Electronic Supplementary Material (ESI) for Nanoscale.

Supporting Information

Electrostatically tunable lateral $MoTe_2$ p-n junction for use in high-performance optoelectronics

*Zhenxing Wang, Feng Wang, Lei Yin, Yun Huang, Kai Xu, Fengmei Wang, Xueying Zhan, Jun He**

CAS Key Laboratory of Nanosystem and Hierarchical Fabrication, National Center for Nanoscience and Technology, Beijing 100190, P. R. China

*To whom correspondence should be addressed: hej@nanoctr.cn

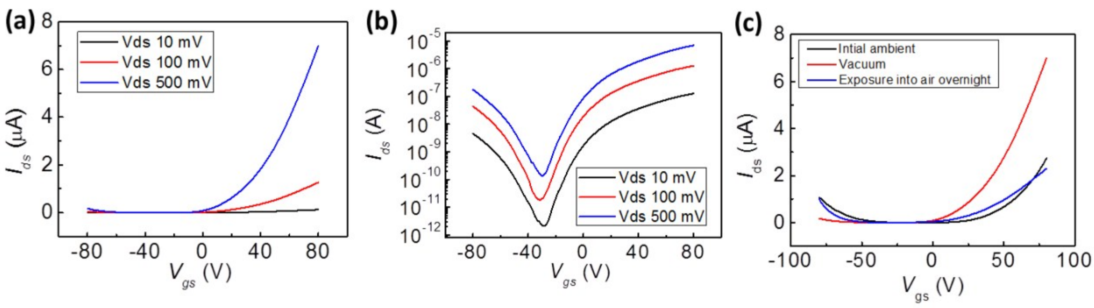

Fig. S1. Same device to Fig. 1. (a) Typical transfer curve of a back-gated $MoTe_2$ FET. The drain voltage was set as 10, 100, 500 mV and the source was grounded. 300 nm thick SiO_2 was used the dielectric layer. (b) Output characteristics of the $MoTe_2$ FET on a logarithmic scale. These data are measured in vacuum (6.1×10^{-5} torr). (c) Comparison of the *I-V* curves in different conditions. Black curve: initial ambient; Red curve: in vacuum; Blue curve: after exposure in air overnight.

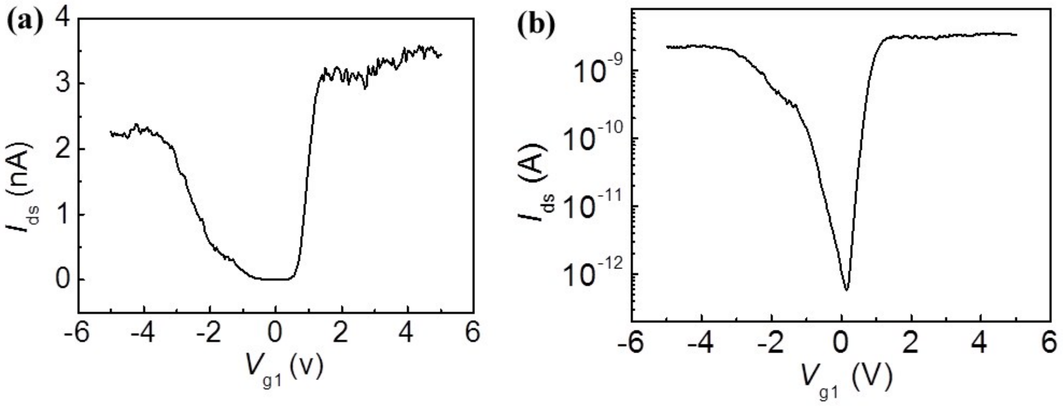

Fig. S2. Same device to Fig. 2. Variation of drain current (I_{ds}) with the V_{g2} when drain voltage (V_{ds}) 500 mV is applied and V_{g2} is set free. (a) the curve is on linearity scale and (b) the curve is on logarithmic scale.

