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# Gate-tunable atomically-thin lateral MoS<sub>2</sub> Schottky junction patterned by electron beam

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**Among atomically-thin two-dimensional (2D) materials, molybdenum disulphide (MoS<sub>2</sub>) is attracting considerable attention because of its direct bandgap in the 2H-semiconducting phase. On the other hand, a 1T-metallic phase has been revealed, bringing complementary application. Recently, thanks to top-down fabrication using electron beam (EB) irradiation techniques, in-plane 1T-metal/2H-semiconductor lateral (Schottky) MoS<sub>2</sub> junctions were demonstrated, opening a path towards the co-integration of active and passive two-dimensional devices. Here, we report the first transport measurements evidencing the formation of a MoS<sub>2</sub> SB junction with barrier height of 0.13 ~ 0.18 eV created at the interface between EB-irradiated (1T)/non-irradiated(2H) regions. Our findings supported by state-of-the-art *ab initio* simulation reveal that the barrier height is highly sensitive to electrostatic charge doping and almost free from Fermi level pinning, a fact unique to atom-thin 1T layers, and a fingerprint of Schottky barrier-based field-effect transistors**

MoS<sub>2</sub>, one of the transition metal dichalcogenides, is much attractive among atomically-thin 2D materials<sup>1-26</sup>, because of its direct bandgap of 1.5 ~ 1.8 eV in 2H semiconducting phase, especially when atom-thin or flexible circuitry is required. On the other hand, the 1T-metallic phase, engineered by chemical doping and laser-beam irradiation, is also useful for some application such as ohmic metallic junction between metal electrode and 2H-MoS<sub>2</sub>, and supercapacitor electrode with capacitance value as high as ~700 F/cm<sup>3</sup><sup>14-19,21</sup>. An electronic transition from the 2H (trigonal prismatic D3h) semiconducting to the 1T (octahedral Oh) metal phases of MoS<sub>2</sub> triggered by EB irradiation (see Fig. 2E) has been recently observed under the in-situ transmission electron microscope (TEM) at high substrate temperature<sup>12</sup>. The two phases can easily be converted from one to the other via intralayer atomic plane gliding, which involves a transversal displacement of one of the *S* planes (Fig. 2E), caused by the charge accumulation and direct momentum transfer from EB combined with substrate heating.

However, to date, such structural observations have not been harnessed to fabricate practical in-plane lateral Schottky junctions and SB devices. It is even unclear whether such lateral SB can be actually formed within atomically thin layers only through atomic-order phase transition. Moreover, if SB devices fabricated with graphene have been already reported, they have been realized with vertically stacked hetero-structures via van der Waals engineering and metal/MoS<sub>2</sub> interfacing, which are not suitable for large scale integration<sup>34-37</sup>. The EB-irradiated top-down fabrication of in-plane 1T/2H Schottky junctions<sup>27-30</sup> and SB field effect transistors (SB-FET)<sup>31-33</sup> is highly important, because the EB-patterned technique could be in principle scalable to large complex in-plane circuitry. Here, we fabricate this atomically thin EB-patterned lateral MoS<sub>2</sub> Schottky junctions and SB-FET. The device characteristics (with confirmation by X-ray photoelectron spectroscopy (XPS), Raman<sup>14,20</sup> and photoluminescence (PL) spectroscopies), highlighted by rectification and SB-FET<sup>27-33</sup> properties and supported by first-principles simulations<sup>38-40</sup>, reveal the formation of 2D SBs<sup>30</sup>, which have high tunability by gate-electrostatic-induced doping (0.13 ~ 0 eV for back-gate voltage ( $V_{bg}$ ) of 0 ~ 4V) and are free from Fermi level ( $E_F$ ) pinning, a fact unique to atomically thin layers with low charge-carrier capability.

In order to create 1T phase embedded into 2H phase, few layer *n*-type MoS<sub>2</sub> flakes with thickness ~8 nm (~7 layers) have been fabricated by mechanical exfoliation of bulk MoS<sub>2</sub> following scotch tape method (Fig. 1A). Two regions on one sample with individual area of 1.5 × 1 μm<sup>2</sup> have been exposed to EB irradiation with different doses (Fig. 1A; 100 Me/nm<sup>2</sup> for region 1 and 160 Me/nm<sup>2</sup> for region 2), without using any dopant at room temperature (see supplementary materials (SM) 1). This was followed by the patterning of two Au/Ti (500nm/20nm thick) electrode pairs on individual

regions (Fig. 1B). Electrode pair 1-2 is contacted to non-EB-irradiated bulk, while, in the electrode pair 3-4, one electrode is contacted to EB irradiated and the other to non-EB-irradiated bulk. From here on, we will refer to the fabricated device on regions 1 and 2 as Devices 1 and 2, respectively. Back gate electrode was also attached on the back-side of Si substrate with thick SiO<sub>2</sub> layer (~300 nm).

