Predicting the Energetic Stabilization of Janus-MoSSe/AlN Heterostructures: A DFT Study

Ramiro M. dos Santos\textsuperscript{a}, Marcelo L. Pereira Júnior\textsuperscript{a}, Luiz F. Roncaratti Júnior\textsuperscript{a} and Luiz A. Ribeiro Júnior\textsuperscript{a,b,}\textsuperscript{*}

\textsuperscript{a}Institute of Physics, University of Brasília, 70910-900, Brasília, Brazil
\textsuperscript{b}PPGCIMA, Campus Planaltina, University of Brasília, 73345-010, Brasília, Brazil

\textbf{ARTICLE INFO}

\textbf{Keywords}: Janus-MoSSe, Aluminum-Nitride, Packing Energy, Improved Lennard-Jones

\textbf{ABSTRACT}

The packing mechanisms between Janus-MoSSe and Aluminum-Nitride (AlN) sheets were systematically investigated by using Density Function Theory calculations. Results show that the stabilization (packing) energies vary from -35.5 up to -17.5 meV depending on the chemical species involved in the interface. The packing energies were obtained using the improved Lennard-Jones (ILJ) potential. The SeMoS/AlN heterostructures, when the MoS face is interacting with the AlN sheet, presented the lowest packing energies due to the sulfur’s higher degree of reactivity. Importantly, the calculated bandgap values ranged within the interval 1.61–1.87 eV, which can be interesting for photovoltaic applications.

1. Introduction

Due to the enormous growth in the global demand for energy consumption in the last decades, novel advances in renewable energy technologies have emerged recently [1–5]. In the establishment of these technologies, transition metal dichalcogenides (TMDs) have been playing an important role [6, 7]. The most known TMD is the molybdenum disulfide (MoS\textsubscript{2}), whose hexagonal monolayer (1H) phase is structurally similar to graphene [8, 9]. One of the greatest advantages of MoS\textsubscript{2} in relation to graphene is its bandgap of 1.9 eV (1.3 eV) for monolayer (multilayer) phase [10, 11]. These values are favorable for optical absorption when exposed to solar radiation [12–15]. In this sense, several works have been developed aiming at designing optoelectronic devices based on MoS\textsubscript{2} [16–20].

TMD-based heterostructures have been both theoretical and experimentally studied [21–26]. Recently, Janus-MoS\textsubscript{2}S\textsubscript{2}-based heterostructures emerged as promising solutions for visible-infrared photocatalysis for water splitting [27–29] and metallic electrodes [30]. Importantly, is was experimentally reported that a Janus-MoS\textsubscript{2}Se monolayer can be obtained through breaking the out-of-plane structural symmetry of the single-layer MoS\textsubscript{2}[31]. In the yielded structure, the sulfur atoms on one side of the monolayer are fully replaced by the selenium ones [31]. Yin and coworkers theoretically studied the role of the intrinsic dipole on photocatalytic water splitting for Janus-MoSSe/Nitrides heterostructures by employing Density Functional Theory (DFT) calculations [32]. Their results showed that MoSSe/XN (X=Al, Ga) configurations with a perfect match between the hexagonal rings are always more stable than other types of stacking regardless of possible atomic positions [32]. Zhao and Schwingenschlögl investigated the van der Waals...
heterostructures constructed from Janus-MoSSe/Germanene through first-principles calculations [30]. The germanene layer was chosen as electrode since it is a Dirac metal with a perfect lattice match to MoSSe [30]. Their findings revealed that an n-type Schottky contact was formed for SeMoS/Ge and a p-type Schottky contact for SMoSe/Ge [30]. A transition from Schottky to Ohmic behavior occurs under tensile strain (∼4% for SeMoS/Ge, ∼8% for SMoSe/Ge), which was explained by modifications of the interface dipole [30]. Albeit relevant studies have been performed to propose feasible applications for Janus-MoSSe-based heterostructures, to the best of our knowledge, the fundamental properties of Janus-MoSSe/Nitrides, such as their packing stabilization, remains not fully understood.

