Titanium disulfide as Schottky/ohmic contact for monolayer molybdenum disulfide

Junsen Gao and Manisha Gupta

2D semiconductors like Molybdenum disulfide (MoS₂) still have issues in forming good metal electrode (Schottky and Ohmic) especially for mono layer (ML) to few layers thick due to strain and metallization issues. Here, we explore a 2D semi-metal, titanium disulfide (TiS₂), for making different types of contacts with ML MoS₂ using density functional theory (DFT). It is observed that ML TiS₂ induces ML MoS₂ to become p-type with a doping density of 3.85 × 10¹⁷ cm⁻³ which becomes larger with thicker TiS₂. Thus, TiS₂ can thus be utilized as a variable contact material ohmic if the MoS₂ is p-type and as Schottky if the MoS₂ is n-type with a Schottky barrier height ranging from 0.3 to 1.35 eV. One of the important results from the study is that compared to a traditional metal–MoS₂ in a TiS₂–MoS₂ contact the bandgap is preserved where in contrast, a traditional metal contact metalizes the monolayer MoS₂ and fill its bandgap with states. Hence, a clear path forward to make pristine contacts is to use 2D semi-metals in conjunction with 2D semiconductors.

INTRODUCTION

In recent years, molybdenum disulfide (MoS₂), one of the transition metal dichalcogenide monolayers (TMDC), has attracted significant attention and has been explored for a variety of applications in a vast range of fields. Inter-layer van der Waals bonding of MoS₂ allows one to obtain monolayer (ML) thickness. Due to its 2D nature, the ML MoS₂ shows planar structure without the presence of the dangling bonds. This gives ML MoS₂ perfect surface smoothness and helps reduce the surface trap states. Compared to other 2D materials, MoS₂ has a non-zero layer-dependent bandgap, which is 1.2 eV indirect bandgap for bulk MoS₂ and 1.8 eV direct bandgap for ML MoS₂. This unique property enables ML or multilayer MoS₂ to act as a semiconductor and thus broadens the application of MoS₂ in the field of electronics and photonics. MoS₂ also has other merits like good flexibility, adequate mobility, and availability of large-scale thin films (synthesis). For these reasons, MoS₂ is fast becoming a promising candidate for the 2D semiconducting channel of the next-generation field effect transistors (FET). Although many MoS₂ FET have been reported, obtaining a good contact for MoS₂ FET is still an important issue. To find both good ohmic and Schottky contacts, extensive research has been conducted to investigate metal–(ML) MoS₂ contacts via both computational and experimental work. However, it is observed that the covalent bonds forming between the metal and MoS₂ introduce defects and metallization effect the MoS₂ structure, which can be seen in Fig. 1a. After creating a contact, the defects generated lower charge mobility. To overcome this issue, some groups have utilized encapsulation technique, the MoS₂ mobility can be preserved by using hexagonal boron nitride (h-BN) nano sheets to enclose the MoS₂ sheet. This encapsulation technique though increases the fabrication complexity of the devices which add difficulty for large-scale manufacturing.

To overcome the existing issues of the metal–MoS₂ contact, the concept of van der Waals contact based on 2D metals and semimetals has been studied earlier. In recent years, many MoS₂ devices integrated with 2D contacts have been fabricated.

Compared with traditional metal contacts, these contacts show higher mobility, smaller structural changes in MoS₂ and smaller metallization is added to MoS₂ along with higher flexibility. The h-BN encapsulation can also be used for these contacts with its deposition by chemical vapor deposition (CVD) or exfoliation to further increase the device mobility. Thus, utilizing 2D metals as a electrode material improves the scalability of the devices. It has been shown that smoothness, absence of dangling bonds, and the ultra-thin layer of the 2D contact enables shorter channel devices in 2D MoS₂ FET. Obtaining good and reliable ohmic and Schottky contacts for MoS₂ will speed up the development of high-performance 2D heterostructure devices.