Figures 1C and 1D show XPS spectra of the sample shown in Fig. 1A, measured including the EB- irradiated region 2 and non-irradiated region (see SM2). The figures show the characteristic Mo 3*d*, S 2*s* (Fig. 1C), and S 2*p* (Fig. 1D) peaks of the 1T phases of MoS<sub>2</sub><sup>14,15</sup>, although the larger area of 2H phase results in higher intensity. Typical Raman spectra for EB-irradiated region 2 are also given in Fig. 1E. We observe two weak but distinct peaks (i.e., J<sub>1</sub> and J<sub>2</sub> around 150 and 216 cm<sup>-1</sup>, respectively). These peak positions are in good agreement with previous reports of Raman spectrum for 1T phase MoS<sub>2</sub><sup>16-20</sup>. Region 1 does not exhibit such peaks. PL map (inset) and spectra measured at selected four points (main panel) are also reported in Fig. 1F(see SM3). Two prominent absorption peaks are clearly identified at ~670 and ~627 nm in the spectra (No. 1-3), which agrees with previous PL reports of 2H-MoS<sub>2</sub> with thickness similar to the present samples<sup>20</sup>, and its entire elimination (No. 4) on EB non-irradiated and irradiated regions, respectively. These results strongly suggest the formation of metal (1T) and semiconductor (2H) phases in the EB-irradiated region 2 and non-irradiated region, respectively. The observed 1T phase is stable even after one month in contradiction to ref. 41. One of the possible reasons might be that in our samples, the 1T phase is not free standing but embedded into 2H phase.

Figure 2 shows the current (*I*) vs voltage (*V*) for two measured devices. Device 1 exhibits a symmetric characteristics for both electrode pairs, with non-negligible current in correspondence of *V* = ±1.5V (Fig. 2A), as expected for conventional metal-semiconductor-metal structures (i.e., (Au/Ti)/bulk 2H-MoS<sub>2</sub>/(Au/Ti) in Fig. 1E)<sup>28</sup>. This suggests that the EB-irradiated region in Device 1 does not show any metallic transition and keeps an electronic fingerprint qualitatively similar to bulk MoS<sub>2</sub>. The EB dose of 100 Me/nm<sup>2</sup> applied to region 1 is too weak to provoke a phase transition. We estimate that the forward voltage (*V<sub>F</sub>*) of our Schottky junction (Au/Ti)/2H-MoS<sub>2</sub> is about ~2V in Fig. 2A (*V<sub>F</sub>* is the voltage at which forward current attains to 4.5 A).

In contrast, *I*<sub>34</sub> vs *V*<sub>34</sub> characteristics for electrode pair 3-4 of Device 2 strongly differ from those of Device 1 (Fig. 2B). Remarkably, a clear asymmetric behavior (i.e., rectification property) is observed with an onset bias voltage of ~+2.5 V. Such an asymmetric electrical feature can be clearly related to the formation of a Schottky junction<sup>27</sup>, with a barrier height seen by electrons different with respect to that seen by holes. As mentioned above, XPS, Raman, and PL spectra suggest the formation of 1T-phase in EB-irradiated region 2. Because 1T-phase is metallic, the observed Schottky behavior can be explained by the formation of a metal-(1T-phase)/semiconductor(bulk 2H) in-plane junction at the surface within ~3 layers (Fig. 2D). Indeed, an electrode pair contacted to a region irradiated by an EB with dose of 160 Me/nm<sup>2</sup> in another sample (Device 2') actually exhibits a metallic characteristic (i.e., a symmetric behavior showing no rectification property) (Fig. 2C). Moreover, electrode pair 1-2 of Device 2 does not drive any current (i.e., *I*<sub>12</sub> < ±200nA at *V*<sub>12</sub> < ±5V). This supports the presence of two Schottky junctions with large barrier heights between electrodes 1 and 2 in Device 2 (Fig. 2E), because reverse bias voltage regime for applied *V*<sub>12</sub> (i.e., corresponding to -*V*<sub>34</sub> regime of Device 2 in Fig. 2B) is dominant for the symmetrically placed two Schottky junctions. In Fig.2B, *V<sub>F</sub>* is as large as ~5V. This is much larger than *V<sub>F</sub>* = 2V of the (Au/Ti)/2H-MoS<sub>2</sub> junction shown in Fig. 2A. Since *V<sub>F</sub>* is basically proportional to Schottky barrier height, the Schottky barrier height for Fig. 2B is thus different as compared that of Au/Ti/2H-MoS<sub>2</sub> junction and, hence, the Schottky barrier for Fig. 2B is attributed to 2H/1T phase junction. From these *V<sub>F</sub>* values, the barrier height of (Au/Ti)/2H phase is estimated to be as small as 0.05eV ~0.07eV, whereas that for 2H/1T is 0.13 ~ 0.18 eV. The former value for (Au/Ti)/2H phase junction is in excellent agreement with previous theoretical modeling<sup>42,43</sup>.