In the present work, we employed DFT calculations to systematically study the stabilization (packing) mechanism of Janus-MoSSe and Aluminum-Nitride (MoSSe/AlN) heterostructures. The computational protocol developed here used the improved Lennard Jones potential (ILJ) [33] and \textit{ab initio} Molecular Dynamics (MD) to obtain the packing energies of van der Waals heterostructures constructed from MoSSe considering both the MoS and MoSe faces interacting with the AlN sheet. The results presented here shed light on the role played by Janus-MoSSe layers in stabilizing van der Waals heterostructures based on TMDs.

2. Methodology

To investigate the structural and electronic properties of MoSSe/AlN heterostructures, we employed DFT calculations as implemented in the SIESTA package [34]. Within the framework of SIESTA, we used the numerical DZP basis set to expand the system wave functions of many atoms [35–37]. The exchange-correlation energies were calculated by using the Local Density Approximation (LDA), as proposed for Ceperley-Alder and Perdew-Wiang (LDA/CA and LDA/PW92, respectively) [38], and the Generalized Gradient Approximation (GGA), as proposed for Perdew-Burke-Ernzerhof and Perdew-Wiang (GGA/PBE, GGA/PW91, respectively) [39]. The relativistic pseudopotentials were parameterized within the Troullier-Martins formalism [40, 41]. These approximations are required to describe the magnetic and electronic properties of materials composed of atoms with many electrons, as is the case of transition metals. A mesh cutoff of 400 Ry is chosen as a parameter for our calculations. The supercells containing MoSSe/AlN were previously converged, with a force criterion of 0.001 eV/Å, to fit in the box that was maintained orthogonal during all optimization. To calculate the bands an MPK mesh of $9 \times 9 \times 3$ was used [42].

The following equation was used to describe the packing energy ($E_p$)

$$E_p(r) = E_{\text{MoSSe/AlN}}^{\text{MoSSe}}(r) - E_{\text{AlN}} - E_{\text{MoSSe}},$$

where $E_{\text{MoSSe/AlN}}^{\text{MoSSe}}(r)$ is the energy of the MoSSe/AlN system that depends on the distance between the two monolayers. $E_{\text{AlN}}$ and $E_{\text{MoSSe}}$ are the energy of the isolated AlN monolayer and the isolated MoSSe monolayer, respectively. The
minimum packing energies and equilibrium distances for all the MoSSe/AlN configurations studied here (see Figure 1) were obtained through the fitting of the interaction energy curves using the ILJ potential [33], as presented in the following

\[ V_{ILJ}(r) = \epsilon \left( \frac{m}{n(r) - m} \left( \frac{r_m}{r} \right)^n - \frac{n(r)}{n(r) - m} \left( \frac{r_m}{r} \right)^m \right). \]

In the equation above, \( \epsilon \) is the background energy of the well, and \( r_m \) is the distance corresponding to \( \epsilon \) (lowest \( E_P \) energy in our case). Here, we assume \( m = 6 \) to account neutral-neutral interactions [33]. Importantly,

\[ n(r) = \beta + 4 \left( \frac{r}{r_m} \right)^2, \]

where \( \beta \) is a parameter related to the hardness of the interaction between the two systems. If \( n(r) \) becomes independent of \( r \), then we obtain the usual relationship for the Lennard-Jones potential [33]. Importantly, \textit{ab initio} MD simulations were also performed, using the SIESTA code, to study the thermodynamical stability of the MoSSe/AlN heterostructures. These simulations were performed using an NPT ensemble with an initial/target temperature set to 300 K and a time-step of 3 fs.

