

## Degenerately Doped $p^+$ -MoS<sub>2</sub> as a High Work Function Electrode Material in van der Waals Heterostructure

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### Abstract

**Fabrication of a low resistance p-type ohmic contact to transition metal dichalcogenide (TMD) semiconductor WSe<sub>2</sub> at low temperatures has been challenging to date. Here, we demonstrate low-temperature ohmic contact to WSe<sub>2</sub> using a van der Waals (vdW) contact of highly p-doped MoS<sub>2</sub> ( $p^+$ -MoS<sub>2</sub>). The  $p^+$ -MoS<sub>2</sub> exhibits a work function comparable to a well-known large work function metal of Pt. In addition to this, due to its layered crystal structure, the  $p^+$ -MoS<sub>2</sub> is easily exfoliatable to obtain atomically flat freshly cleaved surface and stable in the air; thereby, this material can be used for efficient hole-injection contact for TMD semiconductor WSe<sub>2</sub>. We fabricated *h*-BN encapsulated WSe<sub>2</sub> field-effect transistor (FET) having two flakes of exfoliated  $p^+$ -MoS<sub>2</sub> as electrical contacts. The fabricated FET demonstrated ohmic contact behavior under hole doping in the temperature range from room temperature to liquid helium temperature. Owing to the low contact resistance of the  $p^+$ -MoS<sub>2</sub>/WSe<sub>2</sub> junction, we demonstrated quantum oscillation at low temperature under the application of the magnetic field. Our study proves that the  $p^+$ -MoS<sub>2</sub>/WSe<sub>2</sub> vdW contact is an effective low temperature ohmic contact for the application to optoelectronic devices based on vdW heterostructures [1].**

### 1. Introduction

WSe<sub>2</sub> is a transition metal dichalcogenide (TMD) material semiconductor having a layered crystal structure. This material has been extensively studied due to its superior electrical and optical properties compared to other TMD materials. Further, with recent developments of van der Waals (vdW) heterostructure assembly techniques [2], researchers are now able to construct *h*-BN encapsulated high-quality WSe<sub>2</sub>-based heterostructures. These guide the researches to explore the quantum transport or quantum optics of WSe<sub>2</sub> at liquid helium temperature. Nevertheless, a demonstration of low resistance p-type ohmic contact to the WSe<sub>2</sub> in such a low temperature has been still challenging [3]. Fig. 1(a) illustrates the conduction band (CB) and valence band (VB) alignment between different multilayer thick TMD semiconductors and work functions of metallic contacts. Previous studies revealed

that the metal/WSe<sub>2</sub> interface exhibits a strong Fermi-level pinning effect when one fabricates an electrical contact with metal deposited on the surface of WSe<sub>2</sub>. In contrast, the use of metallic 2D material for contact electrode to semiconducting 2D material by constructing a vdW junction [3], enables us to construct an atomically flat as well as a self-cleaning interface on which impurities can be pushed out from the side during construction of the vdW interface. Thus, air-stable p-type vdW metallic contact with WSe<sub>2</sub> is in high demand. Here, we noticed that according to Fig. 1(a), the energy of VB level of MoS<sub>2</sub> relative to the vacuum level is highest among common TMD materials and is almost comparable to that of Pt which is a well-known large work function metal. In addition to this, recently, high p-doping on MoS<sub>2</sub> is demonstrated by Nb doping. Therefore, the Nb-doped  $p^+$ -MoS<sub>2</sub> can be a great candidate for hole injection contact for TMD semiconductors. In this study, we fabricated *h*-BN encapsulated WSe<sub>2</sub> field effect transistors (FET) having two of the exfoliated flakes of  $p^+$ -MoS<sub>2</sub> as contact materials and investigated their low temperature transport properties.

### 2. Results

A schematic illustration of the fabricated devices is shown in Fig. 1(b). A  $\sim 5$  monolayers (ML)-thick WSe<sub>2</sub> flakes are encapsulated between thick ( $\sim 30$  nm) *h*-BN flakes. Flakes of Nb-doped  $p^+$ -MoS<sub>2</sub>, typically thicker than  $\sim 20$  nm, were contacted to the WSe<sub>2</sub> to construct vdW contact between  $p^+$ -MoS<sub>2</sub> and WSe<sub>2</sub> [Fig. 1(c)]. The hole carrier density of Nb-doped  $p^+$ -MoS<sub>2</sub> crystal is  $3 \times 10^{19} \text{ cm}^{-3}$ . Both nondoped-WSe<sub>2</sub> and Nb-doped  $p^+$ -MoS<sub>2</sub> bulk crystals are fabricated by chemical vapor transport (CVT) method and purchased from HQ Graphene Inc. Fabrication of the devices was performed by using vdW pick-up method. Finally, electrical contacts to  $p^+$ -MoS<sub>2</sub> were made by electron beam (EB) lithography to create electrode shape patterns and EB evaporation of 70 nm-thick Au/10 nm-thick Pd as an electrode material.