Next, we focus on the electrical characteristics of electrode pair 3-4 in Device 2, as a function of *V*<sub>34</sub> for different *V<sub>bg</sub>* (Fig. 1E). Figure 3A shows a typical logarithmic *I*<sub>34</sub> vs *V<sub>bg</sub>* characteristics for *V*<sub>34</sub> = +1V (i.e., forward bias voltage region). Under +*V<sub>bg</sub>*, these characteristics resemble that of a n-type SB-FET<sup>31-33</sup>, which consists of (1T-MoS<sub>2</sub> metal)/2H-MoS<sub>2</sub> n-semiconductor/(Ti/Au electrode) (Fig. 3C). As +*V<sub>bg</sub>* increases, the barrier at the Schottky contacts is thinned, and electrons can easily flow from the right contact to the channel and eventually to the left contact, increasing *I*<sub>34</sub>. As it can be seen in Fig. 3A, the current is modulated over 4 orders of magnitude (*I*<sub>on</sub>/*I*<sub>off</sub> ~ 10<sup>4</sup>) and the subthreshold slope (*SS*) is approximately 1 V/decade. The obtained *SS* is almost the same as that observed in CNT-SB-FET and SB-MOSFET with SB height of 0.3 eV and thick back gate oxide<sup>32,33</sup>. This also supports the formation of a SB in Device 2.

Figure 3B shows *I*<sub>34</sub> vs *V<sub>bg</sub>* characteristics for two different reverse biases (i.e., *V*<sub>34</sub> = -1V and -3V). As can be see, larger currents are observed for *V*<sub>34</sub> = -1V. We believe that this effect can be explained as follows. In particular, for this biasing, electrons may accumulate in 1T-MoS<sub>2</sub> metal reservoir, leading to an increase of the *E<sub>F</sub>* (Fig. 3D, where e*V<sub>accum</sub>* is the electrostatic energy due to electron accumulation), to a reduced Schottky barrier and eventually to a larger current in the *V*<sub>34</sub>

= -1V case as compared to the  $V_{34} = -3V$ . As a word of caution, we have to state that other physical effects could explain such a behavior (e.g., reduction of the barrier height due to image-force lowering), which certainly deserves further investigations.

Figs. 4A – 4C show Arrhenius plot for  $I_{34}$  normalized over temperature (i.e.,  $I_{34}/T^{3/2}$  for 2D Schottky junction formula given by eqs. (1 -4)) for different  $V_{bg}$  ( $V_{bg} = 0V, 4V,$  and  $2V,$  respectively) and fixed  $V_{34} = -2V$  (i.e., reverse bias). For Fig. 4A,  $I_{34}$  linearly decreases below  $1/T_c = \sim 0.0067$  as  $1/T$  value increases (i.e.,  $I_{34}$  increases at critical  $T$  ( $T_c$ )  $> 150K$  with increasing  $T$ ), while  $I_{34}$  significantly drops above  $1/T_c$ . In contrast, in Fig. 4B, for  $1/T$  smaller than  $1/T_c$  (i.e., high  $T$ ), the curve becomes constant (i.e.,  $T$ -independent). This can be explained by the fact that for large  $V_{bg}$ , the SB becomes almost transparent and thermal energy does not significantly contribute to increase  $I_{34}$  (as explained for Figs. 4D, 4E, and 5E later).