3. Results

We beggiiing our discussions by presenting the different MoSSe/AlN systems investigated here as well as the protocol used to obtain their most stable packing configurations. In Figure 1 we illustrate the four different cases considered in our simulations: 1(a) SeMoS/Al\( ^{IC} \)N (S-AlN interface), 1(b) SMoSe/AlN\( ^C \) (Se-AlN interface), 1(c) SeMoS/AlN (S-AlN interface), and 1(d) SMoSe/AlN (Se-AlN interface), where N\( ^C \) (Al\( ^C \)) and \( \overline{N} \) denote a configuration in which the nitrogen (aluminum) atoms are localized in the center of the TMD hexagons and the nitrogen atoms are vertically aligned with the molybdenum ones, respectively. These model supercells have the following dimensions: 1(a) 10.87 \( \times \) 6.30 \( \times \) 49.41 Å, 1(b) 10.04 \( \times \) 6.40 \( \times \) 38.86 Å, 1(c) 10.86 \( \times \) 6.29 \( \times \) 49.51 Å, and 1(d) 10.89 \( \times \) 6.31 \( \times \) 39.9 Å. Importantly, the bond-length values obtained here for the optimized structures (see Table 1) are in good agreement with the ones reported in literature [32]. In our computational protocol to predict the most stable packing configuration (with lowest stabilization energy), we performed a systematic variation of the \( r \) distance (see Figure 1) between the TMD and AlN surfaces from 1.9 up to 5.6 Å. The composite systems were initially optimized to adjust cell lengths and the TMD and AlN planes were separated from 3.5 Å. For each \( r \) distance, a single-point calculation was performed to obtain
Energetic Stabilization of Janus-MoSSe/AlN Heterostructures

Figure 1: Schematic representation of the four different cases considered in our simulations: (a) SeMoS/AlCN (S-AlN interface), (b) SMoSe/AlN (Se-AlN interface), (c) SeMoS/AlN (S-AlN interface), and (d) SMoSe/AlN (Se-AlN interface), where N\(^{C}\) (Al\(^{C}\)) and AlN denote a configuration in which the nitrogen (aluminium) is placed in the center of the TMD hexagons and the nitrogen is placed vertically aligned with the molybdenum atoms, respectively.

| Bond Type | SeMoS/AlCN | SMoSe/AlN \(^{C}\) | SeMoS/AlN | SMoSe/AlN |
|-----------|------------|----------------------|------------|------------|
| Mo-S (Å)  | 2.39       | 2.42                 | 2.39       | 2.39       |
| Mo-Se (Å) | 2.50       | 2.51                 | 2.50       | 2.48       |
| S-Se (Å)  | 3.25       | 3.26                 | 3.26       | 3.21       |
| Al-N (Å)  | 1.82       | 1.85                 | 1.81       | 1.83       |

Table 1: Bond-length values obtained here for the optimized MoSSe and AlN structures. Importantly, the values presented here are in good agreement with related ones reported in literature [32].

...the interaction energy. Importantly, the four cases studied here (Figure 1) are solutions of the geometry optimization procedure when the MoSSe and AlN sheets were positioned with/without matching their hexagonal rings. Moreover, \textit{ab initio} MD simulations were also performed to verify the dynamical stability of the interfaces with lowest packing energies.

The stabilization energy curves are shown in Figure 2. These curves were obtained using the set of DFT functionals and potentials described in the previous section. In Figure 2, one can note that the lowest \(E_P\) energy for the SeMoS/Al\(^{C}\)N, SMoSe/Al\(^{C}\)N, Se\textsubscript{MoS}/Al\textsubscript{N}, and SMoSe/Al\textsubscript{N} cases is -4.66 meV (LDA/CA), -4.20 meV (LDA/CA), -5.41 meV (LDA/CA), and -5.50 meV (LDA/PW92), respectively. As expected, the cases with the lowest packing energies are the ones in which the perfect match among the hexagons of both structures takes place (SeMoS/Al\textsubscript{N} and SMoSe/Al\textsubscript{N} cases). The cases where the sulfur atoms are interacting with the AlN surface (SeMoS/Al\(^{C}\)N and Se\textsubscript{MoS}/Al\textsubscript{N}) present the lowest packing energies when contrasted to the selenium ones due to the higher degree of reactivity presented by silicon. Among all the heterostructures, the case with perpendicular configuration between sulfur-aluminum (Se\textsubscript{MoS}/Al\textsubscript{N}) presents the higher packing energy than the related one with unpaired hexagons (SeMoS/Al\(^{C}\)N) due to the lower sulfur-aluminum distances.
Figure 2: Stabilization energy curves obtained using the set of DFT functionals and potentials described in the previous section.