It is thus essential to explore and understand 2D materials suitable for electrode formation with MoS₂. There are quite a few 2D metallic materials and we consider titanium disulfide (TiS₂) for the electrode here. TiS₂ is also a member of TMDC family, but there is a small overlap between the conduction band and valence band of TiS₂. Some references have claimed that TiS₂ has a narrow bandgap of 0.2 eV exhibiting semi-metallic properties. As a semi-metallic material, TiS₂ has already been employed as electrode material of lithium ion batteries and solar cells due to its high electric conductivity. However, compared with graphene, to the best of our knowledge no detailed study has been conducted. Hence, we have conducted a systematic computational study on the 2D TiS₂–MoS₂ (ML) contacts by using first-principles simulation. We found that the intrinsic structure of ML MoS₂ is well preserved after forming a contact with TiS₂. As shown in Fig. 1b, the TiS₂ contact induces ML MoS₂ to demonstrate p-type behavior, while graphene contact induces it to become n-doped. Another interesting finding from our study is that the Schottky barrier height for the TiS₂ contact and ML MoS₂ changes by varying the doping type and concentration of MoS₂. By using the projected local device density of states (PLDOS) analysis, we have extracted the barrier heights of TiS₂–MoS₂ (ML) contacts at different doping type and concentrations along with different TiS₂ thickness. We found that for intrinsic and n-type-doped ML MoS₂, TiS₂ forms a Schottky contact.
whereas for p-type ML MoS2, TiS2 forms an ohmic contact. Thus, we can use TiS2 to obtain high-quality ohmic and Schottky contacts for ML MoS2 for fabrication of high-quality devices.

RESULTS

TiS2 contact formation with ML MoS2

The “Methods” section describes the density functional theory (DFT) techniques used for this research. The contact formation between TiS2–MoS2 leads to two interfaces as seen in Fig. 2d. To confirm this, two geometries are adopted to investigate the contact, which are shown in Fig. 2a, b. A group of TiS2–MoS2 junctions are used to test the electron transport from TiS2 contact to the ML MoS2 sheet at the lateral interface (interface A in Fig. 2d). Another group of FET-like TiS2–MoS2 heterostructures (TiS2–MoS2 FET-like junctions) are used to simulate the electron transportation from the contact region to semiconducting channel region at the vertical interface (interface B in Fig. 2d).

For TiS2–MoS2 FET-like junction, the PLDOS is calculated for revealing the band structure after the contacting of 1–4 layers of TiS2 and ML MoS2 sheet. The configuration after geometrical optimization (GO) is shown by Fig. 2d. The overlap of 1–4 layers of TiS2 and ML MoS2 is 2.5 nm. Due to the limitation of computational capability, the ML-MoS2 channel is set as 8 nm. To increase the accuracy in the transportation direction, the k-point sampling is changed to 10 × 1 × 40. For each of 1–4 layers of TiS2 simulations, the MoS2 channel doping is varied to understand the type of electrode formation as 5 × 10^18 cm^-3 (3.25 × 10^11 cm^-2 for ML MoS2) n-type doping, 1 × 10^19 cm^-3 (6.5 × 10^11 cm^-2 for ML MoS2) n-type doping, 5 × 10^19 cm^-3 (3.25 × 10^12 cm^-2 for ML MoS2) n-type doping, and 5 × 10^19 cm^-3 (3.25 × 10^11 cm^-2 for ML MoS2) p-type doping. Thus, we obtain a ni value of 1.4 × 10^19 cm^-3 for ML MoS2. We chose the doping concentration carefully to meet the calculated upper and lower limits: a large doping concentration will lead to degenerate behavior of the channel and a small doping concentration will cause the depletion length to exceed the length of channel creating artificial results. The overlap region between the TiS2 and MoS2 is undoped. Only the uncovered ML-MoS2 channel is doped with the chosen doping concentrations.

To investigate the charge transport and its mechanism through the interface A in Fig. 2d, the calculation of DOS, ED, average binding energy (EBE), and EDP are conducted after the GO.