The experimental data (Figs. 4A and 4B) are analyzed using the expression of the current ( $I$ ) in a 2D Schottky diode as a function of  $T$ <sup>30</sup>.

$$I = I_{2D} [\exp (qV/\eta k_B T) - 1] \quad (1)$$

$$I_{2D} = W A_{2D}^* T^{\frac{3}{2}} \exp \left( -\frac{q\phi_B}{k_B T} \right) \quad (2)$$

$$A_{2D}^* = q \sqrt{8\pi k_B^2 m^* / h^2} \quad (3)$$

$$m^* = 0.45m_0 \quad (4)$$

where  $\eta$  is the diode ideality factor (i.e., takes into account the presence of generation/recombination phenomena),  $A_{2D}^*$  is the 2D Richardson constant,  $W$  ( $=1.5\mu m$ ) is the junction length,  $\phi_B$  is the SB height,  $k_B$  is the Boltzmann constant,  $m^*$  is the effective mass of  $MoS_2$ , and  $m_0$  is the mass of electron. When a negative  $V_{SD}$  (corresponding to  $-V_{34}$  in our device) is applied, eq. (1) results in  $I = -I_{2D}$ . Thus, the  $T$ -dependence of  $I_{SD}$  agrees with the  $T$ -dependence given by eq. (2).

The linear relationships obtained in Figs. 4a and 4b support the validity of eq. (2) describing the formation of a Schottky junction at the interface between EB-irradiated/non-irradiated (bulk) regions of Device 2, although other physical origins have not been considered as mentioned above. The best fits using eqs. (2) - (4) (dotted lines) give  $\phi_{B1} \sim 0.13$  eV at  $1/T < 0.0067$   $K^{-1}$  and  $\phi_{B2} \sim 0.18$  eV at  $1/T > 0.0067$   $K^{-1}$  in Fig. 4A, and  $\phi_{B3} \sim 0.15$  eV at  $1/T > 0.0067$   $K^{-1}$  in Fig. 4b, when total area of the Schottky junction  $S = 2,500$   $nm^2$ , and  $\eta = 1.07$  are used. The result  $\eta = 1.07$  suggests the presence of small amount of generation/recombination current at the junction, possibly owing to defects introduced by the EB irradiation.

For Fig. 4A, one of the origins of two SB with heights  $\phi_B$  estimated at temperatures above and below  $T_c$  can be understood from the obtained two  $S$  values, which give the best fits.  $\phi_{B1} \sim 0.13$  eV at  $1/T < 0.0067$  and  $\phi_{B2} \sim 0.18$  eV at  $1/T > 0.0067$  give  $S = 5$   $nm \times 300$   $nm$  and  $5$   $nm \times 200$   $nm$ , respectively. For Fig. 4B, an interesting  $T$ -independent  $\phi_B \sim 0$  eV at  $1/T < 0.0067$   $K^{-1}$  is observed. Figure 4C exhibits a result at intermediate  $V_{bg}$  ( $= +2V$ ) between Fig. 4A ( $V_{bg} = 0$ ) and 4b ( $V_{bg} = +4V$ ).  $\phi_B \sim 0.015$  eV at  $1/T < 0.0067$   $K^{-1}$  actually corresponds to intermediate value. Including these results, Fig. 4D reveals the high sensitivity of  $\phi_B$  to applied  $V_{bg}$ , implying highly gate-tunable  $\phi_B$ . The origin is explained in the later part, based on Figs. 4E, and 5E.

To deepen the analysis of the 2H/1T interface, we have performed DFT calculations, considering the geometry of 2H/1T  $MoS_2$  interfaces as experimentally observed with atomistic details given in [12]. This approach allows us to obtain accurate information on the SB forming at the 2H/1T interface, taking into account both the band offset and the formation of dipoles. We neglect the possible contribution of interface defects or recombination centers, which are likely present (suggested experimentally by the Schottky factor  $\eta = 1.07$ , which is larger than 1) and can provide localized states affecting the SB. First-principles DFT calculations are performed using the Quantum Espresso package<sup>38</sup>, utilizing a plane wave basis set, a gradient-corrected exchange-correlation functional<sup>39</sup>, and scalar-relativistic ultrasoft pseudopotentials (US-PPs)<sup>40</sup> (SM4). Figs. 5A and 5B show the computed bands for monolayer 1T and 2H-phase  $MoS_2$ , respectively. Exploiting the information in [12], we built a periodic model of a 2H/1T/2H heterojunction whose atomistic structure is shown in Figs. 5C, 5D, and which represents a realistic model of a 1T-phase embedded within the generating 2H phase.