|     | SeMoS/AlN<sup>C</sup> | SMoSe/AlN<sup>C</sup> | SeMoS/AIN | SMoSe/AIN |
|-----|------------------------|------------------------|-----------|-----------|
| $\epsilon$ (meV)  | 4.90 (±0.10)           | 5.35 (±0.05)           | 5.15 (±0.06) | 2.36 (±0.11) |
| $r_m$ (Å)         | 2.53 (±0.02)           | 3.15 (±0.01)           | 2.92 (±0.03) | 2.80 (±0.01) |

Table 2

ILJ fitting parameters $\epsilon$ and $r_m$ (equilibrium distance and energy, respectively) for the stabilization energy curves for the cases with the lowest packing energies in Figure 2.

Figure 3 shows the fitting for the stabilization energy curves of lowest packing energies in Figure 2, using the ILJ potential (see Equation 2) [33]. In Figure 3, one can note that the ILJ potential accurately describes the curves wheels, predicting packing energies close to the ones obtained in the DFT calculations (see Table 2).

To verify the suitability of the DFT methodologies employed here, we contrast the band structure profiles for the cases presented in Figure 1, that were calculated using the methods described in the previous section. The band structures were obtained by considering the cases with the lowest packing energies, which were obtained through the fitting procedure presented in Figure 3. One can note that all the DFT methodologies present very similar band structure profiles, as illustrated in Figure 4. The bandgap values obtained using each one of them are presented in Table 3. They lie within the range of the visible spectrum and present a direct character between the Y and $\Gamma$ points, making possible the photon absorption conserving electron momentum. Importantly, the calculated bandgap values ($E_{gap}$) ranged within the interval 1.61–1.87 eV, which can be interesting for photovoltaic applications.
Energetic Stabilization of Janus-MoSSe/AlN Heterostructures

(a) SeMoS/AlCN
(b) SMoSe/AlNC
(c) SeMoS/AlN
(d) SMoSe/AlN

Figure 3: Fitting for the stabilization energy curves for the cases with the lowest packing energies in Figure 2, using the ILJ potential (see Equation 2) [33].

| DFT Method   | SeMoS/AlCN | SMoSe/AlNC | SeMoS/AlN | SMoSe/AlN |
|--------------|------------|------------|-----------|-----------|
| LDA/CA - $E_{\text{gap}}$ (eV) | 1.78       | 1.61       | 1.76      | 1.87      |
| LDA/PW92 - $E_{\text{gap}}$ (eV) | 1.78       | 1.61       | 1.76      | 1.87      |
| GGA/PBE - $E_{\text{gap}}$ (eV) | 1.80       | 1.62       | 1.79      | 1.87      |
| GGA/PW91 - $E_{\text{gap}}$ (eV) | 1.80       | 1.61       | 1.80      | 1.87      |

Table 3
Bandgap values obtained for all the DFT methodologies used here. These values are related to the cases with the lowest packing energies, obtained through the fitting procedure presented in Figure 3.