After simulating the DOS of the optimized TiS2–MoS2 structure, the projected partial DOS (PDOS) is shown in Fig. 3. The PDOS of TiS2 after making contact with ML MoS2 is shown in Fig. 3a–d for one–four layers of TiS2. It shows that, after making a contact with ML MoS2, the TiS2 DOS remains the same as the free-standing TiS2. The only difference is that some trap states are added which show as spikes in Fig. 3a–d. These added states are created by the tiny displacement of the atoms in TiS2 layer, which is of the order of 0.01 Å. This indicates that the presence of ML MoS2 has a negligible effect on the TiS2 band structure. The situation of MoS2 is different, as shown in Fig. 3e–i which show the PDOS of ML MoS2 after making contact with one–four layers of TiS2. The plot clearly demonstrates that the TiS2 contact modifies the MoS2 band structure significantly and adds a large amount of p-type doping to the ML MoS2. In Fig. 3e–i, compared with the band structure and DOS of intrinsic ML MoS2 on the left side, for all the cases of ML to four-layer TiS2 contacts, the PDOS of ML MoS2 exhibits Fermi level pinning towards valence band. This shift of Fermi level ranges from 0.40 to 0.45 eV. Even though the three-layer and four-layer TiS2 forming a contact with ML MoS2 show a larger Fermi level shift, the difference in Fermi level shift with change in the number of TiS2 layers is very small. The energy difference between the valence band and Fermi level is 0.05–0.1 eV. The energy difference between the Fermi level and valence band is defined by

\[ \Phi = E_f - E_v, \]

where \( E_f \) and \( E_v \) are the Fermi level and the valence band top, respectively. Knowing the Fermi level shift \( \Phi \), the p-type doping concentration can be determined by calculating the effective DOS in the conduction band \( (N_c) \) and the valence band \( (N_v) \). As there are not too many reported values of \( N_c \) and \( N_v \), we have calculated these to estimate what doping concentration we should use for our electrode simulations for ML MoS2. Hence, the effective density of state values is required only for estimating the doping concentrations of MoS2. After simulating the DOS, the energy difference between the quasi-Fermi level and the valence band can be calculated. These two well-defined equations can be applied to determine \( N_c \) and \( N_v \):

\[ N_c = n \exp \left( \frac{E_c - E_f}{kT} \right), \]

\[ N_v = p \exp \left( \frac{E_v - E_f}{kT} \right), \]

where \( n \) and \( p \) are the electron and hole concentrations, respectively. \( k \) is Boltzmann constant and \( T \) is temperature in K. From the simulation, \( N_c \) and \( N_v \) for ML MoS2 are calculated to be 2 × 10^19 cm^-3 (1.38 × 10^12 cm^-2) and 1 × 10^19 cm^-3 (6.5 × 10^12 cm^-2), respectively.
which are similar to the reported ML and bulk MoS2 values\textsuperscript{36-39}. Using these values, the calculated doping concentration added to the ML MoS2 by TiS2 contacts with different number of layers ranges from 3.85 × 10\textsuperscript{17} to 2.63 × 10\textsuperscript{18} cm\textsuperscript{-3} (2.50 × 10\textsuperscript{10} to 1.71 × 10\textsuperscript{11} cm\textsuperscript{-2}) for ML MoS2. Compared with metal–MoS2 contacts\textsuperscript{14-18}, although the ML MoS2 is p-type doped after forming a contact with TiS2, its bandgap is preserved as shown in Fig. 3e–i; in contrast, the metal contact will metalize the ML MoS2 and fill its bandgap with states as shown in Fig. 1a. The TiS2–MoS2(ML) contact makes ML MoS2 p-type as compared to the n-type in graphene–MoS2 contact (Fig. 1b).

Thus, the DOS simulation indicates that TiS2–MoS2 (ML) contact is a unique contact with less metallization and p-type behavior. It is necessary to conduct a comprehensive analysis on its interfacial bonding condition. ED and EBE are two important criteria to evaluate the bonding between TiS2 and ML MoS2. The average binding energy (EBE), \( E_{B} \), can be defined as

\[
E_{B} = \langle E_{T} + E_{M} - E_{T-M} \rangle / N,
\]

where \( E_{T} \) is the total energy of the free-standing TiS2, \( E_{M} \) is the total energy of the intrinsic ML MoS2, \( E_{T-M} \) is the total energy of the TiS2–MoS2 (ML) contact after GO, and \( N \) can be considered as the number of interfacial sulfur atoms on the MoS2 side.

