrow bandgap of about 0.95 eV. It is worth noting that the direct bandgaps in the MoTe₂/PtS₂ vdWH from the MoTe₂ are 1.33 eV, 1.30 eV, 1.34 eV, 1.31 eV and 1.35 eV for from P1 to P6, respectively.

The type-II band alignment in P1-, P2-, P3- and P6-MoTe₂/PtS₂ vdWHs provides the ability to separate the photoexcited charges, as shown in Figure 2a. With the assistance from the conduction-band offset (CBO), the photoexcited electrons at the conduction-band (CB) of the MoTe₂ continue to flow to the CB of the PtS₂, while the photoexcited holes at the valence-band (VB) of the PtS₂ migrate to the VB of the MoTe₂ under the valence-band offset (VBO). Thus, the photoexcited electrons and the holes induce the hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) at PtS₂ and MoTe₂, respectively, which can be used as a potential photocatalyst. In addition, the intrinsic type-I band structure of P4- and P5-MoTe₂/PtS₂ vdWHs results in a unidirectional flow mode for excited charges, which is a promising light-emitting device.



Figure 1. The projected band structure of the MoTe₂/PtS₂ vdWH with the (**a**) P1, (**b**) P2, (**c**) P3, (**d**) P4, (**e**) P5 and (**f**) P6 stacking configurations.



Figure 2. The photoexcited charge flow path in (**a**) type-II and (**b**) type-II band alignment of the $MoTe_2/PtS_2$ vdWH.

Furthermore, the band edge positions of these $MoTe_2/PtS_2$ vdWHs are obtained by HSE06 calculations in Figure 3, and compared with the HER and OER potential energy for the water-splitting at pH 0. One can see that the P-4 and P-6 $MoTe_2/PtS_2$ vdWHs possess a decent band alignment, which can promote the HER and OER for water-splitting

at pH 0. Additionally, together with a type-II band structure, the P-6 MoTe₂/PtS₂ vdWH can be considered as an advantageous photocatalyst to decompose water. Although the P-4 MoTe₂/PtS₂ vdWH has a type-II band alignment to separate the photogenerated electrons and holes, the suitable band edge positions still have the ability to induce redox for water-splitting. Furthermore, the type-I heterostructure is also reported to show a novel photocatalytic performance [41,42].



Figure 3. The band edge positions of the $MoTe_2/PtS_2$ vdWH with different stacking structures against the redox potential energy of the water-splitting at pH 0.

The interfacial characteristics of the MoTe₂/PtS₂ vdWHs are investigated using the charge density difference and potential drop across the interface. Using Equation (2), the charge density difference in these MoTe₂/PtS₂ vdWHs is calculated, showing that the PtS₂ layer obtained the electrons from the MoTe₂ layer (Figure 4). Additionally, the charge transfer between the MoTe₂ and PtS₂ was investigated by Bader charge analysis [43], as shown in Table 1, which suggests a maximum charge transfer in P6-MoTe₂/PtS₂ vdWH of about 0.047 electrons. Furthermore, the potential drop (shown by Figure 5) in the interface for MoTe₂/PtS₂ vdWHs is addressed in Table 1. One can see that MoTe₂/PtS₂ vdWHs possesses a pronounced potential drop across the interface, ranging from 4.41 eV to 4.67 eV, which is larger than that in the WSSe/BSe vdW heterostructure [44]. Importantly, this potential drop can act as a significant motivating force to separate the photogenerated electrons and holes in type-I and type-II heterostructures [45,46].

The visible-light absorption capacity of these MoTe₂/PtS₂ vdWHs is further investigated, as in Figure 6, which is also a crucial performance using a photocatalyst. The calculated visible-light absorption ability demonstrates that the maximum absorption peaks of the P1-, P2-, P3- and P6-MoTe₂/PtS₂ vdWHs are obtained by 6.40×10^5 cm⁻¹, 7.10×10^5 cm⁻¹, 6.26×10^5 cm⁻¹, 6.28×10^5 cm⁻¹, 6.57×10^5 cm⁻¹ and 6.85×10^5 cm⁻¹, which are located at 369 nm, 379 nm, 369 nm, 378 nm, 380 nm and 376 nm, respectively. Importantly, some absorption peaks also exist, in the range 500–600 nm, for these MoTe₂/PtS₂ vdWHs. The calculated light absorption peak in these MoTe₂/PtS₂ vdWHs, such as CdO/Arsenene (8.47×10^4 cm⁻¹) [47], AlN/Zr₂CO₂ (3.97×10^5 cm⁻¹) [48] and Hf₂CO₂/AlN (3.63×10^5 cm⁻¹) [49]. It is worth noting that the strongest absorption peak in these MoTe₂/PtS₂ vdWHs is 8.12×10^5 cm⁻¹ at 333 nm, for P5-MoTe₂/PtS₂ vdWH. The results show that the MoTe₂/PtS₂ vdWHs possesses a fantastic and tunable optical performance using the stacking configuration.