To validate the thermodynamical stability of the MoSSe/AlN heterostructures studied here, we performed ab initio MD simulations, in which we considered as input the structures with the lowest packing energies (also keeping the related DFT method). In this sense, Figure 5 shows the time evolution of the total potential energy for each system. One can note that the potential energy remains constant during the time. As expected, the systems with lowest potential energies are the ones with a perfect match among the hexagonal rings of both structures (SeMoS/AlN and SMoSe/AlN cases), since they present the lowest packing energies (see Figures 2 and 3). The ab initio MD results suggest that the interaction between MoSSe and AlN layers can yield stable heterostructures. It is worthwhile to stress that these results are in good agreement with the ones reported in literature [32], which showed that MoSSe/XN (X=Al,Ga) configurations with a perfect match between the hexagonal rings are always more stable than other types of stacking regardless of possible atomic positions.
Energetic Stabilization of Janus-MoSSe/AlN Heterostructures

![Graph showing band structure profiles for different heterostructures](image)

**Figure 4:** Band structure profiles for the cases presented in Figure 1 that were obtained using the different DFT methodologies described in the previous section.

### 4. Conclusions

In summary, we used DFT calculations to theoretically investigate the packing mechanism of MoSSe/AlN heterostructures. The computational protocol employed here was based on the ILJ potential and *ab initio* MD simulations to predict the packing energies of van der Waals heterostructures constructed from MoSSe, where both the MoS and MoSe faces interacted with the AlN sheet. The results revealed that the stabilization (packing) energies vary from -35.5 up to -17.5 meV depending on the chemical species involved in the interface. The lowest packing energy for the SeMoS/AlCN, SMoSe/AlNC, SeMoS/AlN, and SMoSe/AlN cases is -4.66 meV, -4.20 meV, -5.41 meV, and -5.50 meV, respectively. The cases with the lowest packing energy are the ones in which the perfect match among the hexagons of both structures takes place (SeMoS/AlN and SMoSe/AlN cases). The cases where the sulfur atoms are interacting with the AlN surface (SeMoS/AlCN and SeMoS/AlN) present the lowest packing energy when contrasted to the selenium ones due to the higher degree of reactivity presented by silicon. The stabilization energy curves were fitted by using the ILJ potential [33]. It was obtained that the ILJ potential can accurately describe the curves wheels, predicting packing energies close to the ones obtained in the DFT calculations. Importantly, all the DFT methodologies used here presented similar band structure profiles. The bandgap values are in the range of 1.61–1.87 eV (visible spectrum) with a direct character. These band structure features can be interesting for photovoltaic applications. Moreover, *ab*
initio MD simulations were performed to validate the thermodynamical stability of the MoSSe/AlN heterostructures studied here. In these simulations, the total potential energies remained constant during the time. Particularly, these results suggest that the interaction between MoSSe and AlN layers can yield stable heterostructures.

Acknowledgments

The authors gratefully acknowledge the financial support from Brazilian Research Councils CNPq, CAPES, and FAPDF and CENAPAD-SP for providing the computational facilities. L.A.R.J. gratefully acknowledges respectively, the financial support from FAP-DF and CNPq grants 00193.0000248/2019-32 and 302236/2018-0.

References

[1] Martin A Green. Third generation photovoltaics: solar cells for 2020 and beyond. Physica E: Low-dimensional Systems and Nanostructures, 14(1-2):65–70, 2002.

[2] Arthur J Nozik, Matthew C Beard, Joseph M Luther, Matt Law, Randy J Ellingson, and Justin C Johnson. Semiconductor quantum dots and quantum dot arrays and applications of multiple exciton generation to third-generation photovoltaic solar cells. Chemical reviews, 110(11):6873–6890, 2010.
Energetic Stabilization of Janus-MoSSe/AlN Heterostructures

[3] Gavin Conibeer, Martin Green, Richard Corkish, Young Cho, Eun-Chel Cho, Chu-Wei Jiang, Thipwan Fangsawanarak, Edwin Pink, Yidan Huang, Tom Puzzer, et al. Silicon nanostructures for third generation photovoltaic solar cells. *Thin solid films*, 511:654–662, 2006.

