Supplementary Information

Heterojunction Hybrid Devices from Vapor Phase Grown MoS_2

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MoS_2 thickness measurements using spectroscopic ellipsometry (SE)

Thickness measurements were conducted using an Alpha SE tool (J. A. Woollam Co., Inc.) operating in the wavelength range of 380 - 900 nm at an angle of incidence of 70 ° with a beam spot size of ~40 mm^2. SE data were analyzed using CompleteEASE 4.72 (J. A. Woollam Co., Inc.). The SE system gathered values of psi (Ψ) and delta (Δ) which represent the amplitude ratio (Ψ) and phase difference (Δ) between p- and s-polarizations, respectively. The two parameters are related to the ratio ρ, defined by the equation of $\rho = r_p/r_s = \tan(\Psi)\exp(i\Delta)$, where r_p and r_s are the amplitude reflection coefficients for the p-polarized and s-polarized light, respectively.[1] A four-layer optical model which consists of a Si substrate, an interface layer between Si and SiO_2, a SiO_2 layer and a MoS_2 layer was built to analyze the SE spectra, and a Tauc-Lorentz (T-L) oscillation model[2] was used to determine the thicknesses of the MoS_2 thin films.

Additional Raman analysis: Scanning Raman map

Raman maps were acquired from the MoS_2 film (~12 nm thick) transferred onto SiO_2 at a power of 250 µW by taking 100 × 100 spectra over a 25 × 25 µm area (10, 000 discrete spectra). Each spectrum had an acquisition time of 0.2 s.

