Supporting Information

Carrier Transport at the Metal-MoS₂ Interface

Faisal Ahmed^{1,2}, Min Sup Choi^{1,3}, Xiaochi Liu^{1,3} and Won Jong Yoo^{1,2,3,*}

¹Samsung-SKKU Graphene Center (SSGC), SKKU Advanced Institute of Nano-Technology (SAINT),

Sungkyunkwan University, 2066, Seobu-ro, Jangan-gu, Suwon, Gyeonggi-do, 440-746, Korea

²School of Mechanical Engineering, Sungkyunkwan University, 2066, Seobu-ro, Jangan-gu, Suwon, Gyeonggi-do, 440-746, Korea

³Department of Nano Science and Technology, SKKU Advanced Institute of Nano-Technology (SAINT), Sungkyunkwan University, 2066, Seobu-ro, Jangan-gu, Suwon, Gyeonggi-do, 440-746, Korea

*Corresponding email: <u>yoowj@skku.edu</u>

S1 (Rc-T Plot of Pd-MoS₂ contact)

Figure S1(a) is the OM image of the Pd/Au contacted device with 9nm thick MoS_2 flake as channel for carrier transport with lengths of 1, 1.5, 2, 2.5, 3 µm respectively. Figure S1(b) shows Rc(T) of Pd-MoS₂ junction and a similar trend to that of Cr-MoS₂, indicating thermionic emission dominant up to 215K followed by tunneling at low temperature.



Figure S1(a) OM image of TLM patterned device with Pd/Au electrode and MoS_2 as channel. (b) the measured contact resistance of the device. Note that the drain bias is swept from -1 to 1 V during output curve measurement.

The higher value of R_c in Fig. S1(b) can be attributed to the large barrier formed across the Pd-MoS₂ contact due to high work function of Pd (5.0eV) with respect to MoS₂.

<u>S2 (Theoretical calculation of current across Cr-MoS₂ interface)</u>

Das *et al* proposed the carrier transport model for holes conduction across metal-MoS₂ interface,¹ but here we implemented that model to the electron conduction at the interface.

The current along the barrier is extracted in three components, one thermionic emission (I_{TH}) current and two of tunneling components $(I_{TN-1} \text{ and } I_{TN-2})$, as shown in Fig. 3(a) of the main manuscript and they are measured by the following equations.

$$I_{TH} = q \int_{\Phi_{B}}^{\chi} M(E + \Psi_{DRIVE} - \Phi_{B}) f(E) dE$$
(1)

$$M(E) = \frac{2}{h^{2}} \sqrt{2m^{*}E} \quad and \quad f(E) = \frac{1}{1 + \exp(\frac{E}{k_{B}T})}$$

$$I_{TN-1} = q \int_{\Phi_{B}-E_{S}}^{\Phi_{B}} M(E + \Psi_{DRIVE} - \Phi_{B})T_{1}(E) f(E) dE$$
(2)

$$T_{1}(E) = \exp(-\frac{8\pi}{3h} \sqrt{2m^{*}(\Phi_{B} - E)^{3}} \times \frac{\lambda}{\Psi_{DRIVE}})$$

$$I_{TN-2} = q \int_{\Phi_{B}-\Psi_{DRIVE}}^{\Phi_{B}-E_{S}} M(E + \Psi_{DRIVE} - \Phi_{B})T_{2}(E) f(E) dE$$
(3)

$$T_{2}(E) = \exp(-\frac{8\pi}{3h} \sqrt{2m^{*}E_{g}^{3}} \times \frac{\lambda}{\Psi_{DRIVE}})$$

$$\Psi_{DRIVE} = q \left[V_{D} + \left| (V_{G} - V_{MIN} - V_{FB}) / \gamma \right| \right]$$
(4)

$$\lambda = \sqrt{t_{ox}t_{body}} \times \frac{\varepsilon_{body}}{\varepsilon_{ox}}$$
(5)

$$R_c = 1 / I.q \tag{6}$$

Here, q is the charge of electron, ΦB denotes the Schottky barrier height for electrons, χ is the electron affinity of MoS₂, M(E) is the number of conduction modes in (eV.m.s)⁻¹, f(E) is the Fermi-Dirac constant, m^* is the effective mass of electrons in MoS₂, $T_1(E)$ and $T_2(E)$ are the tunneling efficiencies of carriers over their respective regions, Ψ_{DRIVE} denotes the amount of band bending by applied bias, γ is the band movement factor, V_{FB} is the flat band voltage and λ is the screening length extracted from equation (5). The parameter values used in our calculations are given in table S1.However, V_{MIN} , V_{FB} , γ and Ψ_{DRIVE} are calculated from transfer curve [Fig. S2 (a) and (b)]. The flat band voltage is approximately equal to the point at which the slope of log(Id) versus Vg-V_{MIN} deviates from linearity *i.e.* 2.9V in Fig. S2(b) and using the linear region slope that is equal to the 60 γ mV/decade, γ is extracted. For our device, it is around 23.8 and ΦB is extracted from thermionic emission theory [Fig. S2(c)].

Gate oxide thickness (t _{ox})	285 nm
Dielectric constant of $SiO_2(\epsilon_{ox})$	3.9
Body thickness (t _{body})	14 nm
Dielectric constant of body $(\epsilon_{body})^1$	7.0
Effective mass (m*) ¹	0.46m
Schottky barrier height (Φ_B)	0.05 eV
Electron affinity (χ)	4.0 eV
Band gap (E _g)	1.2 eV

Table S1. Parameter values used in this work



Figure S2 (a) The transfer curve of Cr-MoS₂ device on log scale showing typical n-type behavior. V_{MIN} is the gate bias at off-state of the device. (b) The calculation of flat band voltage (V_{FB}) and band bending factor (γ). (c) The calculated effective energy barrier variation against gate bias . Inset shows Arrhenius plot. Note that long channel (L₄) is used for these measurements.

From detailed temperature measurement, Schottky barrier height is extracted using thermionic emission theory.² The extracted barrier height for electrons is about 50 meV at estimated flat band voltage as shown in Fig. S2 (c) . The small value of barrier height can be attributed to the Fermi level pinning effect, *i.e.* the Fermi level at the interface is pinned very near to the conduction band edge of MoS_2 .

The extrated values of all these parameters are used in equations from 1 to 5 to calculate all three current components as shown in the band diagram of Fig. 3(a) of the main manuscript, and their reuslts are shown in Fig. 3(b) in units of A/m. Finally, Rc is extracted by applying the Landauer theory,^{3,4} to the measured current components as shown in equation (6), and their results are shown in Fig. 3(c) in the units of ohm mexcept I_{TN-2} .

References

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