ACCEPTED MANUSCRIPT

Status and prospects of ohmic contacts on two dimensional semiconductors

To cite this article before publication: Junhao Ni *et al* 2021 *Nanotechnology* in press <https://doi.org/10.1088/1361-6528/ac2fe1>

Manuscript version: Accepted Manuscript

Accepted Manuscript is “the version of the article accepted for publication including all changes made as a result of the peer review process, and which may also include the addition to the article by IOP Publishing of a header, an article ID, a cover sheet and/or an ‘Accepted Manuscript’ watermark, but excluding any other editing, typesetting or other changes made by IOP Publishing and/or its licensors”

This Accepted Manuscript is © 2021 IOP Publishing Ltd.

During the embargo period (the 12 month period from the publication of the Version of Record of this article), the Accepted Manuscript is fully protected by copyright and cannot be reused or reposted elsewhere.

As the Version of Record of this article is going to be / has been published on a subscription basis, this Accepted Manuscript is available for reuse under a CC BY-NC-ND 3.0 licence after the 12 month embargo period.

After the embargo period, everyone is permitted to use copy and redistribute this article for non-commercial purposes only, provided that they adhere to all the terms of the licence <https://creativecommons.org/licences/by-nc-nd/3.0>

Although reasonable endeavours have been taken to obtain all necessary permissions from third parties to include their copyrighted content within this article, their full citation and copyright line may not be present in this Accepted Manuscript version. Before using any content from this article, please refer to the Version of Record on IOPscience once published for full citation and copyright details, as permissions will likely be required. All third party content is fully copyright protected, unless specifically stated otherwise in the figure caption in the Version of Record.

View the [article online](#) for updates and enhancements.

Status and Prospects of Ohmic Contacts on Two Dimensional Semiconductors

Junhao Ni^{a,#}, Quangui Fu^{a,#}, Kostya (Ken) Ostrikov^b, Xiaofeng Gu^a, Haiyan Nan^{a,*}, and Shaoqing Xiao^{a,*}

^aEngineering Research Center of IoT Technology Applications (Ministry of Education), Department of Electronic Engineering, Jiangnan University, Wuxi 214122, China.
^bSchool of Chemistry and Physics and QUT Centre for Materials Science, Queensland University of Technology (QUT), Brisbane QLD 4000, Australia
*Corresponding author: jnanhaiyan@jiangnan.edu.cn (Haiyan Nan)
xiaosq@jiangnan.edu.cn (Shaoqing Xiao)

#These authors contributed equally.

Abstract

In recent years, two-dimensional materials have received more and more attention in the development of semiconductor devices, and their practical applications in optoelectronic devices have also developed rapidly. However, there are still some factors that limit the performance of two-dimensional semiconductor material devices, and one of the most important is Ohmic contact. Here, we elaborate on a variety of approaches to achieve Ohmic contacts on two dimensional materials and reveal their physical mechanisms. For the work function mismatch problem, we summarize the comparison of barrier heights between different metals and 2D semiconductors. We also examine different methods to solve the problem of Fermi level pinning. For the novel 2D metal-semiconductor contact methods, we analyse their effects on reducing contact resistance from two different perspectives: homojunction and heterojunction. Finally, the challenges of 2D semiconductors in achieving Ohmic contacts are outlined.

Keywords: two-dimensional materials; Ohmic contact; work function; Schottky barrier; Fermi level pinning; transferring electrode; 2D metal-semiconductor contact

1. Introduction

In the past half century, the maturity of complementary metal oxide semiconductor (CMOS) field effect transistor (FET) devices based on silicon (Si) has enabled modern information technology to develop by leaps and bounds [1, 2]. According to Moore's Law, the integration density of FETs on a chip can be doubled and the feature size of FETs can be shrunked greatly in every two years [3]. When the channel length is close to a few nanometers, problems such as short channel effect and high heat dissipation will emerge, indicating that traditional silicon-based devices are approaching their limits. Therefore, it is urgent to explore new alternative materials [4-6]. In this context, 2D semiconductor materials such as graphene [7], transition metal dichalcogenides (TMDC) [8-12], Black Phosphorous (BP)[13, 14], etc. have received more and more attention in recent years. In particular, Ajayan et al. has made a comprehensive summary on the characteristics, preparation and application of different 2D semiconductor materials [15]. The 2D materials are so atomically thin that the channel length of FETs based on such materials can be further reduced without short channel effect. Moreover, due to their unsuspended surface, the devices based on such materials can greatly eliminate carrier scattering, representing an obvious advantage over traditional materials like Si [16-20]. These excellent features of 2D materials have made them promising for a variety of electronic and optoelectronic devices including field effect transistors [21], photodetectors [22], logic devices [23], light-emitting diodes [24] etc.

The contacts between metallic electrodes and semiconductor materials are crucial components of electronic and optoelectronic devices [25], especially for 2D materials that are always accompanied by 3D metallic electrodes. In fact, contacts are the communication bridge between 2D materials and the three-dimensional world [26]. Such contacts are either Ohmic contacts or Schottky junctions. The latter may result in a huge contact resistance and thus hinder the transport of carriers [27, 28], degrade the transconductance [29], switching current ratio and other properties. Therefore, for most devices, Ohmic contact is a guarantee of high performance [26, 30-32]. To this end, researchers have explored many new methods in recent years to achieve Ohmic contacts or reduce 2D contact resistance, such as one-dimensional contact [33-36]; phase engineering [37-39]; electrode transfer [40] and so on. Precise engineering of ohmic contacts in two-dimensional materials is rapidly gaining momentum as summarized in a recent review [41]. This article complements the analysis of the recent advances in this area by examining the effective approaches to fabricate Ohmic contacts on 2D materials as well as the relevant physical mechanisms.

In this review, we will elaborate on the latest research progress of different methods in achieving Ohmic contacts or reducing contact resistances for 2D materials devices. They can be mainly classified into three ones: using metal electrodes with matched work function, solving the problem of Fermi pinning level and using 2D metal-semiconductor contacts. We first examine the work function matching between the most widely studied 2D materials like graphene, TMDCs and BP and different metals, and pinpoint the most suitable metals for these 2D materials in achieving Ohmic contacts. We then study the problem of Fermi level pinning and reveal the physical mechanism. Through different contact engineering, the Fermi level pinning effect at the interface can be weakened and even almost completely suppressed. Finally, in the third part, we shift our sight from 3D to 2D, and focus on effective methods for 2D metal materials to reduce contact resistance from the perspective of homojunction and heterojunction. The main motivation of this review is to establish the associations between different contact methods and the properties of 2D semiconductors to facilitate our understandings toward how to realize Ohmic contacts on 2D semiconductors and improve the performance of their devices.

2. Using metal electrodes with matched work function

In theory, the contact resistance mainly depends on the height of the Schottky barrier. When the metal electrode and the semiconductor interface are in contact, due to the difference between the metal work function and the semiconductor affinity (ionization potential), the energy band will be bent and the Schottky barrier will be generated. Under ideal circumstances, according to Schottky-Mott's law [42, 43]:

$$\Phi_{B,n} = \phi_M - \chi_{SC} \quad (1.)$$

$$\Phi_{B,p} = I_{SC} - \phi_M \quad (2.)$$

where $\Phi_{B,n}$ and $\Phi_{B,p}$ are the Schottky barrier heights for electron and hole injection respectively, ϕ_M is the metal work function, χ_{SC} and I_{SC} are the electron affinity and ionization potentials respectively. In theory, we can minimize the height of the Schottky barrier by selecting a suitable metal electrode to reduce the contact resistance. The minimum of the Schottky barrier is zero corresponding to Ohmic contact. Therefore, we will systematically study the work function matching between different metals and the most widely studied 2D materials like graphene, TMDC (mainly MoS₂), and BP in achieving Ohmic contacts in this section.