Figure 4. The charge density difference between the MoTe₂ and PtS₂ layers in the heterostructure with the (**a**) P1, (**b**) P2, (**c**) P3, (**d**) P4, (**e**) P5 and (**f**) P6 stacking configurations; the purple and cyan marks show losing and obtaining electrons, respectively.



Figure 5. The calculated potential drop across the $MoTe_2/PtS_2$ vdWH interface with different stacking styles.



Figure 6. The HSE06 calculated optical absorption of the $MoTe_2/PtS_2$ vdWH with different stacking styles.

4. Conclusions

Using first-principles simulations, the structural electronic natures of the 2D MoTe₂/PtS₂ vdWHs are addressed. These are formed by different stacking configurations. P-4 and P-5 MoTe₂/PtS₂ vdWHs possess a type-I band structure for a light-emitting device, while others have type-II band alignment to separate the photogenerated electrons and holes. Furthermore, the band edge positions of these MoTe₂/PtS₂ vdWHs are investigated, and the P-6 MoTe₂/PtS₂ vdWHs have suitable potential to induce the redox reactions for water-splitting at pH 0 when used as a promising photocatalyst. The MoTe₂/PtS₂ vdWHs also show stacking-dependent interfacial and excellent optical properties. All these results suggest a theoretical method that could be used to design and tune the performances of a 2D heterostructure.

Supplementary Materials: The following supporting information can be downloaded at: https://www.mdpi.com/article/10.3390/cryst12030425/s1, Figure S1: The HSE06 calculated band structure of the (a) MoTe₂ and (b) PtS₂ monolayers. The Fermi level is set as 0 eV; Figure S2: The MoTe₂/PtS₂ heterostructure constructed by (a) P1, (b) P2, (c) P3, (d) P4, (e) P5 and (f) P6 stacking configurations. The yellow, gray, red, and blue balls represent S, Pt, Mo, and Te atoms, respectively.