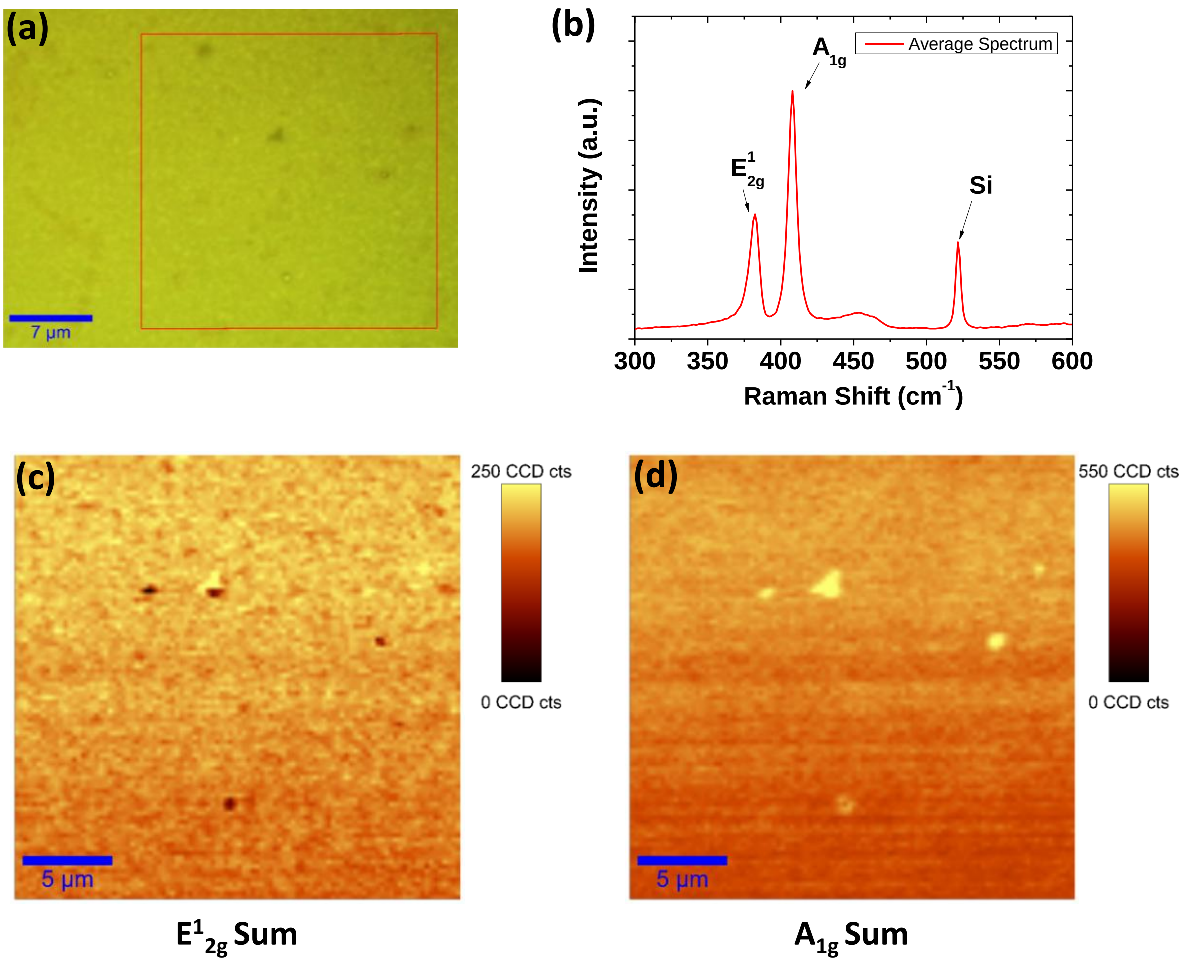
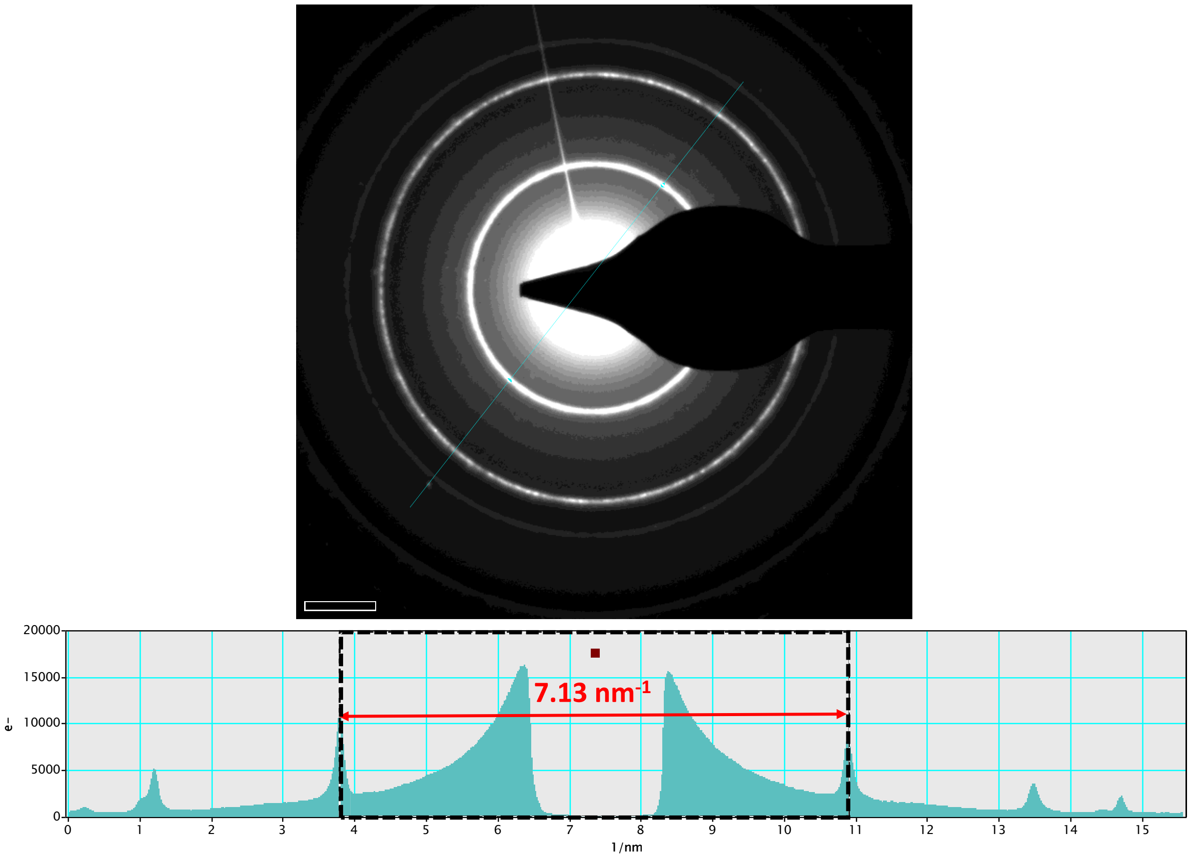