[4] Norasikin ALudin, AM Al-Alwani Mahmoud, Abd Bakar Mohamad, Abd Amir H Kadhum, Kamaruzzaman Sopian, and Nor Shazlinah Abdul Karim. Review on the development of natural dye photosensitizer for dye-sensitized solar cells. *Renewable and Sustainable Energy Reviews*, 31:386–396, 2014.

[5] Albert Polman and Harry A Atwater. Photonic design principles for ultrahigh-efficiency photovoltaics. *Nature materials*, 11(3):174–177, 2012.

[6] Meng-Lin Tsai, Sheng-Han Su, Jan-Kai Chang, Dung-Sheng Tsai, Chang-Hsiao Chen, Chih-I Wu, Lain-Jong Li, Lih-Juann Chen, and Jr-Hau He. Monolayer mos2 heterojunction solar cells. *ACS nano*, 8(8):8317–8322, 2014.

[7] Sungjin Wi, Hyunsoo Kim, Mikai Chen, Hongsuk Nam, L Jay Guo, Edgar Meyhofer, and Xiaogan Liang. Enhancement of photovoltaic response in multilayer mos2 induced by plasma doping. *ACS nano*, 8(5):5270–5281, 2014.

[8] Lakshay Dheer, Satadeep Bhattacharjee, Seung Cheol Lee, and Umesh V Waghmare. Van der waals hetero-structures of 1h-mos2 and n-substituted graphene for catalysis of hydrogen evolution reaction. *Materials Research Express*, 6(12):124006, 2020.

[9] Wenyan Zan, Wei Geng, Huanxiang Liu, and Xiaojun Yao. Influence of interface structures on the properties of molybdenum disulfide/graphene composites: A density functional theory study. *Journal of Alloys and Compounds*, 649:961–967, 2015.

[10] Andrea Splendiani, Liang Sun, Yuanbo Zhang, Tianshu Li, Jonghwan Kim, Chi-Yung Chim, Giulia Galli, and Feng Wang. Emerging photoluminescence in monolayer mos2. *Nano letters*, 10(4):1271–1275, 2010.

[11] Philipp Tonndorf, Robert Schmidt, Philipp Böttger, Xiao Zhang, Janna Börner, Andreas Liebig, Manfred Albrecht, Christian Kloc, Ovidiu Gordan, Dietrich RT Zahn, et al. Photoluminescence emission and raman response of monolayer mos 2, mose 2, and wse 2. *Optics express*, 21(4):4908–4916, 2013.

[12] Yuanxin Li, Ningning Dong, Saifeng Zhang, Xiaoyan Zhang, Yanyan Feng, Kangpeng Wang, Long Zhang, and Jun Wang. Giant two-photon absorption in monolayer mos2. *Laser & Photonics Reviews*, 9(4):427–434, 2015.

[13] A Steinhoff, J-H Kim, F Jahnke, M Rösner, D-S Kim, Ch Lee, Gang Hee Han, Mun Seok Jeong, TO Wehling, and C Gies. Efficient excitonic photoluminescence in direct and indirect band gap monolayer mos2. *Nano letters*, 15(10):6841–6847, 2015.

[14] Eric Singh, Ki Seok Kim, Geun Young Yeom, and Hari Singh Nalwa. Atomically thin-layered molybdenum disulfide (mos2) for bulk-heterojunction solar cells. *ACS applied materials & interfaces*, 9(4):3223–3245, 2017.

[15] Meng-Lin Tsai, Sheng-Han Su, Jan-Kai Chang, Dung-Sheng Tsai, Chang-Hsiao Chen, Chih-I Wu, Lain-Jong Li, Lih-Juann Chen, and Jr-Hau He. Monolayer mos2 heterojunction solar cells. *ACS nano*, 8(8):8317–8322, 2014.