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References

- 1. Li, Y.; Li, Y.-L.; Sa, B.; Ahuja, R. Review of two-dimensional materials for photocatalytic water splitting from a theoretical perspective. *Catal. Sci. Technol.* **2017**, *7*, 545–559. [CrossRef]
- Huo, W.-Y.; Wang, S.-Q.; Zhu, W.-H.; Zhang, Z.-L.; Fang, F.; Xie, Z.-H.; Jiang, J.-Q. Recent progress on high-entropy materials for electrocatalytic water splitting applications. *Tungsten* 2021, *3*, 161–180. [CrossRef]
- 3. Wang, S.; Huo, W.; Fang, F.; Xie, Z.; Shang, J.K.; Jiang, J. High entropy alloy/C nanoparticles derived from polymetallic MOF as promising electrocatalysts for alkaline oxygen evolution reaction. *Chem. Eng. J.* **2022**, *429*, 132410. [CrossRef]
- 4. Geim, A.K.; Novoselov, K.S. The rise of grapheme. *Nat. Mater.* **2007**, *6*, 183–191. [CrossRef]
- Miró, P.; Audiffred, M.; Heine, T. An atlas of two-dimensional materials. *Chem. Soc. Rev.* 2014, 43, 6537–6554. [CrossRef] [PubMed]
- 6. Sun, M.; Schwingenschlögl, U. Structure Prototype Outperforming MXenes in Stability and Performance in Metal-Ion Batteries: A High Throughput Study. *Adv. Energy Mater.* **2021**, *11*, 2003633. [CrossRef]
- Ren, K.; Liu, X.; Chen, S.; Cheng, Y.; Tang, W.; Zhang, G. Remarkable Reduction of Interfacial Thermal Resistance in Nanophononic Heterostructures. *Adv. Funct. Mater.* 2020, *30*, 2004003. [CrossRef]
- 8. Wang, C.; Zhang, C. Discussions on extension of traditional cohesive element for delamination modeling of laminates used in combination with phantom node intraply elements. *Compos. Struct.* **2021**, *261*, 113588. [CrossRef]
- 9. Stoller, M.D.; Park, S.; Zhu, Y.; An, J.; Ruoff, R.S. Graphene-Based Ultracapacitors. Nano Lett. 2008, 8, 3498–3502. [CrossRef]
- Sun, M.; Luo, Y.; Yan, Y.; Schwingenschlögl, U. Ultrahigh Carrier Mobility in the Two-Dimensional Semiconductors B8Si4, B8Ge4, and B8Sn4. *Chem. Mater.* 2021, 33, 6475–6483. [CrossRef]
- 11. Cui, Z.; Luo, Y.; Yu, J.; Xu, Y. Tuning the electronic properties of MoSi2N4 by molecular doping: A first principles investigation. *Phys. E Low-Dimens. Syst. Nanostruct.* **2021**, *134*, 114873. [CrossRef]
- 12. Liu, X.; Gao, J.; Zhang, G.; Zhang, Y.-W. Unusual Twisting Phonons and Breathing Modes in Tube-Terminated Phosphorene Nanoribbons and Their Effects on Thermal Conductivity. *Adv. Funct. Mater.* **2017**, *27*, 1702776. [CrossRef]
- 13. Ren, K.; Qin, H.; Liu, H.; Chen, Y.; Liu, X.; Zhang, G. Manipulating Interfacial Thermal Conduction of 2D Janus Heterostructure via a Thermo-Mechanical Coupling. *Adv. Funct. Mater.* **2022**, 2110846. [CrossRef]
- Qiu, D.Y.; Da Jornada, F.H.; Louie, S.G. Optical Spectrum of MoS₂: Many-Body Effects and Diversity of Exciton States. *Phys. Rev. Lett.* 2013, 111, 216805. [CrossRef]
- 15. Cui, Z.; Wang, M.; Lyu, N.; Zhang, S.; Ding, Y.; Bai, K. Electronic, magnetism and optical properties of transition metals adsorbed puckered arsenene. *Superlattices Microstruct.* **2021**, *152*, 106852. [CrossRef]