Figure S1. (a) Optical microscopy image of MoS_2 film transferred onto SiO_2. The red box indicates the 25 × 25 µm area over which Raman spectra were acquired. (b) Raman spectrum obtained by averaging over 10,000 discrete spectra which comprised the Raman map. Raman maps showing the intensity of the (c) E^1_{2g} and (d) A_{1g} peaks.

Selected area electron diffraction (SAED) patterns of the MoS_2 thin film

(a)



(b)

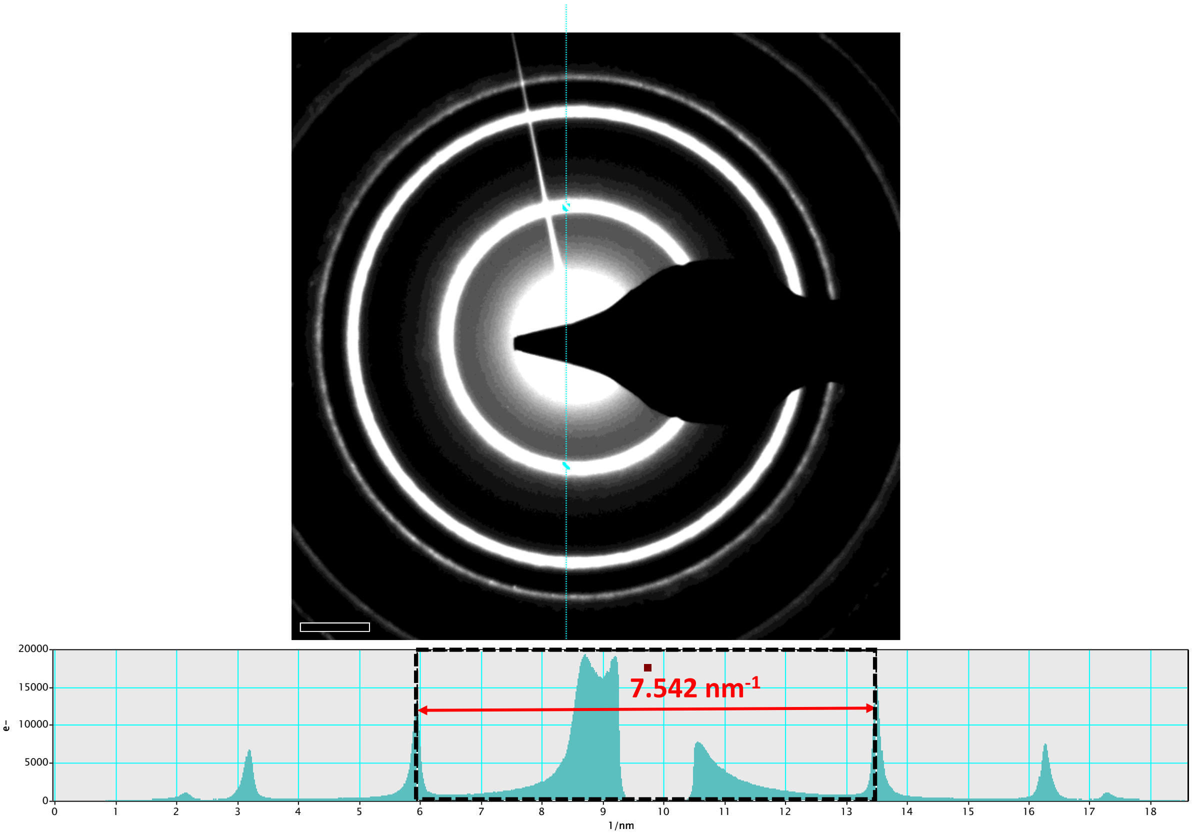


Figure S2. Representative electron diffraction patterns from different areas of the MoS_2 film revealing Mo-Mo lattice spacings of (a) 0.324 nm and (b) 0.306 nm, respectively.