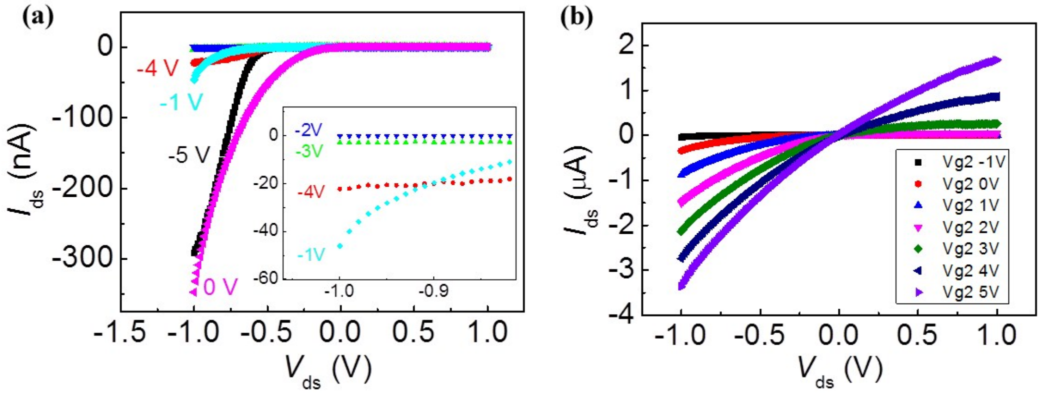

Fig. S3. Same device to Fig. 3. (a) *I-V* curves of $MoTe_2$ p-n junction device with variation of V_{g2} from -5 V to 0 V on a normal scale. (b) *I-V* curves of $MoTe_2$ p-n junction device with variation of V_{g2} from -1 V to 5 V on a normal scale. For both (a) and (b), V_{g1} is fixed as 5V.

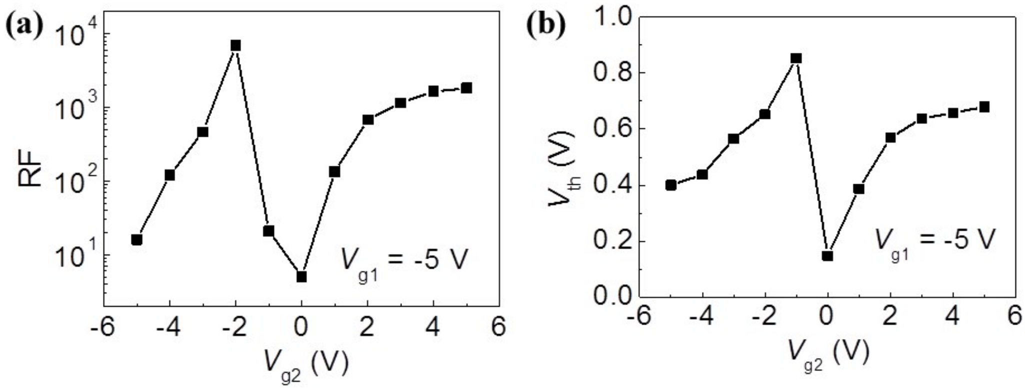

Fig. S4. Different devices to Fig. 3. Variation of (a) RF and (b) Threshold voltage (V_{th}) with V_{g2}. RF is defined as $I_{forward}/I_{reverse}$ at $V_{ds} = \pm 1$ V. V_{th} is the intercept in "V_{ds}" axis by fitting the rectification *I-V* curves.

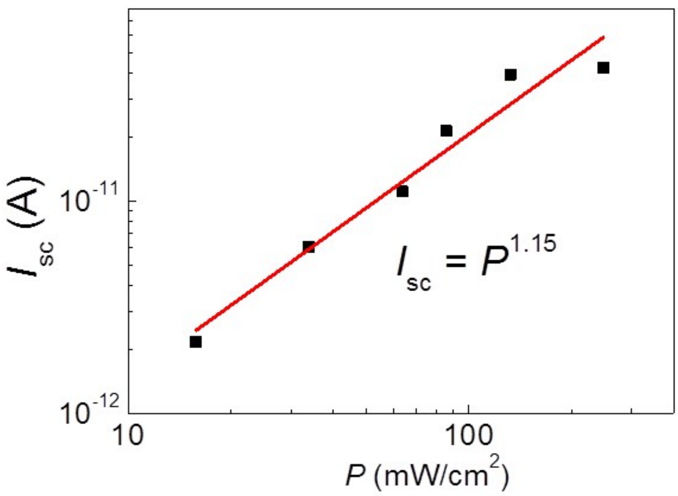

Fig. S5. Different devices to Fig. 4. Short circuit current I_{sc} as a function of laser power density (P) on a logarithmic scale on a double logarithmic scale. Biasing condition: V_{g1} = 5 V and V_{g2} = -5 V.