- 16. Thomas, J.M.; Harris, K.D.M. Some of tomorrow's catalysts for processing renewable and non-renewable feedstocks, diminishing anthropogenic carbon dioxide and increasing the production of energy. *Energy Environ. Sci.* **2016**, *9*, 687–708. [CrossRef]
- 17. Ren, K.; Shu, H.; Huo, W.; Cui, Z.; Yu, J.; Xu, Y. Mechanical, electronic and optical properties of a novel B2P6 monolayer: Ultrahigh carrier mobility and strong optical absorption. *Phys. Chem. Chem. Phys.* **2021**, *23*, 24915–24921. [CrossRef]
- Sun, M.; Schwingenschlögl, U. δ-CS: A Direct-Band-Gap Semiconductor Combining Auxeticity, Ferroelasticity, and Potential for High-Efficiency Solar Cells. *Phys. Rev. Appl.* 2020, 14, 044015. [CrossRef]
- Sun, M.; Schwingenschlögl, U. B2P6: A Two-Dimensional Anisotropic Janus Material with Potential in Photocatalytic Water Splitting and Metal-Ion Batteries. *Chem. Mater.* 2020, 32, 4795–4800. [CrossRef]
- Shen, Z.; Ren, K.; Zheng, R.; Huang, Z.; Cui, Z.; Zheng, Z.; Wang, L. The Thermal and Electronic Properties of the Lateral Janus MoSSe/WSSe Heterostructure. *Front. Mater.* 2022, *9*, 838648. [CrossRef]
- 21. Sun, M.; Chou, J.-P.; Ren, Q.; Zhao, Y.; Yu, J.; Tang, W. Tunable Schottky barrier in van der Waals heterostructures of graphene and g-GaN. *Appl. Phys. Lett.* **2017**, *110*, 173105. [CrossRef]
- Ren, K.; Luo, Y.; Wang, S.; Chou, J.-P.; Yu, J.; Tang, W.; Sun, M. A van der Waals Heterostructure Based on Graphene-like Gallium Nitride and Boron Selenide: A High-Efficiency Photocatalyst for Water Splitting. ACS Omega 2019, 4, 21689–21697. [CrossRef] [PubMed]
- Sun, M.; Chou, J.-P.; Yu, J.; Tang, W. Effects of structural imperfection on the electronic properties of graphene/WSe₂ heterostructures. J. Mater. Chem. C 2017, 5, 10383–10390. [CrossRef]
- 24. Ji, Z.; Hong, H.; Zhang, J.; Zhang, Q.; Huang, W.; Cao, T.; Qiao, R.; Liu, C.; Liang, J.; Jin, C.; et al. Robust stacking-independent ultrafast charge transfer in MoS₂/WS₂ bilayers. *ACS Nano* **2017**, *11*, 12020–12026. [CrossRef] [PubMed]
- 25. Wang, H.; Wei, W.; Li, F.; Huang, B.; Dai, Y. Step-like band alignment and stacking-dependent band splitting in trilayer TMD heterostructures. *Phys. Chem. Chem. Phys.* **2018**, *20*, 25000–25008. [CrossRef]
- Wu, X.; Wang, X.; Li, H.; Zeng, Z.; Zheng, B.; Zhang, D.; Li, F.; Zhu, X.; Jiang, Y.; Pan, A. Vapor growth of WSe₂/WS₂ heterostructures with stacking dependent optical properties. *Nano Res.* 2017, *12*, 3123–3128. [CrossRef]
- Zhou, L.; Xu, K.; Zubair, A.; Liao, A.D.; Fang, W.; Ouyang, F.; Lee, Y.-H.; Ueno, K.; Saito, R.; Palacios, T.; et al. Large-Area Synthesis of High-Quality Uniform Few-Layer MoTe₂. J. Am. Chem. Soc. 2015, 137, 11892–11895. [CrossRef]
- Shao, C.; Ren, K.; Huang, Z.; Yang, J.; Cui, Z. Two-Dimensional PtS₂/MoTe₂ van der Waals Heterostructure: An Efficient Potential Photocatalyst for Water Splitting. *Front. Chem.* 2022, 10, 847319. [CrossRef]
- 29. Qu, D.; Liu, X.; Huang, M.; Lee, C.; Ahmed, F.; Kim, H.; Ruoff, R.S.; Hone, J.; Yoo, W.J. Carrier-Type Modulation and Mobility Improvement of Thin MoTe₂. *Adv. Mater.* **2017**, *29*, 1606433. [CrossRef]