2.1 Graphene

Unlike other 2D materials, graphene has a zero-band gap, so it doesn't form a depletion layer and traditional Schottky barrier when it contacts with metal. The contact between metals with different work functions and graphene will cause graphene to be electrically doped, causing the Fermi level of graphene to move away from the Dirac point. Although graphene has good conductivity, the small density of states near the Dirac point limits the carrier transfer efficiency between metal and graphene, resulting in high contact resistance in the contact area [30]. By using the transmission line model measurement method, Osman et al. measured the contact resistance of Au and graphene to be 630 $\Omega\cdot\mu\text{m}$, Ag-630 $\Omega\cdot\mu\text{m}$, Cu-8800 $\Omega\cdot\mu\text{m}$, Pd-570 $\Omega\cdot\mu\text{m}$ [44] and Ni-2200 $\Omega\cdot\mu\text{m}$ [45]. It is obvious that the contact resistance of Pd and Au is the smallest and this is why we often use Au as the metal electrodes in daily experiments. In addition to a single metal electrode, a combination of multiple metals is generally employed in daily experiments. For this reason, the contact resistance of a combination of multiple metals in contact with graphene is also listed. Au is the most widely used choice among the combined metals. When the previous single metal and Au are combined to serve as the contact, the contact resistance drops significantly. The contact resistance of Cu/Au drops to 92 $\Omega\cdot\mu\text{m}$ [46], which is reduced by two orders of magnitude

Pd/Au-122 $\Omega\cdot\mu\text{m}$ [46]; Ni/Au-400 $\Omega\cdot\mu\text{m}$ [45]; Ti/Au- 23 $\Omega\cdot\mu\text{m}$ [46]. It is clear that Ti/Au and Cu/Au mixed contacts are the most appropriate for graphene in reducing the contact resistance.

2.2 TMDCs and BP

As a typical n-type representative semiconductor of TMDCs, MoS₂ has received extensive attention due to its excellent performance. Here, we mainly study the Schottky barrier height when MoS₂ is in contact with metals with different work functions, and summarize the metal-semiconductor contacts closest to Ohmic contact. The left side of **Figure 1 (a)** is the energy band of MoS₂ and the work function arrangement of commonly used metals, and the right side is the n-type Schottky barrier height where different metals contact with MoS₂. Among them, the red part is the electronic Schottky barrier height obtained through theoretical calculation [9], and the blue part is the Schottky barrier height extracted in the actual experiment [11, 47, 48]. It can be found that the Fermi levels of Sc and Ti are closer to the conduction band of MoS₂, and the Schottky barrier heights between Sc and MoS₂ as well as between Ti and MoS₂ are the smallest. Comparing theoretically calculated barrier heights with actual ones for all the metals, one can find a large difference between them except the metals including Au and Pt. This means that Au and Pt metal electrodes are very hardly affected by the surface states. In addition to Sc and Ti, Kang et al. have also studied metal Mo as an electrode in contact with MoS₂. Because Mo is the constituent metal of the semiconductor material, strong atomic orbital overlap occurs at the contact interface, thus giving rise to a smaller contact resistance than Ti. As show in **Figure 1(b)**, the SBH of Mo-MoS₂ system is much less than Ti-MoS₂ system [49, 50]. In addition, Wang et al. have achieved van der Waals contacts (as shown in **Figure 1(c)**) to reduce contact resistance by evaporating 10 nm thick In between 100 nm thick Au and a single layer of MoS₂ [51]. The experimentally extracted Schottky barrier is about 110 meV, and the contact resistance on the single-layer MoS₂ is measured to be about 3 k $\Omega\mu\text{m}$, and that on the multilayer MoS₂ is 0.8 k $\Omega\mu\text{m}$, which is one of the smallest values so far. This resulted in a huge increase in mobility (**Figure 1(c)**) [51]. In brief, in addition to Sc and Ti with low work function, the special metals Mo and In can also achieve almost Ohmic contact for MoS₂. Similarly, for another n-type TMDCs like WS₂, the most appropriate metals to achieve Ohmic contact are Sc, Ti, W and In [49].

However, for typical p-type TMDCs like WSe₂, the metals with high work function are preferred instead to achieve Ohmic contact. As shown in **Figure 1(d)**, the Schottky barrier heights of holes between WSe₂ and different metals are 1.27, 1.25, 1.13, 0.9 and 0.35eV, corresponding to Ti, W, In, Au, and Pd. Therefore, the most appropriate metals to achieve Ohmic contact for WSe₂ is Pd.

BP shows great potential in 2D electronic and optoelectronic devices because of its high mobility and direct band gap. Few-layer BP flakes with 3-15 layers are often used in practice, which possess a bandgap ranging from 0.3 to 0.6 eV. The band gap can be calculated theoretically: $E_{gap} = 0.39\text{eV} + 1.62/n^{1.4}$ (n=number of layers). As the number of BP layers increases, the band gap decreases. In order to study the influence of different metals and BP contact, Wang et al. listed the Schottky barrier heights extracted from five different metals Ti, Ni, Ag, Sc, Er in contact with BP under the alumina package [52] (**Figure1(e)**). It can be seen from the figure that Ni has the lowest hole barrier, which is more conducive to hole injection, so as to achieve high-quality p-type contact, which is also proved by experimental results. Zhi-peng et al. reported that when using Ni in contact with 12nm thick BP, the extracted Schottky barrier is 92meV; when using 15nm BP in contact with Ni, Ni₂P is formed after annealing at 300°C, making the contact potential barrier reduced to 12 meV [53]. Compared with low work function metals Co and Ti as contact metals (extracted Schottky barriers are 206meV [54] and 325meV [55], respectively), Ni shows obvious advantages. In addition to Ni, high work function metal Pd is also a common metal. Yuqiang Ma et al. synthesized Pd-H alloy by reacting with H₂ to increase the work function of the metal, thereby reducing the barrier height and making the contact resistance from 7.1 $\Omega\cdot\text{mm}$ is reduced to 1.05 $\Omega\cdot\text{mm}$ [56]. As a supplement to BP performance, bipolar transport can be obtained by using Al ($\phi_{Al}=4.2\text{eV}$) with BP contact, which provides more possibilities for the application of BP in CMOS [57, 58].

