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Supplementary Information

Gate-Tunable Rectification and Photoresponse in a $MoTe_2/SnS_2$ Van der Waals Heterostructure P-N Diode.

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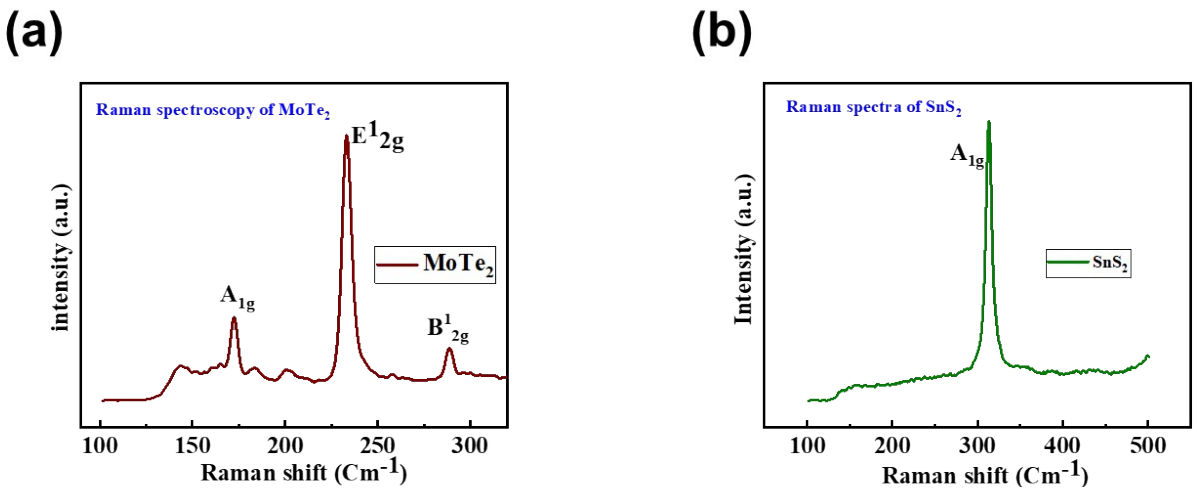

Figure S1: (a) Raman spectroscopy of $MoTe_2$. (b) Raman spectroscopy of SnS_2 flake. Two peaks can be seen in the Raman spectra of $MoTe_2$ at 173.33 cm^{-1}, 233.10 cm^{-1}, respectively. These peaks correspond to the out-of-plane vibrational mode A_{1g} and the in-plane vibrational mode E^1_{2g}, and the A_{1g} mode at 313.7 cm^{-1} corresponds to SnS_2.

We have evaluated approximately the band alignment of two materials $MoTe_2$ and SnS_2 by XPS. The peak positions are given as

Sn 3d5/2= 486.281 eV, **Sn 3d3/2**= 494.704 eV

S 2p3/2= 161.318 eV, **S 2p1/2**= 162.491 eV

Mo 3p5/2= 228.247 eV, **Te 3d5/2**= 572.870 eV

Mo 3p3/2= 231.397 eV, **Te 3d3/2**= 583.262 eV

The approximate valence band offset (VBO) of $MoTe_2$-SnS_2 is calculated using the energy difference among the core levels relative to the respective VBM of $MoTe_2$ and SnS_2. Hence the VBO of MoTe-SnS_2 can be evaluated by the formula [1].

$$\Delta E_v = \text{Energy of } MO3d_{5/2} - VBM_{MoTe2} + (\text{Energy of } Sn3d_{5/2} - \text{Energy of } Mo3d_{5/2}) - (\text{Energy of } Sn3d_{5/2} - VBM_{SnS2})$$

$$= 228.24 - 0.10 + (486.28 - 228.24) - (486.28 - 1.53) \approx \mathbf{1.43\ eV}$$

Based on VBO approximate data attained by XPS, we have calculated the conduction band offset (CBO) of MoT_2-SnS_2 by the following formula:

