Supporting Information

Electrostatically tunable lateral MoTe$_2$ p-n junction for use in high-performance optoelectronics

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**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 ($6.1 \times 10^{-5}$ 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 $I_{\text{forward}}/I_{\text{reverse}}$ 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 2\( \mu \)m. (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.
The metal Cr work function is around 4.5 eV. Electron affinity ($\chi$) 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. So it 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’.

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

When further increasing $V_{g2}$ to 5 V, a nn junction was formed. RF further decreases.
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.