3. Solving pinning effect

Ideally, the height of the Schottky barrier between a metal and a semiconductor is determined by the metal work function, but in practice, the Φ_B in formula (1) is usually insensitive to Φ_M . This is mainly due to the fact that the Fermi level of the system is typically pinned to a nearly fixed position in the semiconductor bandgap, varying little with respect to different metals used. The Schottky-Mott law should be rewritten as following when considering the Fermi pinning effect [59]:

$$\Phi_B = S(\phi_M - \phi_{CNL}) + (\phi_{CNL} - \chi) \quad (3.)$$

where S is the Schottky pinning coefficient ($S = d\phi_B/d\phi_M$), χ is the electron affinity of the semiconductor, and ϕ_{CNL} is the charge intermediate performance level under a relative vacuum level. Generally, the Fermi level will be pinned near ϕ_{CNL} , it is given by the following formula:

$$\phi_{CNL} = \frac{\chi + b}{1 - S} \quad (4.)$$

where b is the y-intercept of the ϕ_B versus ϕ_M graph, S depends on the interface state density per unit area N and the length δ extending into the semiconductor as:

$$S = \frac{1}{1 + \frac{q^2 N \delta}{\epsilon_0 \epsilon_r}} \quad (5.)$$

where $\epsilon_0 \epsilon_r$ is the absolute permittivity of the interface. When S is equal to 0, strong Fermi level pinning effect dominates so that SBH has nothing to do with the work function of the metal; when S is close to 1, the Barding limit converges to the Schottky limit.

The origin of Fermi level pinning may be mainly due to the existence of interface dipoles and metal-induced interstitial states (MIGS) [60]. The interface dipoles will change the metal work function, and the metal-induced interstitial states will weaken the layer Molybdenum-sulfur bond through the interaction between the metal and the chalcogenide element, thereby pinning the Fermi level [60]. In addition, the existence of defects is considered to be one of the main reasons for Fermi level pinning [61, 62]. The SBH difference between theoretical and experimental values as illustrated in Section 1.2 may be caused by the defect state, which is attributed to atomic vacancies and process-induced defects [63]. Studies on the pinning factor of the defect area and the original surface show that in most cases, the pinning factor of the defect area is observed to be about 30-40% smaller than that of the original surface, which indicates that the FLP is stronger at the defect location [64]. Guo et al.'s study of Schottky barrier heights for a variety of metals showed that any defects formed at the interface will cause additional pinning and reduce the S value [65]. Therefore, improving the quality of the interface is essential for achieving high-performance Ohmic contacts.

3.1 Reducing interface impact

One of the main methods to alleviate the Fermi level pinning effect is to insert an ultra-thin oxide layer between the metal and the semiconductor to realize the MIS structure. The insertion of the oxide layer can isolate the direct contact between the metal and the 2D semiconductor, and thus suppress the Fermi level pinning effect by reducing the metal-induced interstitial state. Also, the insertion of the oxide layer can ensure the cleanness of the interface. Various metal oxides have been used as insulating layers to reduce the pinning effect, such as MoO_x , MgO , Ta_2O_5 , TiO_2 and so on [66-69]. As early as 2013, Chen et al. found that by inserting MgO between Co and MoS_2 , the height of the Schottky barrier can be reduced by 84% [66]. In addition to MgO , TiO_2 is also a commonly used oxide. In 2014, Dankert et al. also used Co as a contact and changed the interface state by inserting a TiO_2 insulating layer between Co and MoS_2 . As a result, the height of the extracted Schottky barrier was reduced from 121 meV to 27 meV, and the on-state current of the transistor increased by two orders of magnitude, as shown in **Figures 2(a) and 2(b)** [67]. Recently, Kim has further studied the reason why the oxide layer alleviates the Fermi level pinning effect by inserting 1nm TiO_2 between various metals and MoS_2 . As shown in **Figures 2(c) and 2(d)**, the pinning coefficient S is increased from 0.02 to 0.24 after inserting TiO_2 , showing a stronger work function dependence. The Fermi level pinned in the intermediate state is moved more toward their ideal position through the reduced interface state of the oxide layer, thereby weakening the pinning effect [68]. Lee et al. reduced the barrier height from 95 meV to 29 meV by inserting Ta_2O_5 between MoS_2 and metal contacts [69]. As shown in **Figure 2(e)**, the authors believed that the MIS structure can alleviate the Fermi level pinning mainly due to two points: (1) The metal will make the semiconductor Fermi level move to the charge middle performance level, and the oxide layer can weaken this effect; (2) Interfacial dipoles will be formed on the interface of oxide and semiconductor, and the opposite electric field of the interfacial dipoles will also restrict the Fermi energy level to move to the charge middle performance level. At the same time, Lee et al. also found that the thickness of the oxide layer also has an effect on the barrier height. The barrier height will increase as the oxide layer thickness increases [69].

In addition to the oxide layer, inserting h-BN to form the MIS structure can also effectively suppress the Fermi level pinning effect [70, 71] with similar physical mechanisms. BN can help form a high-quality interface with 2D semiconductors to prevent the formation of defects and traps. Wang et al. reduced the barrier height from 158 meV to 31 meV and the contact resistance from 5.1 $\text{k}\Omega\mu\text{m}$ to 1.8 $\text{k}\Omega\mu\text{m}$ by inserting h-BN between MoS_2 and Ni/Au [70]. In addition to intercalation, it is also a feasible method to reduce the Fermi level pinning effect by treating

the metal surface. Min et al. weakened the Fermi level pinning effect by atomically passivating gold, reducing the barrier height to 0.12 eV, almost realizing Ohmic contact [72]. In addition, ultra-high vacuum deposition of metal electrodes can make the metal/semiconductor interface extremely clean and thus greatly reduce the contact resistance. For example, the contact resistance of MoS₂/Au contact with the metal electrode deposited under ultra-high vacuum conditions (10⁻⁹ Torr) is three times lower than that under normal conditions (10⁻⁶ Torr) [73]. Recently, Matkovic, et al. successfully adjusted the work function of the metal electrode by using a self-assembled monolayers (SAMs) containing pyrimidine, so that the contact resistance between MoS₂ monolayer and metal electrode was reduced by two orders of magnitude. This work brings a new but well-understood approach in organic electronics to realize ohmic contact in the field of 2D materials [74].

3.2 Transferring electrode

The above-mentioned multiple methods can partially reduce the Fermi level pinning effect, while transferring electrode as proposed and demonstrated by Liu et al. can almost completely eliminate the Fermi level pinning effect [40]. By pre-fabricating metal electrodes and transferring them onto the two-dimensional semiconductor surface via physical lamination, related chemical barriers and defect-induced gap states are completely eliminated. As shown in **Figures 3(a)** and **3(b)**, compared to the metal/semiconductor interface prepared by traditional deposition method, that prepared by transferring electrode method has an atomically sharp and clean interface, without defects, strain, metal diffusion, etc. Physical contact without direct chemical bonding can greatly inhibit the generation of interstitial states induced by interface dipoles and metals, thereby eliminating Fermi level pinning. **Figure 3(c)** shows the transfer characteristic curves of MoS₂ FETs with electron beam deposited metal electrodes. It can be seen that regardless of the different work function of the contact metals, all curves show n-type behaviour. This indicates that there is a strong Fermi level pinning effect near the MoS₂ conduction band. On the contrary, for the FETs with transferring metal electrodes, as shown in **Figure 3(c)**, the transfer curves can exhibit different polarities with the change of the work function of different metals. For low work function metal like Ag, a good n-type transfer curve is observed; as the work function of the metal increases, it shows a transition from n-type to bipolar and then to p-type. By using the extracted Schottky barrier height, the Fermi level pinning coefficient is fitted in **Figure 3(d)**. For the FET devices with deposited metal, the extracted S parameter is 0.09, which is consistent with the previous results. For the devices with transferring electrode, the fitted S parameter is 0.96, which is approaching the Schottky-Mott limit, indicating that the height of the Schottky barrier depends dominantly on the metal work function.