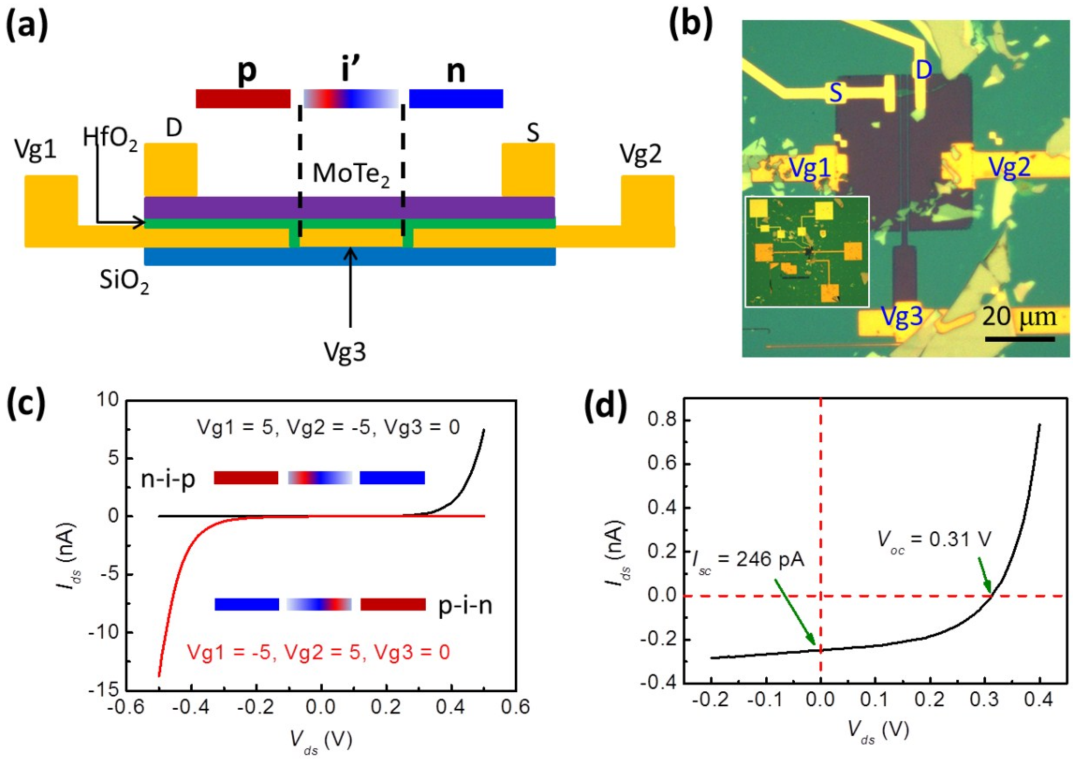

Figure S6. (a) The scheme and (b) optical image of the three gate device. The gap between V_{g1} and V_{g2} is around 2μm. (c) Rectifying characteristics of the device. P-i-n junction (red curve, V_{g1} = -5 V, V_{g2} = 5 V and V_{g3} is set electrically floating), n-i-p junction (black curve, V_{g1} = 5 V, V_{g2} = -5 V and V_{g3} is set electrically floating). (d) *I-V* curve under illumination of 473 nm laser with a power density of 248.0 mW/cm^2, where V_{g1} = 5 V, V_{g2} = -5 V and V_{g3} is set electrically floating.

Figure S6a and b is the scheme and optical image of the device configuration, respectively. Here, when we set V_{g3} electrically floating and V_{g1}, V_{g2} with opposite polarity, clear rectifying characteristics can be observed, as shown in Figure S6c. These results are similar to those from the device with 200 nm gap. In addition, the photovoltaic effects of the device are also studied using a 473 nm laser with a power density of 248 mW/cm^2. As shown in Figure S6d, the short circuit current I_{sc} = 246 pA and open circuit voltage V_{oc} = 0.31 V. Compared with the data demonstrated in our manuscript based on the 200 nm gap device, the open circuit voltage is similar (0.28 V), however, the short circuit current becomes much larger (246 pA *vs.* 28 pA). This may be attributed to the p-i-n structures despite. Actually, Lieber CM did a lot of p-i-n nanowires for photovoltaic applications (*Nano Lett.* **2008**, 8, 3456; *Nature* **2007**, 449, 885; *Chem. Soc. Rev.* **2009**, 38, 16). The larger gap may bring up better performance on photovoltaic devices because of the "p-i-n" junctions.