The ED of the TiS2–MoS2 junctions are shown by Fig. 4a–d for one–four layers of TiS2. As seen in the plot, there is a clear gap between the TiS2 layer and MoS2 with no charge distribution in it. The overlap of the electron gas between TiS2 and MoS2 is very limited, as can be observed from the contour plot. The plot of the projected electron density (ED) in the y direction also clearly shows that the ED overlap at the contact interface is very similar to those between TiS2 layers, indicating that the bonding between TiS2 and MoS2 is not much stronger than interfacial bonding within TiS2 layers. The buckling distance can also be extracted from both the ED plot and GO. For TiS2–MoS2(ML) junctions, the optimized buckling distance for TiS2–MoS2 contacts are: 3.2282 Å for TiS2(ML)–MoS2(ML), 2.8112 Å for TiS2(2L)–MoS2(ML), 2.8069 Å for TiS2(3L)–MoS2 (ML), and 2.7381 Å for TiS2(4L)–MoS2(ML). For comparison, the inter-layer distance for TiS2 and MoS2 is 2.8678 and 2.9754 Å, respectively. It is clear that thicker TiS2 has larger attractive force to ML MoS2 and leads to smaller inter-layer distance. These ED results reveal that the bonding between the TiS2 contact and ML MoS2 in TiS2–MoS2 (ML) junctions is Van der Waals bonding. Unlike the covalent bond, the delocalization of interfacial electron gas would not exist in these cases.

By using this definition, the EBE for TiS2–MoS2(ML) interface is 0.7426 eV, while this value is 0.7157 eV for the Van der Waals bonds of bilayer MoS2. This result further confirms the previous results and demonstrates that TiS2–MoS2 (ML) contact is a Van der Waals contact.

The tunneling barrier at the TiS2–MoS2 (ML) interface will determine the charge transport through the interface A. To evaluate the impedance to the current transportation added by the tunneling barrier, the electrostatic difference potential (EDP) of the TiS2–MoS2 contact is simulated. As shown in Fig. 4e, the potential between the TiS2 and MoS2 is considered as the tunneling barrier. The shape of the potential barrier can be estimated as a rectangle. The tunneling probability, from the TiS2 to the ML MoS2, can be defined as, of carriers tunneling through the barrier, \( T_{B} \)

\[
T_{B} = \exp \left( -4\pi \frac{\sqrt{2m\Delta V}}{h} W_{b} \right),
\]

where \( \Delta V \) is the barrier height, which is defined by the length of the rectangle, \( h \) is the Planck constant, and \( W_{b} \) is the barrier width, which is defined as the half width of the rectangle. \( \Delta V \) and \( W_{b} \) can be directly extracted from Fig. 4e: \( \Delta V \) is 0.404620 eV and \( W_{b} \) is 0.35412 Å. By using these parameters and Eq. (4), we calculate \( T_{B} \) as 79.4%. A large \( T_{B} \) indicates small impedance and a higher charge injection. It is very clear that even though the tunneling barrier at the interface A resists the charge transport vertically through the interface, the possibility of tunneling is high for carriers because of a
Fig. 3  **The partial density of states (PDOS) of TiS$_2$ and MoS$_2$ within TiS$_2$(ML to 4L)–MoS$_2$(ML) contacts.**  

a–d PDOS of TiS$_2$ (from ML to 4L). In the plot, the dashed line indicates the position of Fermi level, which is set as zero point. The red line represents the DOS of free-standing TiS$_2$, as a comparison. 

e–i PDOS of ML MoS$_2$. On the top is the DOS of free-standing ML MoS$_2$, as a comparison. The Fermi level of each plot has been aligned to the same energy value. The label ML-TiS$_2$ to 4L-TiS$_2$ indicate the TiS$_2$ contact thickness.
very tiny barrier width (0.354 Å). For this reason, the charge injection at the lateral interface can be ignored. However, the interfacial tunneling barrier within the TiS$_2$ contact may scatter the electrons and holes. This scattering effect can be reduced by using a thinner TiS$_2$ film. Thus, we also address scaling down the thickness of TiS$_2$ contacts after meeting the stability requirement.