4. 2D-semiconductor-metal contact

Using 2D metal materials instead of traditional metals to contact 2D semiconductors is also a good strategy to eliminate the Fermi level pinning effect. Homogeneous structures or heterostructures formed by 2D metals and 2D semiconductors can strongly inhibit the formation of metal-induced interstitial states in semiconductors, thereby reducing the Fermi level pinning effect. In this section, we thus elaborate on effective methods for 2D metal materials to reduce contact resistance from the perspective of homojunction and heterojunction.

4.1 Homojunction

For TMDCs, in addition to the 2H phase semiconductor state, they also have 1T and 1T' metal states. As shown in **Figure 4(a)**, both 2H and 1T (1T') phases possess the same lattice constant so that their in-plane connections are perfectly aligned without any interface defects [75, 76]. For example, as shown in **Figure 4(b)**, it is effective to grow lateral homojunction consisting of 2H MoTe₂ and 1T MoTe₂ by chemical vapor deposition via adjusting growth temperature since the energy difference between the 1T phase and the 2H phase is very small (35 meV per unit cell) [77, 78]. Compared with the traditional contact consisting of 2H semiconducting phase MoTe₂ and metal electrode where a Schottky contact is always formed, a novel contact consisting of 2H/1T' homojunction and metal electrode is fabricated where a stable covalent bond is formed between the 1T' phase and the 2H phase. In this case, the 1T' metallic phase serves as the transition region between 2H semiconducting phase and metal electrode. As a result, the contact resistance is reduced significantly and the conductance of the 2H semiconducting channel is increased by two orders of magnitude. As shown in **Figure 4(c)**, the height of the Schottky barrier is reduced greatly from 150 meV for the traditional contact consisting of 2H MoTe₂ and metal electrode to 22 meV for the novel contact consisting of 2H/1T' homojunction and metal electrode. Such Chemical Vapor Deposition (CVD) method can also be applicable to the fabrication of WSe₂ 2H/1T homojunction for reducing the Fermi level pinning effect [79, 80].

In addition, phase engineering of existing 2H-phase TMDCs to transform them into metallic phases is also a commonly used method [37, 38, 81]. As early as 2014, Kappera et al. [37] transformed the 2H phase of MoS₂ into 1T phase through a local induction method, as shown in **Figure 4(d)**. The contact resistance measured under zero grid bias is only 200 $\Omega\cdot\mu\text{m}$, which is the lowest value ever for MoS₂ [37]. Cho et al. also realized the transformation of MoTe₂ from 2H phase to 1T' phase by laser burning method and systematically studied their Schottky barriers. The Schottky barrier height in the 1T' phase is only 10 meV and the field-effect mobility is increased by 50 times [82], indicating that Ohmic contact is nearly realized.

Interestingly, for some specific 2D materials such as PtSe₂, the phase state depends on the thickness of the material. The thick layer behaves as a metal state, while the few layers become a semiconductor state. In such case, homogeneous junction can be fabricated by superimposing two PtSe₂ layers with different thicknesses. Indeed, Das et al. achieved a low-resistance Ohmic contact by transferring multiple layers of PtSe₂ onto three layers of PtSe₂ (**Figure 4(e)**) [83]. The barrier height was reduced from 140 meV for the traditional contact consisting of 3L PtSe₂ and metal electrode to 35 meV for the novel contact consisting of ML PtSe₂/3L PtSe₂ and metal electrode [83].

4.2 Heterojunction

In addition to fabricating 2D metal/semiconductor homojunctions made of different phases of the same material to reduce the contact resistance, fabricating 2D metal/semiconductor heterojunctions made of different 2D materials is also an alternative choice. Graphene, as a metallic 2D material with adjustable Fermi level, is usually used as the intermediate metal layer [84, 85]. As shown in **Figure 5(a)**, Chee et al. fabricated the MoS₂ transistor by using graphene as the intermediate metal layer between MoS₂ and Ag electrode [84]. The output characteristics of the controlled MoS₂ transistor without using graphene and the one with 2D metal/semiconductor heterojunctions under different gate bias are presented in **Figure 5(b)**, clearly demonstrating that the contact resistance of the latter device is reduced to 1.4% of the controlled one [84]. Apart from graphene, there are many metallic 2D materials such as VS₂, VSe₂, NbS₂ the 1T or 1T' phase TMDs mentioned in Section 4.1. Ji et al. transferred the thin layer VS₂ (<10 nm) produced by the CVD method onto MoS₂, and the source-drain current under the same bias voltage was increased by 4 times in comparison with that of the MoS₂ device with the traditional Ni/Au electrode. Compared to 1T-MoS₂ or 1T'-MoTe₂, 1T-VS₂ exhibits stronger thermal stability, and its performance does not decline even after a few months [86].

Compared to the above transferring method, 2D semiconductor/metal heterojunctions grown directly by chemical vapor deposition have higher interface quality. Recently, Leong et al. have directly grown the lateral MoS₂/VS₂ heterostructure by CVD method. As shown in **Figure 5(d)**, the lateral heterostructure shows good contact characteristics. The Schottky barrier height of the lateral heterostructure is only 30 meV, while the Schottky barrier height of the MoS₂-Ni contact is as high as 163 meV, and the field effect mobility is increased by 6 times [87]. Such clean vdW interface can greatly suppress the interface dipole and metal-induced interstitial states. Further, by selectively forming nucleation points on semiconductor-TMDs, the growth of metallic-TMDs can be precisely controlled to form the van der Waals heterostructure arrays, as shown in **Figure 5(e)**. In particular, WSe₂ is used as the channel material, and the adjacent VSe₂ layers are used as the source and drain electrodes respectively, so that 2D semiconductor/metal heterojunctions serve as the contact. The output curve shows a satisfactory Ohmic contact, as shown in **Figure 4(f)**. The calculated mobility is as high as 137 cm²V⁻¹S⁻¹, which is one of the highest values of WSe₂ reported so far [88].

Conclusion and Outlook

In conclusion, realizing Ohmic contact is essential to achieve good device performance. Work function mismatch and Fermi level pinning are the main factors that hinder the formation of Ohmic contact. By comparing the barrier heights between different metals and 2D materials, we summarized the most suitable metals for different 2D materials including graphene, commonly used TMDs and BP. However, due to the existence of Fermi level pinning, the influence of the metal work function is weakened. We then mainly provided the mathematical representation of Fermi level pinning and presented two main methods namely intercalating an ultrathin insulating layer and transferring electrodes to reduce the influence of Fermi level pinning. Finally, we elaborated on 2D metal/semiconductor contacts including homojunction and heterojunction to reduce the contact resistance.

In addition, the use of the emerging two-dimensional materials such as silicene, germanene and borobenzene as electrodes to realize ohmic contact has also been reported recently. Yang et al. constructed Ge and MoSSe contacts on different surfaces by taking advantage of the lattice matching between Ge and MoSSe, and thus transformed the Schottky contact into ohmic contact via changing the tensile strain [89]. Also, Zhao et al.

systematically studied the interface properties of β_{12} phase borophene and commonly used two-dimensional materials, and found that it can form ohmic contacts with most group V-enes (such as BP) [90].