Device preparation

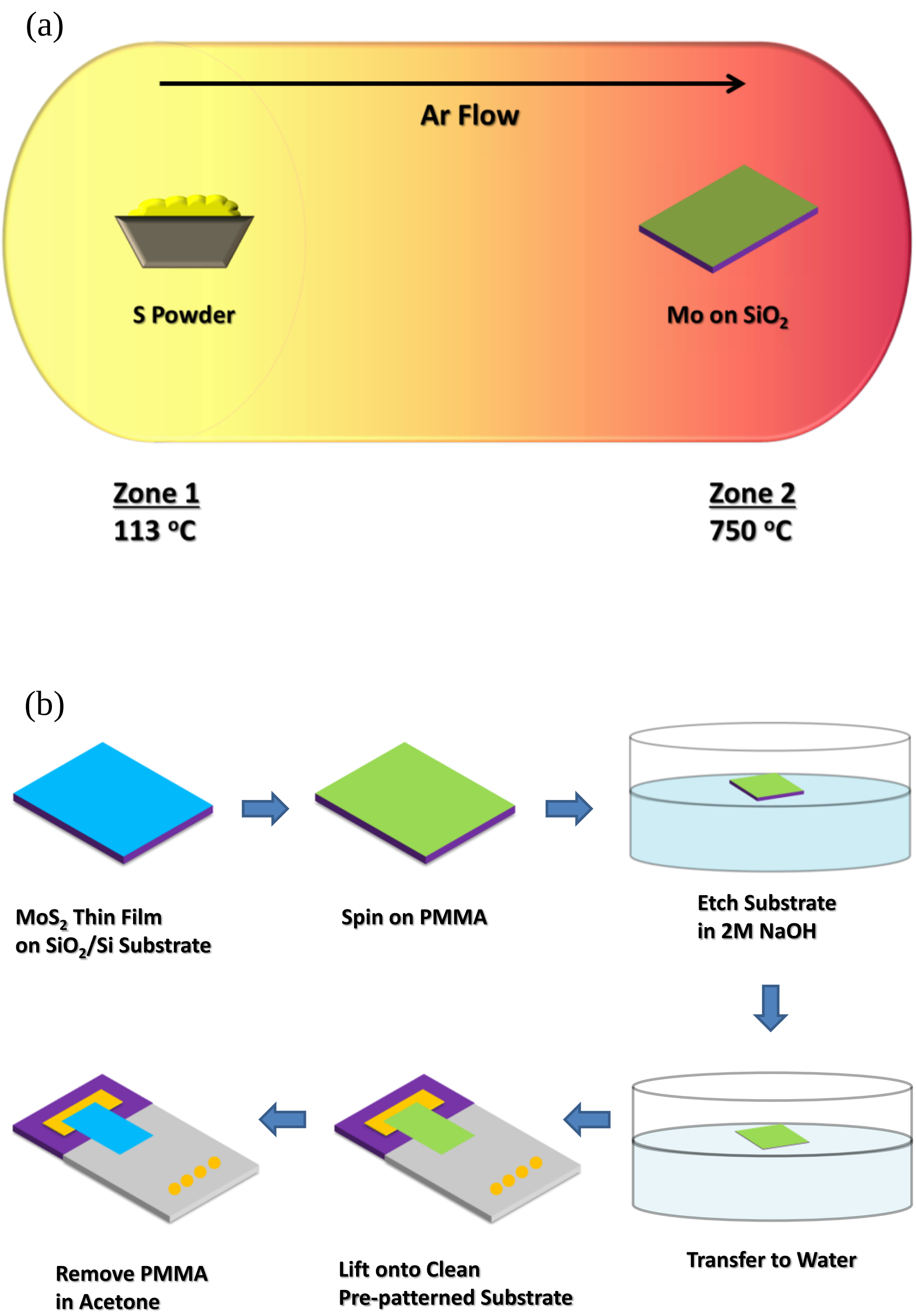


Figure S3. (a) Schematic diagram of the vapor phase sulfurization process. (b) Transfer process of as-grown MoS_2 thin films onto the pre-patterned substrate.

Diode parameter extraction from the *J-V* measurements of the MoS_2/p-Si diode

The forward *J-V* characteristics of a diode in dark conditions can be expressed using the flowing diode equation,

$$J = J_S[\exp\left(\frac{qV_D}{nk_BT}\right) - 1], \quad (1)$$

where J is the current density of the diode, V_D is the voltage drop across the junction, J_S is the reverse saturation current density, n is the ideality factor, k_B is the Boltzmann constant, q is the elementary charge and T is the absolute temperature in Kelvin. When the effect of series resistance (R_S), an additional secondary resistance component observed in the high forward bias region of practical diode devices, is taken into account, for $V_D > 3k_BT/q$, by replacing V_D with $V – JAR_S$, Eq (1) can be written as follows,