- 30. Shi, D.; Wang, G.; Li, C.; Shen, X.; Nie, Q. Preparation and thermoelectric properties of MoTe₂ thin films by magnetron co-sputtering. *Vacuum* **2017**, *138*, 101–104. [CrossRef]
- Nguyen, C.V.; Bui, H.D.; Nguyen, T.D.; Pham, K.D. Controlling electronic properties of PtS₂/InSe van der Waals heterostructure via external electric field and vertical strain. *Chem. Phys. Lett.* 2019, 724, 1–7. [CrossRef]
- 32. Colibaba, S.A.; Körbel, S.; Motta, C.; El-Mellouhi, F.; Sanvito, S. Interlayer dielectric function of a type-II van der Waals semiconductor: The HfS₂/PtS₂ heterobilayer. *Phys. Rev. Mater.* **2019**, *3*, 124002. [CrossRef]
- Ren, K.; Tang, W.; Sun, M.; Cai, Y.; Cheng, Y.; Zhang, G. A direct Z-scheme PtS₂/arsenene van der Waals heterostructure with high photocatalytic water splitting efficiency. *Nanoscale* 2020, *12*, 17281–17289. [CrossRef] [PubMed]
- 34. Kresse, G.; Furthmüller, J. Efficiency of ab-initio total energy calculations for metals and semiconductors using a plane-wave basis set. *Comput. Mater. Sci.* **1996**, *6*, 15–50. [CrossRef]
- 35. Kresse, G.; Furthmüller, J. Efficient iterative schemes for ab initio total-energy calculations using a plane-wave basis set. *Phys. Rev. B* **1996**, *54*, 11169. [CrossRef]
- 36. Kresse, G.; Joubert, D. From ultrasoft pseudopotentials to the projector augmented-wave method. *Phys. Rev. B* **1999**, *59*, 1758. [CrossRef]
- 37. Perdew, J.P.; Burke, K.; Ernzerhof, M. Generalized gradient approximation made simple. Phys. Rev. Lett. 1996, 77, 3865. [CrossRef]
- Grimme, S.; Antony, J.; Ehrlich, S.; Krieg, H. A consistent and accurate ab initio parametrization of density functional dispersion correction (DFT-D) for the 94 elements H-Pu. *J. Chem. Phys.* 2010, 132, 154104. [CrossRef]
- 39. Heyd, J.; Peralta, J.; Scuseria, G.E.; Martin, R.L. Energy band gaps and lattice parameters evaluated with the Heyd-Scuseria-Ernzerhof screened hybrid functional. *J. Chem. Phys.* **2005**, *123*, 174101. [CrossRef]
- Ren, K.; Sun, M.; Luo, Y.; Wang, S.; Yu, J.; Tang, W. First-principle study of electronic and optical properties of two-dimensional materials-based heterostructures based on transition metal dichalcogenides and boron phosphide. *Appl. Surf. Sci.* 2019, 476, 70–75. [CrossRef]
- Wang, S.; Guan, B.Y.; Wang, X.; Lou, X.W.D. Formation of Hierarchical Co9S8@ZnIn2S4 Heterostructured Cages as an Efficient Photocatalyst for Hydrogen Evolution. J. Am. Chem. Soc. 2018, 140, 15145–15148. [CrossRef] [PubMed]
- Do, T.-N.; Idrees, M.; Binh, N.T.T.; Phuc, H.V.; Hieu, N.N.; Hoa, L.T.; Amin, B.; Van, H. Type-I band alignment of BX–ZnO (X = As, P) van der Waals heterostructures as high-efficiency water splitting photocatalysts: A first-principles study. *RSC Adv.* 2020, 10, 44545–44550. [CrossRef]
- Sanville, E.; Kenny, S.D.; Smith, R.; Henkelman, G. Improved grid-based algorithm for Bader charge allocation. *J. Comput. Chem.* 2007, 28, 899–908. [CrossRef] [PubMed]
- Zhu, Z.; Ren, K.; Shu, H.; Cui, Z.; Huang, Z.; Yu, J.; Xu, Y. First-Principles Study of Electronic and Optical Properties of Two-Dimensional WSSe/BSe van der Waals Heterostructure with High Solar-to-Hydrogen Efficiency. *Catalysts* 2021, 11, 991. [CrossRef]
- 45. Lou, J.; Ren, K.; Huang, Z.; Huo, W.; Zhu, Z.; Yu, J. Electronic and optical properties of two-dimensional heterostructures based on Janus XSSe (X = Mo, W) and Mg(OH)₂: A first principles investigation. *RSC Adv.* **2021**, *11*, 29576–29584. [CrossRef]
- 46. Wang, S.; Tian, H.; Ren, C.; Yu, J.; Sun, M. Electronic and optical properties of heterostructures based on transition metal dichalcogenides and graphene-like zinc oxide. *Sci. Rep.* **2018**, *8*, 12009. [CrossRef]
- 47. Ren, K.; Zheng, R.; Yu, J.; Sun, Q.; Li, J. Band Bending Mechanism in CdO/Arsenene Heterostructure: A Potential Direct Z-scheme Photocatalyst. *Front. Chem.* 2021, *9*, 788813. [CrossRef]
- Ren, K.; Zheng, R.; Lou, J.; Yu, J.; Sun, Q.; Li, J. Ab Initio Calculations for the Electronic, Interfacial and Optical Properties of Two-Dimensional AlN/Zr₂CO₂ Heterostructure. *Front. Chem.* 2021, *9*, 796695. [CrossRef]
- 49. Ren, K.; Zheng, R.; Xu, P.; Cheng, D.; Huo, W.; Yu, J.; Zhang, Z.; Sun, Q. Electronic and Optical Properties of Atomic-Scale Heterostructure Based on MXene and MN (M = Al, Ga): A DFT Investigation. *Nanomaterials* **2021**, *11*, 2236. [CrossRef]