One important area for future research and development of nanofabrication techniques is the formation of edge contacts. Using plasma etching in combination with photoresist mask to expose the complete boundary of two-dimensional materials such as graphene, and then depositing electrodes to form edge contacts. Such edge contacts offer the advantages of strong orbital overlap and no current crowding [33,34]. However, due to the complexity of the process, it is currently challenging to achieve pure edge contact with standard lithography technology, because the photoresist will inevitably form a trapezoidal slope during the process of revealing and hiding, resulting in the formation of short and small top contact between electrodes and materials. Therefore, it is necessary to overcome this limitation and use more accurate methods to make edge ohmic contacts (for example, using h-BN packaging [91], etc.), which requires more exploration in the future.

Although great strides have been made on how to reduce the contact resistance of 2D devices, there are still some challenges that need to be overcome. First of all, the Fermi level pinning effect is widespread in the contact between metal and 2D semiconductor, but its root cause has not been clearly explained so far. For specific materials, the role of metal interstitial states and interface dipoles can be explained as energy level pinning. But there is still no specific theoretical explanation. Secondly, for traditional semiconductor materials, Ohmic contact is mainly and effectively achieved through high doping. However, the reliable and controllable doping of 2D materials is limited, which needs further investigation. Finally, 2D metal materials are an effective means to achieve Ohmic contact. However, compared with 2D semiconductor materials, the number of 2D metal materials is very limited. Therefore, new methods for the preparation of 2D metal materials need to be further explored.

Acknowledgements

This work is partially supported by the National Nature Science Foundation under Grants 62074070 and 11704159, the Natural Science Foundation of Jiangsu Province, China under Grant BK20170167, the Fundamental Research Funds for the Central Universities of China under Grants JUSRP221015, the 111 Project under Grant B12018, as well as by the Australian Research Council (ARC).

References

- [1] R. Schaller R 1997 Moore's law: past, present and future *IEEE spectrum* **34** 52-59
- [2] D.J. Frank, R.H. Dennerd, E. Nowak 2001 Device scaling limits of Si MOSFETs and their application dependencies *Proceedings of the IEEE* **89** 259-288
- [3] G.E. Moore 1965 Cramming more components onto integrated circuits *Proceedings of the IEEE* **86** 114-117
- [4] G. Yeric 2015 Moore's Law at 50: Are we planning for retirement? *IEEE International Electron Devices Meeting* **2015** 1.1.1-1.1.8
- [5] M. Chhowalla, D. Jena, H. Zhang 2016 Two-dimensional semiconductors for transistors *Nat Rev Mater* **1** 16052
- [6] Y. Gong, G. Shi, Z. Zhang, W. Zhou, J. Jung, W. Gao, L. Ma, Y. Yang, S. Yang, G. You, R. Vajtai, Q. Xu, A.H. MacDonald, B.I. Yakobson, J. Lou, Z. Liu, P.M. Ajayan 2014 Direct chemical conversion of graphene to boron- and nitrogen- and carbon-containing atomic layers *Nat Commun* **5** 3193
- [7] K.S. Novoselov, A.K. Geim, S.V. Morozov 2014 Electric Field Effect in Atomically Thin Carbon Films *science* **306** 666-669
- [8] A. Rai, H. Movva, A. Roy, D. Taneja, S. Chowdhury, S. Banerjee 2018 Progress in Contact, Doping and Mobility Engineering of MoS₂: An Atomically Thin 2D Semiconductor *Crystals* **8**
- [9] Y. Pan, J. Gu, H. Tang, X. Zhang, J. Li, B. Shi, J. Yang, H. Zhang, J. Yan, S. Liu, H. Hu, M. Wu, J. Lu 2019 Reexamination of the Schottky Barrier Heights in Monolayer MoS₂ Field-Effect Transistors *ACS Applied Nano Materials* **2** 4717-4726
- [10] N. Haiyan, J. Jie 2019 Soft hydrogen plasma induced phase transition in monolayer and fewlayer MoTe₂ *Nanotechnology* **30** 034004
- [11] H. Tang, B. Shi, Y. Pan, J. Li, X. Zhang, J. Yan, S. Liu, J. Yang, L. Xu, J. Yang, M. Wu, J. Lu 2019 Schottky Contact in Monolayer WS₂ Field-Effect Transistors *Advanced Theory and Simulations* **2**
- [12] X. Zhang, H. Nan, S. Xiao, X. Wan, X. Gu, A. Du, Z. Ni, K.K. Ostrikov 2019 Transition metal dichalcogenides bilayer single crystals by reverse-flow chemical vapor epitaxy *Nat Commun* **10** 598
- [13] H. Nan, X. Wang, J. Jiang, K. Ostrikov, Z. Ni, X. Gu, S. Xiao 2021 Effect of the surface oxide layer on the stability of black phosphorus *Applied Surface Science* **537**
- [14] R. Quhe, Y. Wang, M. Ye, Q. Zhang, J. Yang, P. Lu, M. Lei, J. Lu 2017 Black phosphorus transistors with van der Waals-type electrical contacts *Nanoscale* **9** 14047-14057
- [15] P. Ajayan, P. Kim, K. Banerjee 2016 Two-dimensional van der Waals materials *Physics Today* **69** 38-44