By analyzing the ED, EBE, and GO for configuration A, it can be concluded that TiS$_2$ tends to form Van der Waals bond with ML MoS$_2$, with thicker TiS$_2$ creating stronger bonding. The DOS in Fig. 3 shows that less metallization is created due to the weak Van der Waals bonding and the bandgap of ML MoS$_2$ is preserved. DOS results also show that TiS$_2$ will add p-type doping to the ML MoS$_2$. The EDP results in Fig. 4 show that the tunneling barrier is small at interface A, which means that the current injection would not be seriously impeded.

To understand the source-to-channel/channel-to-drain working mechanism for the TiS$_2$–MoS$_2$ (ML) contacts applied in 2D FET, the PLDOS is adopted to sketch out the framework of the band structure at the interface B of the TiS$_2$–MoS$_2$ FET-like junctions. The PLDOS uses a contour plot to map the DOS projected onto the geometry configuration is integrated in the plot, which is shown on the bottom. It shows that at the interface A, there is a small tunneling barrier. The scale bar is from 0.0 to 3.0 Å$^{-3}$.
the c-axis, which is the transportation direction. The band structure can be determined by plotting the boundary between the states-filled region (bright region) and the no-states region (dark region). The extraction of the barrier height and contact type of TiS$_2$-MoS$_2$ contact can be achieved by evaluating the PLDOS. Two reasons let us dope the ML MoS$_2$. First, the intrinsic carrier concentration of ML MoS$_2$ is small; therefore, it is a good choice to dope the MoS$_2$ channel to improve the conductivity. For this reason, it is of great interest to investigate the contact consisting of the intrinsic carrier concentration very close to degeneration, the Schottky barrier height is 0.30 eV for 5 × 10$^{18}$ cm$^{-3}$ and 0.40 eV for 1 × 10$^{19}$ cm$^{-3}$. In testing MoS$_2$ doping-dependent contact formation with TiS$_2$ doping concentration of 1 × 10$^{19}$ cm$^{-3}$, the Schottky barrier height of the contacts are large: 1.03 eV for 2L cases and 1.07 eV for 4L cases. The simulation results are shown in Table 1. Figure 5 shows that a larger doping concentration will reduce the barrier height, the modiﬁcation of doping concentration very close to degeneration, the Schottky barrier height is 0.7 eV for ML MoS$_2$ and TiS$_2$ cannot be extracted directly from the PLDOS, the barrier height and contact type of doped cases can still be extracted accurately.

MoS$_2$ doping-dependent contact formation with TiS$_2$

Four different doping concentrations: 5 × 10$^{18}$, 1 × 10$^{19}$, and 5 × 10$^{19}$ cm$^{-3}$ n-type doping and 5 × 10$^{18}$ cm$^{-3}$ p-type doping is tested. The simulation results are shown in Table 1. Figure 5 shows only the results of the TiS$_2$(4L)-MoS$_2$(ML) cases and the variation of the band structures with different doping concentrations.

For n-type doping concentrations smaller than $N_0$, the Schottky barrier height of the contacts are large: 1.03–1.07 eV for 5 × 10$^{18}$ cm$^{-3}$, and 0.88–0.95 eV for 1 × 10$^{19}$ cm$^{-3}$, as shown in Table 1 and Fig. 5b, c. Table 1 also clearly shows that for the cases with ML TiS$_2$, $\Phi_n$ of the contact is larger than $\Phi_p$ of 2L–4L cases with the same doping concentration. For the n-type doping concentration of 5 × 10$^{18}$ cm$^{-3}$, $\Phi_n$ is 0.67 eV for ML but 0.21–0.25 eV for 2L–4L. For n-type doping concentration of 1 × 10$^{19}$ cm$^{-3}$, $\Phi_n$ is 0.7 eV for ML but 0.40–0.44 eV for 2L–4L. By summing $\Phi_n$ and $\Phi_p$, the modified $E_g$ is 1.70 eV for the ML case doped n-type with concentration 5 × 10$^{18}$ cm$^{-3}$, and for 2L–4L cases doped with this concentration, $E_g$ ranges from 1.26 to 1.32 eV. For n-type doping of concentration 1 × 10$^{19}$ cm$^{-3}$, $E_g$ is 1.65 eV for ML and 1.32 eV for 2L–4L.