[16] Zongyou Yin, Hai Li, Hong Li, Lin Jiang, Yumeng Shi, Yinghui Sun, Gang Lu, Qing Zhang, Xiaodong Chen, and Hua Zhang. Single-layer mos2 phototransistors. *ACS nano*, 6(1):74–80, 2012.

[17] Yexin Deng, Zhe Luo, Nathan J Conrad, Han Liu, Yongji Gong, Sina Najmaei, Pulickel M Ajayan, Jun Lou, Xianfan Xu, and Peide D Ye. Black phosphorus–monolayer mos2 and van der waals heterojunction p–n diode. *ACS nano*, 8(8):8292–8299, 2014.

[18] Fengping Li, Wei Wei, Pei Zhao, Baibiao Huang, and Ying Dai. Electronic and optical properties of pristine and vertical and lateral heterostructures of janus mosse and wsse. *The journal of physical chemistry letters*, 8(23):5959–5965, 2017.

[19] Deependra Kumar Singh, Rohit Pant, Arun Malla Chowdhyury, Basanta Roul, Karuna Kar Nanda, and Saluru Baba Krupanidhi. Defect-mediated transport in self-powered, broadband, and ultrafast photoresponse of a mos2/alin/si-based photodetector. *ACS Applied Electronic Materials*, 2(4):944–953, 2020.

[20] Xiaobin Liao, Yunlong Zhao, Junhui Wang, Wei Yang, Lin Xu, Xiaocong Tian, Yi Shuang, Kwadwo Asare Owusu, Mengyu Yan, and Liqiang Ramiro Marcelo dos Santos et al.: Preprint submitted to Elsevier Page 9 of 11
Energetic Stabilization of Janus-MoSSe/AlN Heterostructures

Mai. Mos 2/mno 2 heterostructured nanodevices for electrochemical energy storage. *Nano Research*, 11(4):2083–2092, 2018.

[21] Željko Šljivančanin and Milivoj Belić. Graphene/mos₂ heterostructures as templates for growing two-dimensional metals: Predictions from ab initio calculations. *Phys. Rev. Materials*, 1:044003, Sep 2017.

[22] Dongyuan Chen, Weixiang Chen, Lin Ma, Ge Ji, Kun Chang, and Jim Yang Lee. Graphene-like layered metal dichalcogenide/graphene composites: synthesis and applications in energy storage and conversion. *Materials Today*, 17(4):184 – 193, 2014.

[23] Georg Duesberg. Heterojunctions in 2d semiconductors: A perfect match. *Nature materials*, 13:1075–6, 11 2014.

[24] Miguel M Ugeda, Aaron J Bradley, Su-Fei Shi, H Felipe, Yi Zhang, Diana Y Qiu, Wei Ruan, Sung-Kwan Mo, Zahid Hussain, Zhi-Xun Shen, et al. Giant bandgap renormalization and excitonic effects in a monolayer transition metal dichalcogenide semiconductor. *Nature materials*, 13(12):1091–1095, 2014.

[25] Martin Gmitra and Jaroslav Fabian. Graphene on transition-metal dichalcogenides: A platform for proximity spin-orbit physics and optospintronics. *Phys. Rev. B*, 92:155403, Oct 2015.

[26] Amin Azizi, Sarah Eichfeld, Gayle Geschwind, Kehao Zhang, Bin Jiang, Debangshu Mukherjee, Lorraine Hossain, Aleksander F Piasecki, Bernd Kabius, Joshua A Robinson, et al. Freestanding van der waals heterostructures of graphene and transition metal dichalcogenides. *ACS nano*, 9(5):4882–4890, 2015.

[27] Lin Ju, Mei Bie, Jing Shang, Xiao Tang, and Liangzhi Kou. Janus transition metal dichalcogenides: superior platform for photocatalytic water-splitting. *Journal of Physics: Materials*, 3, 03 2020.

[28] Yimin Xu, Yongsheng Yao, Wenjin Yin, Juexian Cao, Mingyang Chen, and Xiaolin Wei. Intrinsic defect engineered janus mosse sheet as a promising photocatalyst for water splitting. *RSC Advances*, 10(18):10816–10825, 2020.