- [16] R. Xu, H. Jang, M.H. Lee, D. Amanov, Y. Cho, H. Kim, S. Park, H.J. Shin, D. Ham 2019 Vertical MoS₂ Double-Layer Memristor with Electrochemical Metallization as an Atomic-Scale Synapse with Switching Thresholds Approaching 100 mV *Nano Lett* **19** 2411-2417
- [17] Y. Zhu, Y. Li, G. Arefe, R.A. Burke, C. Tan, Y. Hao, X. Liu, X. Liu, W.J. Yoo, M. Dubey, Q. Lin, J.C. Hone 2018 Monolayer Molybdenum Disulfide Transistors with Single-Atom-Thick Gates *Nano Lett* **18** 3807-3813
- [18] J. Kang, W. Cao, X. Xie, D. Sarkar, W. Liu, K. Banerjee, Micro- and Nanotechnology Sensors, Systems, and Applications VI **2014**.
- [19] F. Schwierz, J. Pezoldt, R. Granzner 2015 Two-dimensional materials and their prospects in transistor electronics *Nanoscale* **7** 8261-8283
- [20] D. Akinwande, N. Petrone, J. Hone 2014 Two-dimensional flexible nanoelectronics *Nat Commun* **5** 5678
- [21] T. ROy, M. Tosun, J.S. Kang 2014 Field-Effect Transistors Built from All Two-Dimensional Material Components *ACS Nano* **8** 6259-6264
- [22] J.D. Mehew, S. Unal, E. Torres Alonso, G.F. Jones, S. Fadhil Ramadhan, M.F. Craciun, S. Russo 2017 Fast and Highly Sensitive Ionic-Polymer-Gated WS₂ -Graphene Photodetectors *Adv Mater* **29**
- [23] X. Liu, D. Qu, R. J 2016 P-type polar transition of chemically doped multilayer MoS₂ transistor *Advanced Materials* **28** 2345-2351
- [24] C.H. Liu, G. Clark, T. Fryett, S. Wu, J. Zheng, F. Hatami, X. Xu, A. Majumdar 2017 Nanocavity Integrated van der Waals Heterostructure Light-Emitting Tunneling Diode *Nano Lett* **17** 200-205
- [25] S.M. Sze, D.C. Mattis 1970 Physics of Semiconductor Devices *Physics Today* **23.6** 75-75
- [26] D.S. Schulman, A.J. Arnold, S. Das 2018 Contact engineering for 2D materials and devices *Chem Soc Rev* **47** 3037-3058
- [27] W. Luo, M. Zhu, G. Peng, X. Zheng, F. Miao, S. Bai, X.-A. Zhang, S. Qin 2018 Carrier Modulation of Ambipolar Few-Layer MoTe₂ Transistors by MgO Surface Charge Transfer Doping *Advanced Functional Materials* **28**
- [28] Y. Sheng, L. Zhang, F. Li, X. Chen, Z. Xie, H. Nan, Z. Xu, D.W. Zhang, J. Chen, Y. Pu, S. Xiao, W. Bao 2021 A novel contact engineering method for transistors based on two-dimensional materials *Journal of Materials Science & Technology* **69** 15-19
- [29] A. Avsar, K. Marinov, E.G. Marin, G. Iannaccone, K. Watanabe, T. Taniguchi, G. Fiori, A. Kis 2018 Reconfigurable Diodes Based on Vertical WSe₂ Transistors with van der Waals Bonded Contacts *Adv Mater* **30** e1707200
- [30] F. Giubileo, A. Di Bartolomeo 2017 The role of contact resistance in graphene field-effect devices *Progress in Surface Science* **92** 143-175
- [31] K.K. Ng, W.T. Lynch 1987 The Impact of Intrinsic Series Resistance on MOSFET Scaling *IEEE transactions on electron devices* **34** 503-511
- [32] T.H. Ning, Y. Taur 1998 Fundamentals of Modern VLSI Devices *Cambridge University Press*
- [33] Y. Chai, R. Ionescu, S. Su, R. Lake, M. Ozkan, C.S. Ozkan 2016 Making one-dimensional electrical contacts to molybdenum disulfide-based heterostructures through plasma etching *physica status solidi (a)* **213** 1358-1364
- [34] D.W. Yue, C.H. Ra, X.C. Liu, D.Y. Lee, W.J. Yoo 2015 Edge contacts of graphene formed by using a controlled plasma treatment *Nanoscale* **7** 825-831
- [35] M. Shaygan, M. Otto, A.A. Sagade 2017 Low resistive edge contacts to CVD-grown graphene using a CMOS compatible meta *Annalen der Physik* **529** 1600410
- [36] X. Cui, G.H. Lee, Y.D. Kim, G. Arefe, P.Y. Huang, C.H. Lee, D.A. Chenet, X. Zhang, L. Wang, F. Ye, F. Pizzocchero, B.S. Jessen, K. Watanabe, T. Taniguchi, D.A. Muller, T. Low, P. Kim, J. Hone 2015 Multi-terminal transport measurements of MoS₂ using a van der Waals heterostructure device platform *Nat Nanotechnol* **10** 534-540
- [37] R. Kappera, D. Voiry, S.E. Yalcin, B. Branch, G. Gupta, A.D. Mohite, M. Chhowalla 2014 Phase-engineered low-resistance contacts for ultrathin MoS₂ transistors *Nat Mater* **13** 1128-1134
- [38] J. Zhu, Z. Wang, H. Yu, N. Li, J. Zhang, J. Meng, M. Liao, J. Zhao, X. Lu, L. Du, R. Yang, D. Shi, Y. Jiang, G. Zhang 2017 Argon Plasma Induced Phase Transition in Monolayer MoS₂ *J Am Chem Soc* **139** 10216-10219
- [39] H. Nan, R. Zhou, X. Gu, S. Xiao, K. Ken Ostrikov 2019 Recent advances in plasma modification of 2D transition metal dichalcogenides *Nanoscale* **11** 19202-19213
- [40] Y. Liu, J. Guo, E. Zhu, L. Liao, S.J. Lee, M. Ding, I. Shakir, V. Gambin, Y. Huang, X. Duan 2018 Approaching the Schottky-Mott limit in van der Waals metal-semiconductor junctions *Nature* **557** 696-700
- [41] Y. Zheng, J. Gao, C. Han, W. Chen 2021 Ohmic Contact Engineering for Two-Dimensional Materials *Cell Reports Physical Science* **2**
- [42] N.F. Mott 1939 The theory of crystal rectifiers *Proceedings of the Royal Society of London. Series A. Mathematical and Physical Sciences* **171** 27-38
- [43] R.T. Tung 2014 The physics and chemistry of the Schottky barrier height *Applied Physics Reviews* **1**
- [44] O. Balci, C. Kocabas 2012 Rapid thermal annealing of graphene-metal contact *Applied Physics Letters* **101**
- [45] A. Gahoi, S. Wagner, A. Bablich, S. Kataria, V. Passi, M.C. Lemme 2016 Contact resistance study of various metal electrodes with CVD graphene *Solid-State Electronics* **125** 234-239
- [46] H.Y. Park, W.S. Jung, D.H. Kang, J. Jeon, G. Yoo, Y. Park, J. Lee, Y.H. Jang, J. Lee, S. Park, H.Y. Yu, B. Shin, S. Lee, J.H. Park 2016 Extremely Low Contact Resistance on Graphene through n-Type Doping and Edge Contact Design *Adv Mater* **28** 864-870