$$\Delta E_C = E_{gMoTe2} - \Delta E_v - E_{gSnS2}$$

$$\Delta E_C = 1.10eV + 1.43 - 2.28 \approx \mathbf{0.25eV}$$

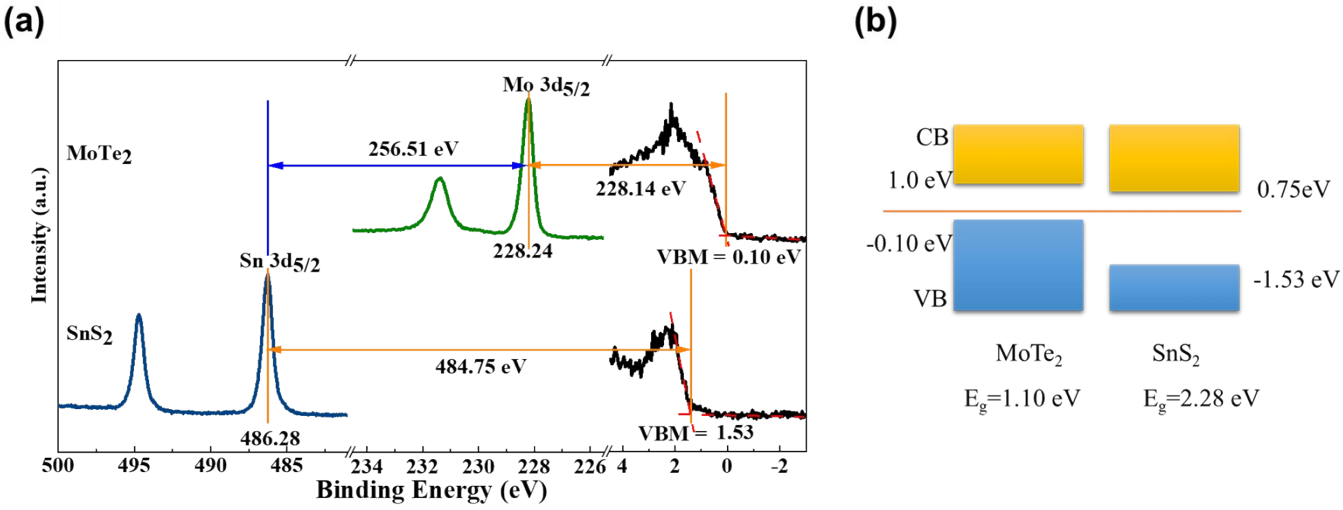

Figure S2: The distance between VBM and Mo $3d_{5/2}$ for $MoTe_2$, the distance between, VBM and Sn $3d_{5/2}$**.** (b) Band arrangement of $MoTe_2$-SnS_2 heterojunction.

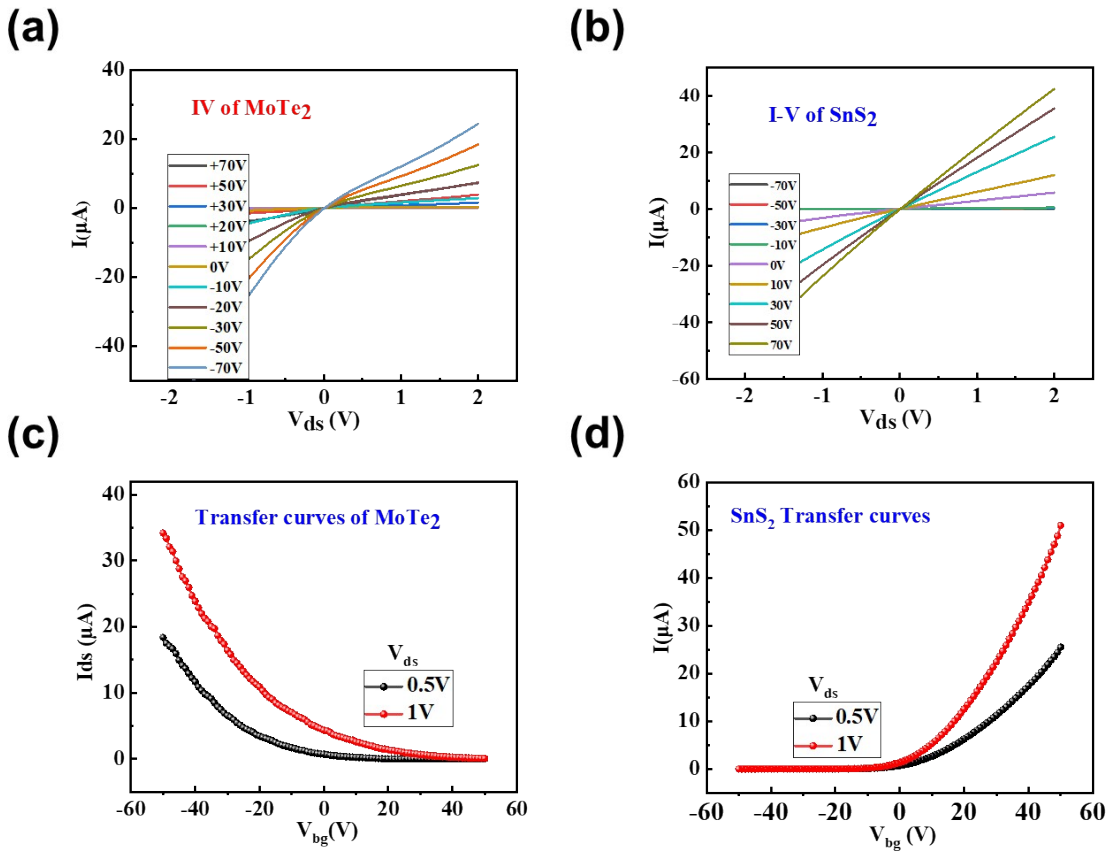

Figure S3: (a) I-V characteristics of $MoTe_2$ at various back gate voltages. (b) I-V characteristics of SnS_2 at various back gate voltages. (c) Transfer curves of $MoTe_2$ at V_{ds}=0.5 and 1V. (d) Transfer curves of SnS_2 at V_{ds}=0.5V and 1V.