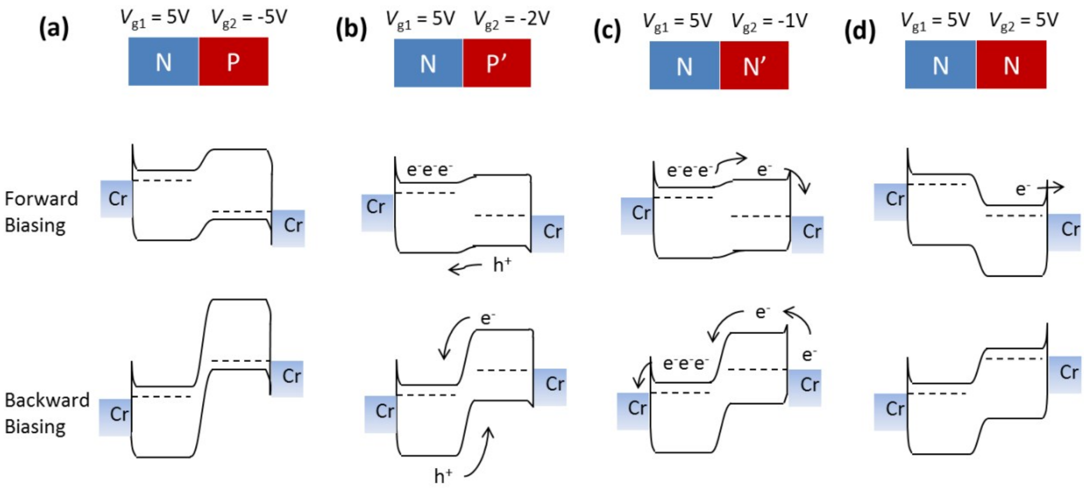

Figure S7. Band diagrams during the transition from "np" to "nn".

The metal Cr work function is around 4.5 eV. Electron affinity (χ) and band gap of $MoTe_2$ is around 3.8 eV and 1.0 eV, respectively (Appl. Phys. Lett. 2016, 108, 043503). According the band alignment of Cr and $MoTe_2$, we draw the band diagram of the device. Figure S7 shows the transition process from 'np' to 'pn', which is a very complex process. Here, we try to find a tentative explanation. At the start where V_{g1} = 5 V and V_{g2} = -5 V, the device forms a 'np' junction, which has the highest built-in electric field and consequently generate largest V_{th}. Since the right part of the device (p zone) has the highest hole density at V_{g2} = -5 V, the device owns the largest forward current. Meanwhile, for 'np' junctions, the backward current was almost constant, which determined by the minor carriers (semiconductor theory). When reducing the V_{g2}, both built-in electric field and hole density decreases. So we can see the RF and V_{th} decrease with the V_{g2} reducing up to -2V, as shown in Figure 3c and d. When further lowering V_{g2} to -1 V, the right part of the device was converted to 'n' type and a nn' was formed. At this time, since the right contact has a large Schottky Barrier and the right part has relatively low electron density, the backward current is almost same to np junction. However, the forward current becomes much larger than that of np junction. That is because the major carrier of the channel is electron. On one hand, the electron has much higher mobility than hole. On the other hand, the forward nn' junction generates current without the drifting and recombination process, happened in np junctions. SoIt can be observed the RF abruptly increased, shown in Figure 3c. Another thing should be noted that the band bending direction at the right contact becomes reversibly, as shown in Figure S7c. Here a contact barrier occurs at the right contact, so V_{th} also become larger than np'. That is seen in Figure 3d. When further increasing V_{g2} to 5 V, a nn junction was formed. RF further decreases. In spite that a sharp triangle barrier was formed at the right contact, however, tunneling easily happened. So V_{th} also decreases with the transition from n’ to n.