- [47] M. Abraham, S.E. Mohny 2017 Annealed Ag contacts to MoS₂ field-effect transistors *Journal of Applied Physics* **122**
- [48] C. Maurel, F. Ajustron, R. Péchou, G. Seine, R. Coratger 2006 Electrical behavior of the Au/MoS₂ interface studied by light emission induced by scanning tunneling microscopy *Surface Science* **600** 442-447
- [49] J. Kang, W. Liu, D. Sarkar 2014 Computational Study of Metal Contacts to Monolayer Transition-Metal Dichalcogenide Semiconductors *Physical Review X* **4** 031005
- [50] J. Kang, W. Liu, K. Banerjee 2014 High-performance MoS₂ transistors with low-resistance molybdenum contacts *Applied Physics Letters* **104**
- [51] Y. Wang, J.C. Kim, R.J. Wu, J. Martinez, X. Song, J. Yang, F. Zhao, A. Mkhoyan, H.Y. Jeong, M. Chhowalla 2019 Van der Waals contacts between three-dimensional metals and two-dimensional semiconductors *Nature* **568** 70-74
- [52] C.H. Wang, J.A.C. Incorvia, C.J. McClellan, A.C. Yu, M.J. Mleczko, E. Pop, H.P. Wong 2018 Unipolar n-Type Black Phosphorus Transistors with Low Work Function Contacts *Nano Lett* **18** 2822-2827
- [53] Z.P. Ling, S. Sakar, S. Mathew, J.T. Zhu, K. Gopinadhan, T. Venkatesan, K.W. Ang 2015 Black Phosphorus Transistors with Near Band Edge Contact Schottky Barrier *Sci Rep* **5** 18000
- [54] M.V. Kamalakar, B.N. Madhushankar, A. Dankert, S.P. Dash 2015 Low Schottky barrier black phosphorus field-effect devices with ferromagnetic tunnel contacts *Small* **11** 2209-2216
- [55] H.-M. Chang, K.-L. Fan, A. Charnas, P.D. Ye, Y.-M. Lin, C.-I. Wu, C.-H. Wu 2018 Experimental analysis of the Schottky barrier height of metal contacts in black phosphorus field-effect transistors *Journal of Physics D: Applied Physics* **51**
- [56] Y. Ma, C. Shen, A. Zhang, L. Chen, Y. Liu, J. Chen, Q. Liu, Z. Li, M.R. Amer, T. Nilges, A.N. Abbas, C. Zhou 2017 Black Phosphorus Field-Effect Transistors with Work Function Tunable Contacts *ACS Nano* **11** 7126-7133
- [57] D.J. Perello, S.H. Chae, S. Song, Y.H. Lee 2015 High-performance n-type black phosphorus transistors with type control via thickness and contact-metal engineering *Nat Commun* **6** 7809
- [58] Y. Deng, N.J. Conrad, Z. Luo 2014 Towards High-Performance Two-Dimensional Black Phosphorus Optoelectronic Devices: the Role of Metal Contacts *IEEE International Electron Devices Meeting* **2014** 5.2.1-5.2.4
- [59] K. Soththewes, R. van Bremen, E. Dollekamp, T. Boulogne, K. Nowakowski, D. Kas, H.J.W. Zandvliet, P. Bampoulis 2019 Universal Fermi-Level Pinning in Transition-Metal Dichalcogenides *J Phys Chem C Nanomater Interfaces* **123** 5411-5420
- [60] C. Gong, L. Colombo, R.M. Wallace, K. Cho 2014 The unusual mechanism of partial Fermi level pinning at metal-MoS₂ interfaces *Nano Lett* **14** 1714-1720
- [61] Y. Guo, D. Liu, J. Robertson 2015 Chalcogen vacancies in monolayer transition metal dichalcogenides and Fermi level pinning at contacts *Applied Physics Letters* **106**
- [62] D. Liu, Y. Guo, L. Fang, J. Robertson 2013 Sulfur vacancies in monolayer MoS₂ and its electrical contacts *Applied Physics Letters* **103**
- [63] C. Kim, I. Moon, D. Lee, M.S. Choi, F. Ahmed, S. Nam, Y. Cho, H.J. Shin, S. Park, W.J. Yoo 2017 Fermi Level Pinning at Electrical Metal Contacts of Monolayer Molybdenum Dichalcogenides *ACS Nano* **11** 1588-1596
- [64] Y. Liu, P. Stradins, S.H. Wei 2016 Van der Waals metal-semiconductor junction: Weak Fermi level pinning enables effective tuning of Schottky barrier *Science advances* **2** e1600069
- [65] Y. Guo, D. Liu, J. Robertson 2015 3D Behavior of Schottky Barriers of 2D Transition-Metal Dichalcogenides *ACS Appl Mater Interfaces* **7** 25709-25715
- [66] J.R. Chen, P.M. Odenthal, A.G. Swartz, G.C. Floyd, H. Wen, K.Y. Luo, R.K. Kawakami 2013 Control of Schottky barriers in single layer MoS₂ transistors with ferromagnetic contacts *Nano Lett* **13** 3106-3110
- [67] A. Dankert, L. Langouche, M.V. Kamalakar 2014 High-Performance Molybdenum Disulfide Field-Effect Transistors with Spin Tunnel Contacts *ACS Nano* **8** 476-482
- [68] G.S. Kim, S.H. Kim, J. Park, K.H. Han, J. Kim, H.Y. Yu 2018 Schottky Barrier Height Engineering for Electrical Contacts of Multilayered MoS₂ Transistors with Reduction of Metal-Induced Gap States *ACS Nano* **12** 6292-6300
- [69] S. Lee, A. Tang, S. Aloni, H.S. Wong 2016 Statistical Study on the Schottky Barrier Reduction of Tunneling Contacts to CVD Synthesized MoS₂ *Nano Lett* **16** 276-281
- [70] J. Wang, Q. Yao, C.W. Huang, X. Zou, L. Liao, S. Chen, Z. Fan, K. Zhang, W. Wu, X. Xiao, C. Jiang, W.W. Wu 2016 High Mobility MoS₂ Transistor with Low Schottky Barrier Contact by Using Atomic Thick h-BN as a Tunneling Layer *Adv Mater* **28** 8302-8308
- [71] X. Cui, E.M. Shih, L.A. Jauregui, S.H. Chae, Y.D. Kim, B. Li, D. Seo, K. Pistunova, J. Yin, J.H. Park, H.J. Choi, Y.H. Lee, K. Watanabe, T. Taniguchi, P. Kim, C.R. Dean, J.C. Hone 2017 Low-Temperature Ohmic Contact to Monolayer MoS₂ by van der Waals Bonded Co/h-BN Electrodes *Nano Lett* **17** 4781-4786
- [72] K.-A. Min, J. Park, R.M. Wallace, K. Cho, S. Hong 2016 Reduction of Fermi level pinning at Au-MoS₂ interfaces by atomic passivation on Au surface *2D Materials* **4**
- [73] C.D. English, G. Shine, D.V. E 2016 Improved Contacts to MoS₂ Transistors by Ultra-High Vacuum Metal Deposition *Nano letters* **16** 3824-3830
- [74] A. Matković, A. Petritz, G. Schider, M. Krammer, M. Kratzer, E. Karner-Petritz, A. Fian, H. Gold, M. Gärtner, A. Terfort, C. Teichert, E. Zojer, K. Zojer, B. Stadlober 2020 Interfacial Band Engineering of MoS₂/Gold Interfaces Using Pyrimidine-Containing Self-Assembled Monolayers: Toward Contact-Resistance-Free Bottom-Contacts *Advanced Electronic Materials* **6**