Figure 5E shows a plot of the vacuum level potential profile with respect to  $E_F$  showing the formation of dipoles at the hetero-interfaces. DFT calculations provide a value of 0.73 eV for the energy difference between the electron affinity of 2H  $MoS_2$  and the work function of 1T  $MoS_2$ . From this information, we plot in Figure 5F the conduction band edge profile in the structure relative to the  $E_F$ , and extract a  $\phi_B$  of 0.47 eV, in reasonably good agreement with the experimental results. The

residual discrepancy between predicted and observed values of the Schottky barrier can be ascribed to several effects. One likely effect is the change in the work function of the 1T phase due to doping by the contact electrode: indeed, from test calculations we found that such a doping induces an upward shift in the background potential of the 1T phase by  $\sim 0.3\text{-}0.4$  eV which could easily account for the observed discrepancy (see SM5). Other possibilities include the mentioned defects and recombination centers at the interface which can induce mid-gap states, thus reducing the effective  $\Phi_B$ . Indeed, a dependence of the Schottky barrier on the work function has been observed in other Schottky junctions: for example the  $\Phi_B$  of non-hydrogenated and hydrogenated Pd/few-layer MoS<sub>2</sub> SBs were reported to be 0.25 eV and 0.15 eV, respectively. Hydrogenation of Pd reduced the work function of Pd and subsequently reduced the  $\Phi_B$  to  $\sim 0.1$  eV<sup>31</sup>. Moreover, a value of 0.3 eV for  $\Phi_B$  was reported in SB-MOSFET with  $S$  value ( $\sim 1\text{V}/\text{decade}$ ) similar to ours as mentioned above<sup>32</sup>.

One can also see in Fig. 5E that the potential in the 1T phase shows some variations at the interface, because 1T MoS<sub>2</sub> has a relatively low density of states (in this sense it is not an ideal metal). This also explains the observed highly  $V_{\text{bg}}$ -sensitive  $\Phi_B$  (Fig. 4D). As the  $V_{\text{bg}}$  is increased, electrons doped from substrate accumulate in the 1T-phase region under  $-V_{34}$ , increasing  $E_F$  with respect to the conduction band (Fig. 4E;  $-e(V_{34} + V_{\text{accm}})$ ), hence decreasing  $\Phi_B$  to  $\Phi_B'$ . When  $E_F$  in the 1T-metal region coincides with the top of the Schottky junction by further increasing  $V_{\text{bg}}$ ,  $\Phi_B'$  becomes zero and, thus, electrons feel no SB. Therefore, a T-independent zero- $\Phi_B$  value appears. The dependence of  $\Phi_B$  on T is likely to depend on the energy and nature of localized states at the hetero-interface. This tunable Fermi level  $E_F$ , highly sensitive to electrostatic carrier doping via. back-gate electrode, is unique to the present SB consisting of 1T phase of atomically thin ( $\sim 3$  layers) MoS<sub>2</sub>. It also implies that the  $E_F$  is almost free from pinning by defects at the SB despite of the presence of generation/recombination center, particularly in the high T regime. This is also a significant benefit of the atomically thin layers, in which pinned  $E_F$  can be easily shifted by increased electro-static potentials induced by the accumulation of the doped charge carriers in 1T area. This high tunability can be highly useful in future atomically-thin in-plane device applications.