For a larger n-type doping concentration (5 × 10$^{19}$ cm$^{-3}$), as shown in both Table 1 and Fig. 5a, the Schottky barrier height is 0.30–0.45 eV, which is much smaller than the cases with n-type doping concentrations of 5 × 10$^{18}$ and 1 × 10$^{19}$ cm$^{-3}$. This reduction in barrier height may be brought about by multiple causes. One possible reason is the imaging force created by the larger amount of excess charge, as a result of the larger doping concentration. It is observed that $\Phi_p$ increases with lower doping concentrations. $\Phi_p$ is 0.92–0.97 eV for the 1–4L cases. $E_g$ for this concentration is 1.27–1.37 eV.

The simulation results and mapped band structures in Fig. 5a–c for n-type-doped TiS$_2$–MoS$_2$(ML) contacts show that, normally, n-type-doped TiS$_2$–MoS$_2$(ML) contacts show a large barrier height, which is around 1.0 eV below a degenerate doping. Even though Fig. 5 shows that a larger doping concentration will reduce the barrier height for n-type carriers, it is obvious that, even for a doping concentration very close to degeneration, the Schottky barrier height is still larger for TiS$_2$–MoS$_2$(ML) contacts. The inference from Fig. 5 is that since the majority carriers in these n-type-doped contacts are always faced with a large Schottky barrier height, the n-type-doped TiS$_2$–ML MoS$_2$ Schottky diodes can probably act as high-power switches or Schottky barrier MOSFETs based on tunneling.

Unlike the n-type contacts, the p-type-doped TiS$_2$–MoS$_2$(ML) contacts show zero barrier height when the p-type doping concentration reaches 5 × 10$^{18}$ cm$^{-3}$. In Fig. 5d, it is observed that, at this doping concentration, the depletion width vanishes and the band is flat. The Schottky barrier at the interface shows both a small barrier height and a small built-in potential, which indicates the contact is an ohmic contact for ML MoS$_2$-doped p-type at a concentration of 5 × 10$^{19}$ cm$^{-3}$.

For the cases with p-type doping concentration of 5 × 10$^{18}$ cm$^{-3}$, only the ML and 2L cases show a very small barrier height $\Phi_p$ (0.13 eV for ML and 0.05 eV for 2L). For the 3L and 4L cases, there is zero barrier height, $\Phi_p$ is 1.35 eV for ML and 1.18 eV for 2–4L, as shown in Table 1. For the cases with p-type doping concentration of 5 × 10$^{19}$ cm$^{-3}$, the bandgap shrinks to 1.48 eV for ML TiS$_2$ and 1.18 eV for 2–4L.

As inferred from Fig. 5d, when the doping is p-type with a concentration of 5 × 10$^{19}$ cm$^{-3}$, the contact is ohmic for p-type carriers while the barrier for n-type carriers is still large. As mentioned earlier, the doping concentration $P_e$ was added to the ML MoS$_2$ within the contact region ranges from 3.85 × 10$^{17}$ to 2.63 × 10$^{18}$ cm$^{-3}$. When the p-type doping of channel MoS$_2$ reaches the value of $P_e$, the band will become flat, and the contact