- [75] S. Liu, J. Li, B. Shi, X. Zhang, Y. Pan, M. Ye, R. Quhe, Y. Wang, H. Zhang, J. Yan, L. Xu, Y. Guo, F. Pan, J. Lu 2018 Gate-tunable interfacial properties of in-plane ML MX₂ 1T'-2H heterojunctions *Journal of Materials Chemistry C* **6** 5651-5661
- [76] Z.Q. Fan, X.W. Jiang, J. Chen, J.W. Luo 2018 Improving Performances of In-Plane Transition-Metal Dichalcogenide Schottky Barrier Field-Effect Transistors *ACS Appl Mater Interfaces* **10** 19271-19277
- [77] D.H. Keum, S. Cho, J.H. Kim, D.-H. Choe, H.-J. Sung, M. Kan, H. Kang, J.-Y. Hwang, S.W. Kim, H. Yang, K.J. Chang, Y.H. Lee 2015 Bandgap opening in few-layered monoclinic MoTe₂ *Nature Physics* **11** 482-486
- [78] J.H. Sung, H. Heo, S. Si, Y.H. Kim, H.R. Noh, K. Song, J. Kim, C.S. Lee, S.Y. Seo, D.H. Kim, H.K. Kim, H.W. Yeom, T.H. Kim, S.Y. Choi, J.S. Kim, M.H. Jo 2017 Coplanar semiconductor-metal circuitry defined on few-layer MoTe₂ via polymorphic heteroepitaxy *Nat Nanotechnol* **12** 1064-1070
- [79] Y. Ma, B. Liu, A. Zhang 2015 Reversible Semiconducting-to-Metallic Phase Transition in Chemical Vapor Deposition Grown Monolayer WSe₂ and Applications for Devices *ACS Nano* **9** 7383-7391
- [80] C.S. Lee, S.J. Oh, H. Heo, S.Y. Seo, J. Kim, Y.H. Kim, D. Kim, O.F. Ngome Okello, H. Shin, J.H. Sung, S.Y. Choi, J.S. Kim, J.K. Kim, M.H. Jo 2019 Epitaxial van der Waals Contacts between Transition-Metal Dichalcogenide Monolayer Polymorphs *Nano Lett* **19** 1814-1820
- [81] S. Cho, S. Kim, J.H. Kim 2015 Phase patterning for ohmic homojunction contact in MoTe₂ *Science* **349** 625-628
- [82] L. Zhang, H. Nan, X. Zhang, Q. Liang, A. Du, Z. Ni, X. Gu, K.K. Ostrikov, S. Xiao 2020 2D atomic crystal molecular superlattices by soft plasma intercalation *Nat Commun* **11** 5960
- [83] T. Das, E. Yang, J.E. Seo, J.H. Kim, E. Park, M. Kim, D. Seo, J.Y. Kwak, J. Chang 2021 Doping-Free All PtSe₂ Transistor via Thickness-Modulated Phase Transition *ACS Appl Mater Interfaces* **13** 1861-1871
- [84] S.S. Chee, D. Seo, H. Kim, H. Jang, S. Lee, S.P. Moon, K.H. Lee, S.W. Kim, H. Choi, M.H. Ham 2019 Lowering the Schottky Barrier Height by Graphene/Ag Electrodes for High-Mobility MoS₂ Field-Effect Transistors *Adv Mater* **31** e1804422
- [85] Y. Sata, R. Moriya, S. Masubuchi 2017 N- and p-type carrier injections into WSe₂ with van der Waals contacts of two-dimensional materials *Japanese Journal of Applied Physics* **56** 04CK09
- [86] Q. Ji, C. Li, J. Wang 2017 Metallic vanadium disulfide nanosheets as a platform material for multifunctional electrode applications *Nano letters* **17** 4908-4916
- [87] W.S. Leong, Q. Ji, N. Mao, Y. Han, H. Wang, A.J. Goodman, A. Vignon, C. Su, Y. Guo, P.C. Shen, Z. Gao, D.A. Muller, W.A. Tisdale, J. Kong 2018 Synthetic Lateral Metal-Semiconductor Heterostructures of Transition Metal Disulfides *J Am Chem Soc* **140** 12354-12358
- [88] J. Li, X. Yang, Y. Liu, B. Huang, R. Wu, Z. Zhang, B. Zhao, H. Ma, W. Dang, Z. Wei, K. Wang, Z. Lin, X. Yan, M. Sun, B. Li, X. Pan, J. Luo, G. Zhang, Y. Liu, Y. Huang, X. Duan, X. Duan 2020 General synthesis of two-dimensional van der Waals heterostructure arrays *Nature* **579** 368-374
- [89] N. Zhao, U. Schwingenschlogl 2020 Transition from Schottky to Ohmic contacts in Janus MoSSe/germanene heterostructures *Nanoscale* **12** 11448-11454
- [90] J. Yang, R. Quhe, S. Feng, Q. Zhang, M. Lei, J. Lu 2017 Interfacial properties of borophene contacts with two-dimensional semiconductors *Phys Chem Chem Phys* **19** 23982-23989
- [91] B. Karpiak, A. Dankert, A.W. Cummings, S.R. Power, S. Roche, S.P. Dash 2017 1D ferromagnetic edge contacts to 2D graphene/h-BN heterostructures *2D Materials* **5**

Figure 1: TMDCs and BP are in contact with metals with different work functions. (a) The energy band of MoS_2 and the work function arrangement of commonly used metals (left side), and the n-type Schottky barrier height where different metals contact with MoS_2 (right side). The red part is the electronic Schottky barrier height obtained through theoretical calculation [9], and the blue part is the Schottky barrier height extracted in the actual experiment [11, 47, 48]. (b) Band structure of Mo-MoS_2 and Ti-MoS_2 [50]; (c) Van der Waals contact between In and MoS_2 [51]; (d) Barrier heights of five different metals in contact with WSe_2 [49]; (e) The Schottky barrier heights of five commonly used metals in contact with BP (N-SBH, p-SBH)[52].

Figure 2: Oxide intercalation weakens the Fermi level pinning effect. (a) MoS₂ output curve before and after oxide intercalation under zero gate voltage. (b) The height of the Schottky barrier extracted from Figure 2(a) [67]. (c) Schematic diagram of the structure of MS S/D contact and MISS/D contact. (d) The height of the Schottky barrier extracted before and after TiO₂ intercalation, and the fitted pinning coefficient S [68]. (e) Schematic diagram of the Fermi level of MoS₂ pinning, and two explanations for reducing the Fermi pinning effect [69]. (f) Inserting h-BN to form the MIS structure reducing the barrier height from 158 meV to 31 meV (the illustration is the device structure diagram) [70].

Figure 3: (a)-(b) Cross-sectional schematics and TEM images of the transferred Au electrode on top of MoS₂ and conventional electron-beam-deposited Au electrode on top of MoS₂. The transferred metal-semiconductor surface is very clean and atomically sharp, while electron beam evaporation creates considerable damage to the MoS₂ surface, producing a glassy layer with apparent defects, interface diffusion, chemical bonding and atomic disorder. (c) Transfer characteristic curves of MoS₂ transistors with deposited and transferred metal electrodes. (d) Experimentally determined Schottky barrier height for different transferred metals and evaporated metals [40].

Figure 4: 2D metal and 2D semiconductor homojunction. (a) In-plane atomic connection diagrams for 1T-MX₂ and 2H-MX₂ as well as 1T'-MX₂ and 2H-MX₂ homojunctions[76]. (b) Schematic and SEM image of the growth of lateral homojunction consisting of 2H MoTe₂ and 1T MoTe₂ by chemical vapor deposition via adjusting growth temperature[78]. (c) The extracted Schottky barrier heights for the novel contact consisting of 2H/1T' homojunction and metal electrode as well as the traditional contact consisting of 2H MoTe₂ and metal electrode [78]. (d) MoS₂ is transformed from 2H phase to 1T phase through phase engineering, and the contact resistance of the corresponding transistor is calculated under zero gate bias[37]. (e) A false-color top-view SEM image of the representative few layer PtSe₂ FETs and the corresponding extracted Schottky barrier height[83].

Figure 5: 2D metal and 2D semiconductor heterojunction. (a) Schematic diagram of graphene being transferred to MoS₂ as an electrode. (b) Output characteristics of MoS₂ FETs with Ag and graphene/Ag contacts under different gate bias voltage[84]. (c) Schematics showing monolayer MoS₂ field-effect transistors (FETs) with the lateral VS₂ contacts (upper) and vertical Ni contacts (lower). (d) Schottky barrier heights (Φ_B) of VS₂- and Ni-contacted MoS₂ devices, as a function of V_G. Dashed arrows indicate flat-band Φ_B[87]. (e) Typical optical microscopy images of rectangular periodic arrangements of VSe₂/WSe₂ vdWH arrays. (f) Comparison of output curves of van der Waals contacts and WSe₂ transistors with direct deposition metal contacts [88].