In conclusion, we demonstrated the first EB-patterned gate-tunable in-plane atomically-thin Schottky junction and SB-FET fabricated with a top-down approach, by inducing a structural phase change in few-layer MoS<sub>2</sub> through an EB irradiation dose of  $160 \text{ Me}/\text{nm}^2$  at room temperature. Observation of XPS, Raman, and PL spectra exhibit presence of 1T metallic phase on the EB irradiated region. Experimental measurements and ab-initio simulations provide a coherent physical picture of the properties of the 2D Schottky junction created at the interface of EB-irradiated (1T) /non-irradiated (2H) regions. The difference between the experimentally observed SB height ( $\sim 0.13 - 0.18$  eV) and the one obtained by theory (0.47 eV) highlight the presence of defects and recombination centers introduced by EB irradiation. Electrostatic-induced carrier doping by  $V_{\text{bg}}$  enables tuning the SB height due to low density of states of 1T phase (0.13  $\sim$  0 eV for  $V_{\text{bg}}$  of 0  $\sim$  4V), resulting in the T-independent zero-SB height. This EB top-down patterning opens the possibility to fabricate in-plane lateral heterostructure FETs<sup>9</sup>, which have shown promising scaling prospects in the nm range<sup>10</sup>, and/or local interconnects directly with metallic phase (1T) between (2H)MoS<sub>2</sub> transistors, resulting in ultimate flexible and wearable in-plane integration circuits without using 3D metal wirings. After this initial work, more efforts are needed to mitigate the presence of interface defects and to establish the atomic-scale in-plane SB devices as building blocks of 2D electronic and optoelectronic circuits.

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## Author contributions

Y. K., T. N., A. I., C. O., and Y.K.F. performed experiments. T.C., A. F., G.I. and G. F. performed theoretical calculation. J. H., S. K., T. N., M. H. designed the experiments. J.H. and A.I. analyzed the data. J. H., T.C., A.F., S.R., G. I., and G. F. wrote the manuscript.

## Notes

The authors declare no competing financial interest.

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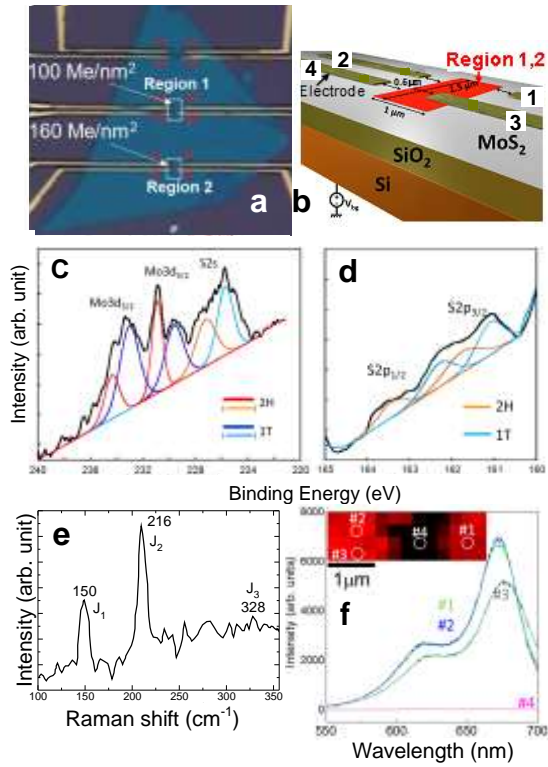