| Number of TiS$_2$ layers/ML MoS$_2$ doping conc. and type | Depletion width $W_D$ (nm) | Vertical barrier height for electrons $\Phi_n$ (eV) | Vertical barrier height for holes $\Phi_p$ (eV) | Effective band gap after formation of junction $E_g$ (eV) |
|----------------------------------------------------------|-----------------------------|--------------------------------------------------|---------------------------------|------------------|
| 1L, 5 × 10$^{18}$ (p-type)                              | –                           | 1.35                                             | 0.13                            | 1.48             |
| 2L, 5 × 10$^{18}$ (p-type)                              | –                           | 1.18                                             | 0.05                            | 1.23             |
| 3L, 5 × 10$^{18}$ (p-type)                              | –                           | 1.18                                             | 0                                | 1.18             |
| 4L, 5 × 10$^{18}$ (p-type)                              | –                           | 1.18                                             | 0                                | 1.18             |
| 1L, 5 × 10$^{18}$ (n-type)                              | 6.4                         | 1.03                                             | 0.67                            | 1.70             |
| 2L, 5 × 10$^{18}$ (n-type)                              | 6.3                         | 1.05                                             | 0.21                            | 1.26             |
| 3L, 5 × 10$^{18}$ (n-type)                              | 5.8                         | 1.07                                             | 0.25                            | 1.32             |
| 4L, 5 × 10$^{18}$ (n-type)                              | 5.8                         | 1.03                                             | 0.23                            | 1.26             |
| 1L, 1 × 10$^{19}$ (n-type)                              | 3.6                         | 0.95                                             | 0.70                            | 1.65             |
| 2L, 1 × 10$^{19}$ (n-type)                              | 4.9                         | 0.92                                             | 0.40                            | 1.32             |
| 3L, 1 × 10$^{19}$ (n-type)                              | 4.6                         | 0.90                                             | 0.42                            | 1.32             |
| 4L, 1 × 10$^{19}$ (n-type)                              | 4.8                         | 0.88                                             | 0.44                            | 1.32             |
| 1L, 5 × 10$^{19}$ (n-type)                              | 1.6                         | 0.35                                             | 0.95                            | 1.30             |
| 2L, 5 × 10$^{19}$ (n-type)                              | 1.5                         | 0.45                                             | 0.92                            | 1.37             |
| 3L, 5 × 10$^{19}$ (n-type)                              | 1.2                         | 0.30                                             | 0.97                            | 1.27             |
| 4L, 5 × 10$^{19}$ (n-type)                              | 1.2                         | 0.30                                             | 0.97                            | 1.27             |
becomes an ohmic contact. Thus, TiS$_2$ can be used as an either an ohmic or Schottky contact depending on the doping of the ML MoS$_2$.

**DISCUSSIONS**

We propose a design for a ML MoS$_2$ with two different contacts namely TiS$_2$ on one side and graphene on the other to achieve tunable functionalities as shown in the schematic in Fig. 6. Since TiS$_2$ junction with ML MoS$_2$ induces $p$-type doping, while graphene contact induces $n$-type doping as reported$^{35}$. The heterostructure shown in Fig. 6 consists of TiS$_2$ contact on the left side and graphene contact on the right with ML MoS$_2$ channel. The working principle of the device depends on the doping condition of the channel. If the channel is $p$-type doped, it tends to form Ohmic contact with graphene while forming a Schottky contact on the right side. This would flip if the channel is $n$-type. This device would turn on only if the Schottky barrier is overcome. In addition, if an oxide and gate are added to the MoS$_2$ to obtain better control over the channel. This device can be made using $p$ and $n$-type ML MoS$_2$ doping using the same materials for electrode and obtain complementary devices. In addition, from our simulation studies, we observe that the covalent-bonding contacts add metallization to the MoS$_2$. Thus, for a good contact that preserves the doping concentration of the MoS$_2$ one would prefer a material which forms van der Waal bond with it although...
it will introduce some loss due to the inter-layer impedance. Hence, one can utilize 2D materials to obtain high performance devices.