A two-terminal current-voltage ( $I$ - $V_{SD}$ ) characteristic of the device 1 has been measured at 1.6 K under the application of different back-gate voltage ( $V_{BG}$ ) values to doped Si substrate and results are shown in Fig. 2(a). This measures all of bulk and junction resistances of Au/Pd/ $p^+$ -MoS<sub>2</sub>/WSe<sub>2</sub>/ $p^+$ -

MoS<sub>2</sub>/Pd/Au structure. As we show later, dominant resistance contribution is p<sup>+</sup>-MoS<sub>2</sub>/WSe<sub>2</sub>/p<sup>+</sup>-MoS<sub>2</sub> structure; the resistance contribution from two of Au/Pd/p<sup>+</sup>-MoS<sub>2</sub> junction is playing a minor role (~1 kΩ in total). At the highest  $V_{BG}$  value of -70 V, the device demonstrated linear  $I$ - $V_{SD}$  and ohmic behavior even at 1.6 K. With increasing  $V_{BG}$  to  $V_{BG} = -60$  and -50 V, the  $I$ - $V_{SD}$  curve is changing to non-ohmic behavior.  $I$ - $V_{SD}$  curves at room temperature (RT) in Fig. 2(b) show ohmic behavior in wider range of  $V_{BG}$  values such that it is ohmic at  $V_{BG} \leq -30$  V. Overall, our WSe<sub>2</sub> transistor works as p-type FET as depicted in the back-gated transfer characteristics in Fig. 3.

The high quality of the fabricated 5ML-WSe<sub>2</sub> FET exhibited quantum oscillation with two-terminal resistance measurement at 1.6 K under the application of perpendicular magnetic field of  $B$  and  $V_{BG} = -70$  V as shown in Fig. 4. Here, resistance measurement was performed under the application of AC current of 100 nA and detect AC voltage with lock-in amplifier. In the inset figure, we show oscillating component of resistance  $\Delta R$  extracted by subtracting the background, non-oscillating component of  $R$  using polynomial function. Above the magnetic field  $B = 4$  T, a quantum oscillation in WSe<sub>2</sub> is clearly visible. This is a piece of evidence that p<sup>+</sup>-MoS<sub>2</sub>/WSe<sub>2</sub> interface is having low junction resistance and at the same time, WSe<sub>2</sub> channel is maintained its high quality.

## Figures

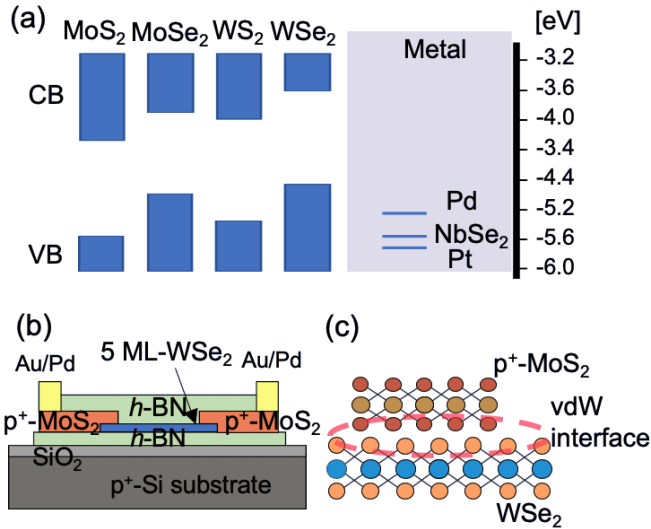


Fig. 1: (a) The energy levels of conduction band (CB) and valence band (VB) of different TMD materials and work function of common metals. (b) Schematic illustrations of the device structure. (c) An illustration of vdW interface at p<sup>+</sup>-MoS<sub>2</sub>/WSe<sub>2</sub>.

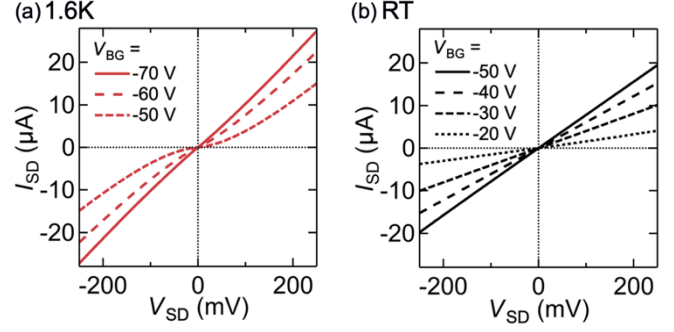


Fig. 2: (a,b) Two-terminal  $I_{SD}$ - $V_{SD}$  characteristics of the device at (a) 1.6 K and (b) RT measured at different  $V_{BG}$  values.

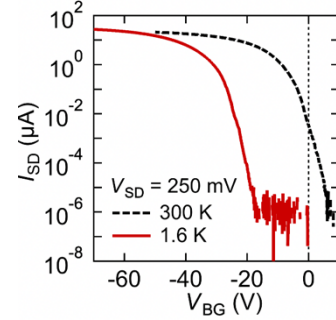


Fig. 3: The  $I_{SD}$ - $V_{BG}$  characteristics of the device at two different temperatures measured under the application of  $V_{SD} = 250$  mV.

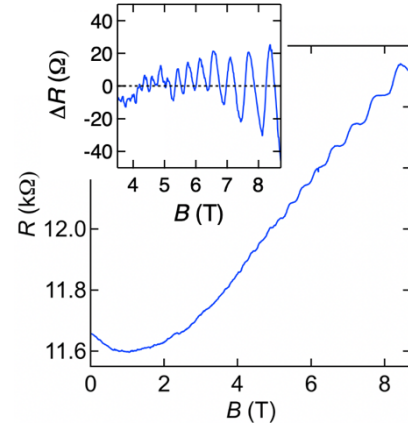


Fig. 4: Two-terminal resistance  $R$  as a function of out-of-plane magnetic field  $B$  measured at 1.6 K. Inset:  $\Delta R$  as a function of  $B$ .

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