Figure 1

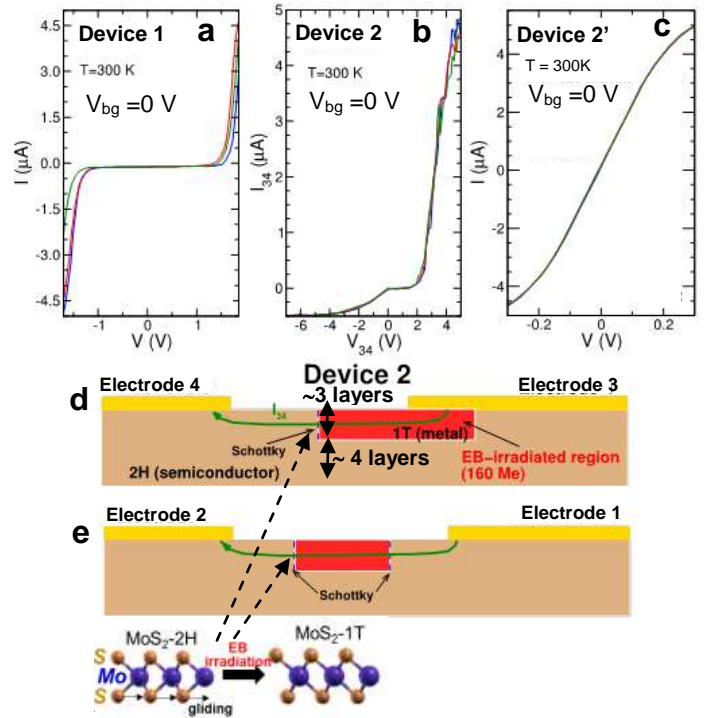


Figure 2

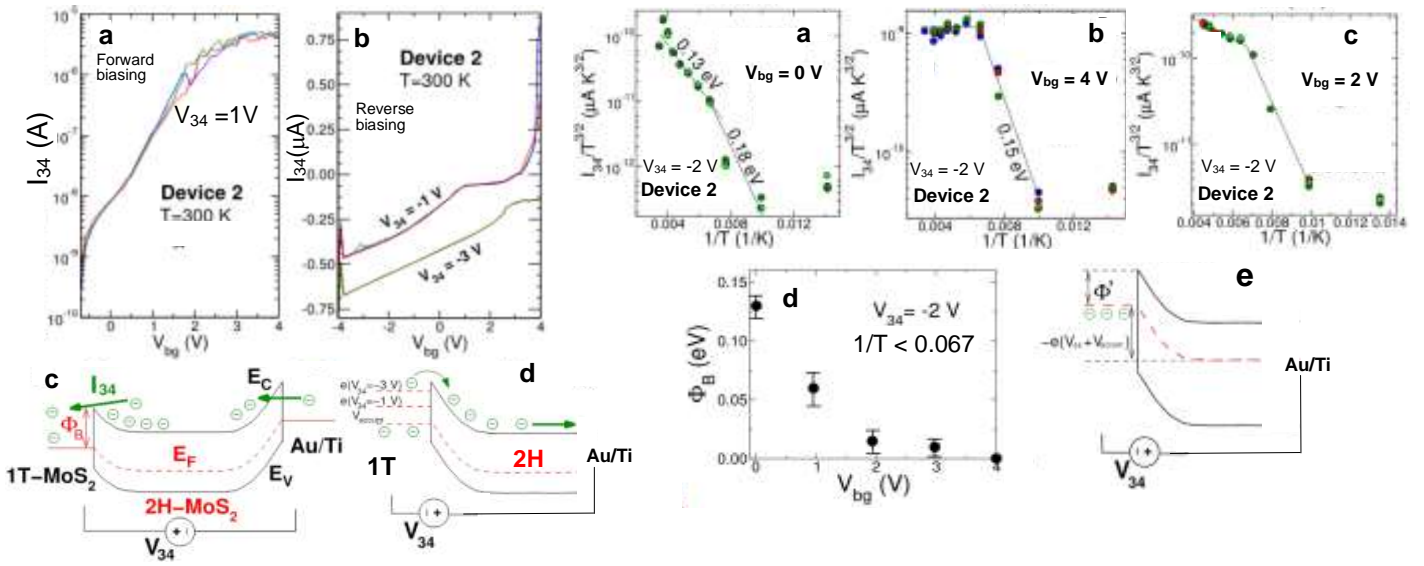


Figure 3

Figure 4

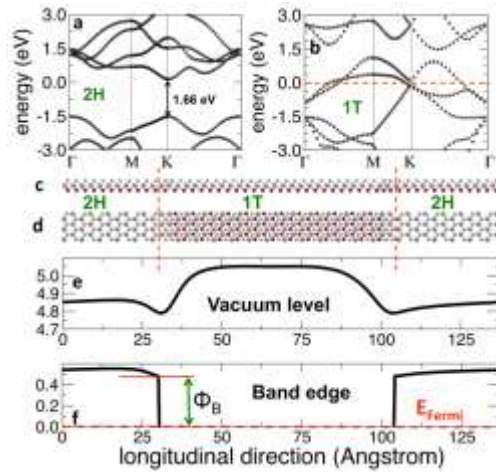


Figure 5



## Figure captions

**Figure 1.** Structural information of few-layer MoS<sub>2</sub> and characterization. **(a)** Optical microscope image of few-layer MoS<sub>2</sub>, mechanically exfoliated from bulk, with two EB irradiation regions and two electrode pairs patterned on individual regions. **(b)** Schematic view of an electrode pair on one EB-irradiated region of (a). **(c, d)** XPS spectra of sample shown in (a), which have been measured including the EB-irradiated region 2 and non-irradiated region, showing the Mo 3*d*, S 2*s* (c), and S 2*p* (d) peaks of the 1T phases of MoS<sub>2</sub>. Typical experimentally measured spectra are shown in black and fits are shown in red (for the 2H phase component) and blue (for the 1T phase component). **(e)** Typical Raman spectra of EB-irradiated region 2 in (a), showing three peaks unique to the 1T phases of MoS<sub>2</sub>. **(f)** PL spectra (via. laser wavelength with 488 nm) of area including region 2 in (a) (see **inset**), exhibiting two absorption peaks due to direct excitonic transitions unique to 2H-MoS<sub>2</sub> (No. 1,2,3) and its complete quench (No.4) on EB non-irradiated and irradiated regions, respectively. **Inset**; PL map with 0.25 μm<sup>2</sup> space resolution, corresponding to wave length of 102 nm (black) ~ 686 nm (red). The number 1-4 correspond to those in main panel.

**Figure 2.** Room-temperature I vs. V relationships for individual electrode pairs formed around two EB-irradiated regions of Fig. 1(a) for **(a)** Device 1, **(b)** electrode pair 3-4 of Device 2, and **(c)** electrode pair formed on EB-irradiated region with 160 Me/nm<sup>2</sup> in another sample (Device 2'). Results of three-times measurements are shown in different colors on individual figures. **(d, e)** Schematic cross sections of Device 2 for electrode pairs (d) 3-4 and (e) 1-2, corresponding to Fig. 1e. Number of layers of ~4 at bottom-side 2H MoS<sub>2</sub> of EB-irradiated region has been confirmed by Raman peak observed around 407 cm<sup>-1</sup> (A<sub>1g</sub> peak). That of ~3 at upper-side 1T MoS<sub>2</sub> has been determined by subtracting the 4 layers from total layer number of 7. **Inset of (e)**: Schematic views of two-different-atomic structured mono-layer MoS<sub>2</sub> crystals; 2H semiconducting and 1T metal phases.