Ideality factor calculation

The ideality factor was calculated for the forward-biased zone by fitting the logarithmic I-V characteristics to the Shockley diode equation.

$$I_D = I_S\left[exp\left(\frac{qV}{nk_BT}\right) - 1\right]$$

where I_D represents the diode current, I_S represents the reverse bias saturation current, V denotes the applied voltage, η symbolizes an ideality factor, T signifies temperature, q symbolizes

electronic charge, and k_B indicates Boltzmann's constant. For applied voltages larger than k_BT (e.g., > 0.1 V), the term "-1" in the preceding equation can be ignored.

$$\ln(I_D) = \ln(I_S) + \left(\frac{q}{nK_BT}\right)V$$

$$\eta = \frac{1}{Slope}\left(\frac{q}{K_BT}\right)$$

$$\eta = \frac{1}{Slope}\left(\frac{1.6 \times 10^{-16}C}{1.38 \times 10^{-23}JK^{-1} \times 300K}\right)$$

Slope= 30.82

$$\eta = \frac{38.6}{30.82} = 1.25 \quad \text{at } V_{bg}\text{=-30V}$$

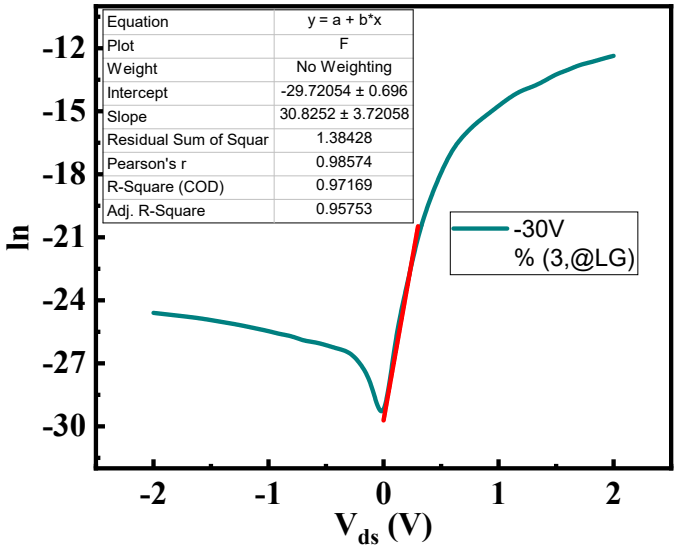

Figure S4: Ideality factor calculation at back gate voltage V_{bg}= -30V.

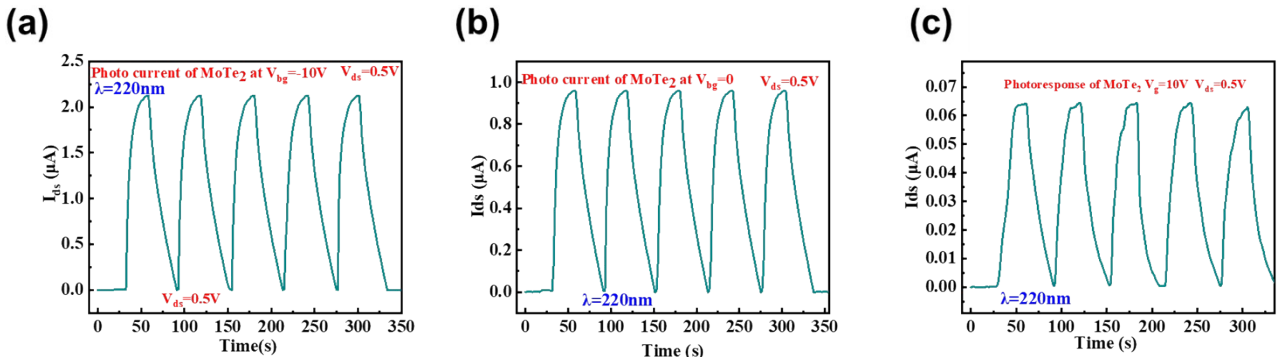

Figure S5: (a) Photocurrent of $MoTe_2$ with the light (DUV) at V_{bg}=-10V and V_{ds}=0.5V. (b) Photocurrent of $MoTe_2$ with the light (DUV) at V_{bg}=0V and V_{ds}=0.5V. (c) Photocurrent of $MoTe_2$ with the light (DUV) at V_{bg}=+10V and V_{ds}=0.5V.