[29] M Idrees, HU Din, Shafiq Ur Rehman, M Shafiq, Yasir Saeed, HD Bui, Chuong V Nguyen, and Bin Amin. Electronic properties and enhanced photocatalytic performance of van der waals heterostructures of zno and janus transition metal dichalcogenides. *Physical Chemistry Chemical Physics*, 22(18):10351–10359, 2020.

[30] Ning Zhao and Udo SchwingenschlÃ/uni0171gl. Transition from schottky to ohmic contacts in janus mosse/germanene heterostructures. *Nanoscale*, 12:11448–11454, 2020.

[31] Ang-Yu Lu, Hanyu Zhu, Jun Xiao, Chih-Piao Chuu, Yimo Han, Ming-Hui Chiu, Chia-Chin Cheng, Chih-Wen Yang, Kung-Hwa Wei, Yiming Yang, et al. Janus monolayers of transition metal dichalcogenides. *Nature nanotechnology*, 12(8):744–749, 2017.

[32] Wenjin Yin, Bo Wen, Qingxia Ge, Daifeng Zou, Ying Xu, Mingwei Liu, Xiaolin Wei, Mingyang Chen, and Xiaoli Fan. Role of intrinsic dipole on photocatalytic water splitting for janus mosse/nitrides heterostructure: A first-principles study. *Progress in Natural Science: Materials International*, 29(3):335 – 340, 2019. Special Issue of Computational Materials.

[33] Fernando Pirani, Simona Brizi, Luiz F. Roncaratti, Piergiorgio Casavecchia, David Cappelletti, and Franco Vecchiocattivi. Beyond the lennard-jones model: a simple and accurate potential function probed by high resolution scattering data useful for molecular dynamics simulations. *Phys. Chem. Chem. Phys.*, 10:5489–5503, 2008.

[34] José M Soler, Emilio Artacho, Julian D Gale, Alberto García, Javier Junquera, Pablo Ordejón, and Daniel Sánchez-Portal. The SIESTA method forab initioorder-nmaterials simulation. *Journal of Physics: Condensed Matter*, 14(11):2745–2779, 2002.

[35] W. Kohn and L. J. Sham. Self-consistent equations including exchange and correlation effects. *Phys. Rev.*, 140:A1133–A1138, 1965.

[36] P. Hohenberg and W. Kohn. Inhomogeneous electron gas. *Phys. Rev.*, 136:B864–B871, 1964.

[37] James P. Lewis, Kurt R. Glaesemann, Gregory A. Voth, Jürgen Fritsch, Alexander A. Demkov, José Ortega, and Otto F. Sankey. Further developments in the local-orbital density-functional-theory tight-binding method. *Phys. Rev. B*, 64:195103, Oct 2001.

[38] David C. Langreth and M. J. Mehl. Beyond the local-density approximation in calculations of ground-state electronic properties. *Phys. Rev.*
Energetic Stabilization of Janus-MoS\textsubscript{2}/AlN Heterostructures

\textit{B}, 28:1809–1834, Aug 1983.

[39] John P. Perdew, Kieron Burke, and Matthias Ernzerhof. Generalized gradient approximation made simple. \textit{Phys. Rev. Lett.}, 77:3865–3868, 1996.

[40] Warren E. Pickett. Pseudopotential methods in condensed matter applications. \textit{Computer Physics Reports}, 9(3):115 – 197, 1989.

[41] N. Troullier and José Luís Martins. Efficient pseudopotentials for plane-wave calculations. ii. operators for fast iterative diagonalization. \textit{Phys. Rev. B}, 43:8861–8869, Apr 1991.

[42] Hendrik J. Monkhorst and James D. Pack. Special points for brillouin-zone integrations. \textit{Phys. Rev. B}, 13:5188–5192, Jun 1976.