**Figure 3.** Room-temperature back-gate voltage (V<sub>bg</sub>) dependence of Fig. 2b (Electrode pair 3-4 in Device 2). **(a, b)** I<sub>34</sub> vs. V<sub>bg</sub> relationships for the forward (a) and reverse (b) V<sub>34</sub>. Y-axis of (a) is a logarithmic. Results of three-time measurements are shown in different colors on individual figures. Note that current limiter of the measurement facility is set to 5 μA through all measurements. **(c, d)** Schematic energy band diagrams of (c) Schottky barrier (SB) FET consisting of (1T-metal)/(2H-semiconductor)/(Ti/Au electrode 3) under forward bias voltage (+V<sub>34</sub>) and +V<sub>bg</sub>, and (d) 1T/2H-phase MoS<sub>2</sub> Schottky junction under reverse bias voltage (-V<sub>34</sub>) and +V<sub>bg</sub> (see Fig. 2e). In (d), eV<sub>accm</sub> is the electrostatic energy caused by electron accumulation by applying +V<sub>bg</sub>.

**Figure 4.** Temperature dependence of I<sub>34</sub> (Arrhenius plot and 2D Schottky formula) of Fig. 3a and gate tunability. **(a, b)** I<sub>34</sub> normalized by temperature (I<sub>34</sub>/T<sup>3/2</sup>) vs. 1/T at V<sub>bg</sub> = 0V (a) and 4V (b) under fixed V<sub>34</sub> = -2V. **(c)** that for intermediate V<sub>bg</sub> = 2V under V<sub>34</sub> = -2V. Dotted lines are obtained by data fitting using eqs. (1) – (4). **(d)** Gate-tunability of Φ<sub>B</sub>, including results of (a) – (c). The error bars show the results of three samples. **(e)** Schematic energy band of 1T/2H-phase MoS<sub>2</sub> Schottky junction under reverse bias voltage (-V<sub>34</sub>) and +V<sub>bg</sub> to explain (d).

**Figure 5** Calculation results based on density functional theory (DFT). **(a)** 2H-MoS<sub>2</sub> monolayer bands. **(b)** 1T-MoS<sub>2</sub> monolayer bands. **(c)** Side and **(d)** top atomistic schematic representation of the 2H/1T/2H MoS<sub>2</sub> heterostructure. **(e)** Vacuum level and **(f)** Band edges of the structure, as computed from DFT calculations. E<sub>F</sub> of the hetero-structure has been considered as the reference potential for both potentials shown in **(e)** and **(f)**.