Using the first-principle DFT simulation, a comprehensive and detailed study on TiS$_2$-(ML) MoS$_2$ contact has been conducted. The simulation shows that, unlike most other contact materials, it is unique that the presence of a TiS$_2$ contact adds p-type doping to the ML MoS$_2$ sheet. The Fermi level shift and smaller metallization effect in the contact region preserves the intrinsic nature of ML MoS$_2$. A tunneling barrier model is employed and we have extracted the transmission rate by using quantum mechanical calculations. The transmission rate $T_0$ (79.4%) is very high at the interface. However, thinner contacts are necessary to reduce carrier scattering. We thus observe that TiS$_2$ forms a n-type Schottky contact with intrinsic ML MoS$_2$ at the vertical interface, but the barrier heights for both electrons and holes are large. The barrier height for electrons ($\Phi_e$) and the holes ($\Phi_h$) at vertical interface can be reduced having either n-type or p-type doping in the channel region. The barrier height is small for p-type-doped channels and TiS$_2$ can form either an ohmic contact or a Schottky contact with low barrier height, which depends on the p-type doping concentration of MoS$_2$. Hence, our simulation results demonstrate that TiS$_2$ is a promising 2D electrode material for ML MoS$_2$, because it does not disturb the structure of the ML MoS$_2$ much as compared to the metals which metallize the MoS$_2$ strongly. This merit makes TiS$_2$ contact viable for a variety of applications for ML MoS$_2$ heterostructure devices like p–n hetero device. Also, in addition to its utility as a good electrode material TiS$_2$ also can be used as a p-type dopant for MoS$_2$.

**METHODS**

Density functional theory

The computational study based on DFT\(^{40}\) has been conducted for this research using Atomistix ToolKit (ATK)\(^{41}\). For all the simulations, TiS$_2$–MoS$_2$ junctions and TiS$_2$–MoS$_2$–MoS$_2$ FET-like junctions, the thickness of the TiS$_2$ was chosen to range from ML to 4L (four layers) to impact the created by the variation of the TiS$_2$ thickness, while the MoS$_2$ channel is set as ML. The mean absolute strain is set as 3.46% for the lattice mismatch between the TiS$_2$ layer and ML MoS$_2$ for the simulations. It means the $5 \times \sqrt{3}$ unit cell of the Ti matches the $3 \times \sqrt{3}$ unit cell of ML MoS$_2$. The Ti atoms in the TiS$_2$ layer occupy both on-top sites and hollow sites of the MoS$_2$ layer. This combination gives a much smaller total energy compared with the pure structure (which is possible for TiS$_2$ and MoS$_2$ because both of them are TMDCs). Since the periodic boundary condition (PBC) is applied in the simulation, a vacuum buffer of 30 Å is added in vertical direction to both groups of configurations to let the electrostatic potential decay softly at the boundary.

Perdew–Burke–Ernzerhof variant of generalized gradient approximation (GGA)\(^{42}\) is applied for the DFT calculation. For simulation, the Hartwigsen–Goedecker–Hutter (HGH)\(^{43}\) basis set is adopted to expand the ED. A DFT-D2\(^{44}\) correction is applied to make a correction to the interfacial Van der Waals bonding. Since the spin–orbital interaction is not taken into consideration in our simulation no correction was applied for it. The k-point sampling for TiS$_2$–MoS$_2$ junction is $12 \times 4 \times 1$ while it is $10 \times 1 \times 1$ for TiS$_2$–MoS$_2$–MoS$_2$ FET-like junction. All the k-point samplings are defined after a convergence test, which ensures that the total energy is converged to $< 1.0 \times 10^{-5}$ eV. By conducting the convergence test, the energy cut-off for the simulation is set as 200 Ry. The maximum force, which determines the convergence of the geometry optimization (GO), is set at 0.05 eVÅ$^{-1}$. The DOS, ED, and EDP also have been conducted utilizing this set-up.

**DATA AVAILABILITY**

The data that support the findings of this study are available from the corresponding author upon request.

Received: 30 March 2020; Accepted: 8 July 2020; Published online: 31 July 2020

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ACKNOWLEDGEMENTS

We would like to acknowledge Natural Sciences and Engineering Research Council of Canada award #06096 for funding this work.

AUTHOR CONTRIBUTIONS

J.G. conducted all the simulations. J.G. and M.G. analyzed and wrote the manuscript.

COMPETING INTERESTS

The authors declare no competing interests.

ADDITIONAL INFORMATION

Correspondence and requests for materials should be addressed to M.G.

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