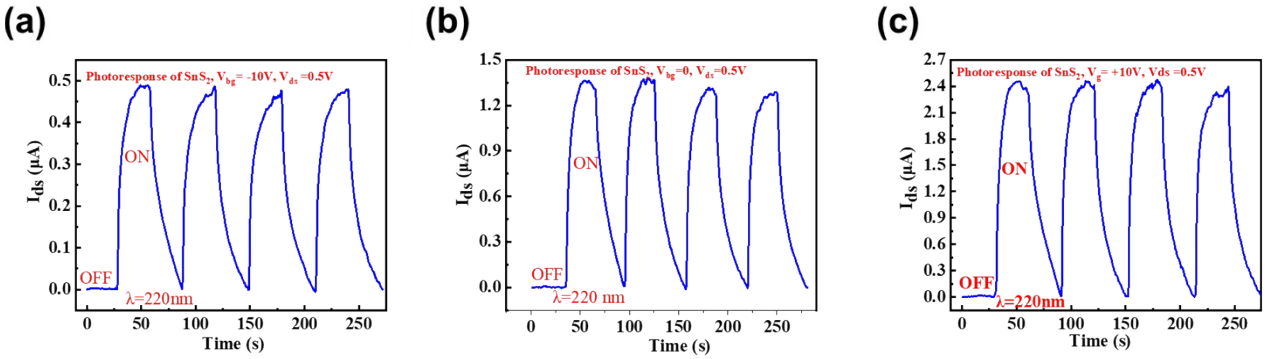

Figure S6: (a) Photocurrent of SnS_2 with the light (DUV) at V_{bg}=-10V and V_{ds}=0.5V. (b) Photocurrent of SnS_2 with the light (DUV) at V_{bg}= 0V and V_{ds} = 0.5V. (c) Photocurrent of SnS_2 with the light (DUV) at V_{bg}= +10V and V_{ds} = 0.5V.

By fitting the data collected using photocurrent, rising and decaying times were identified. **Figure S7** depicts the fitting of rise and decay times.

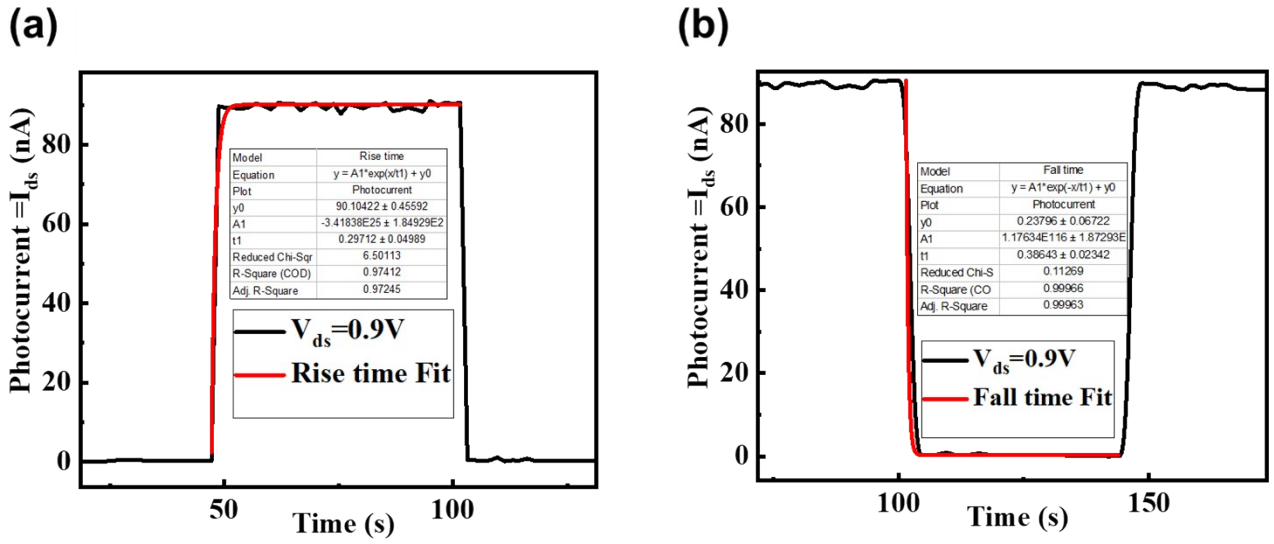

Figure S7: (a) The rise time for the photocurrent at V_{ds}=0.9V. (b) The fall time at V_{ds}=0.9V.

References

1. Kraut, E., et al., *Precise determination of the valence-band edge in x-ray photoemission spectra: application to measurement of semiconductor interface potentials.* Physical Review Letters, 1980. **44**(24): p. 1620.