$$J = J_s \exp[\frac{q(V-JAR_S)}{nk_BT}], \quad (2)$$

where V is the total voltage drop across the series combination of the junction and R_S, and A is the effective contact area of the diode. This can be modified in terms of V and J and rewritten as the following equation.

$$V = JAR_S + \frac{nk_BT}{q}\ln\left(\frac{J}{J_S}\right), \quad (3)$$

Differentiating Eq. (3) in terms of J, we obtain

$$\frac{dV}{dJ} = AR_S + \frac{nk_BT}{qJ}. \quad (4)$$

According to Eq (4), dV/dJ is linearly proportional to $1/J$. Thus, the ideality factor ($n \geq 1$) of a diode, which represents how closely the diode follows ideal diode behavior and has a value of unity in the ideal case, and the series resistance, can be extracted by extrapolating the linear region of the plot of dV/dJ vs. $1/J$. The dV/dJ vs. $1/J$ plot of the 12.52 nm device is shown in

Figure S4, giving a series resistance value of 7.3 kΩ from the y-axis intercept and an ideality factor value of 1.68 from the slope.

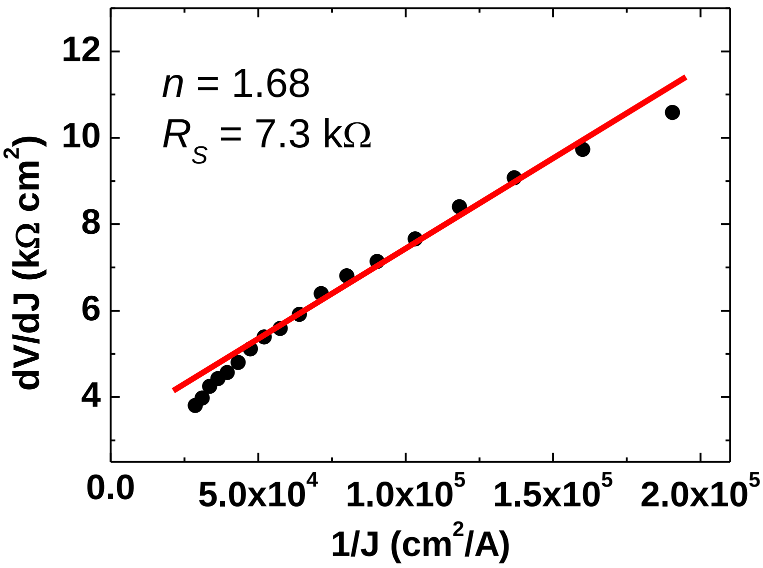
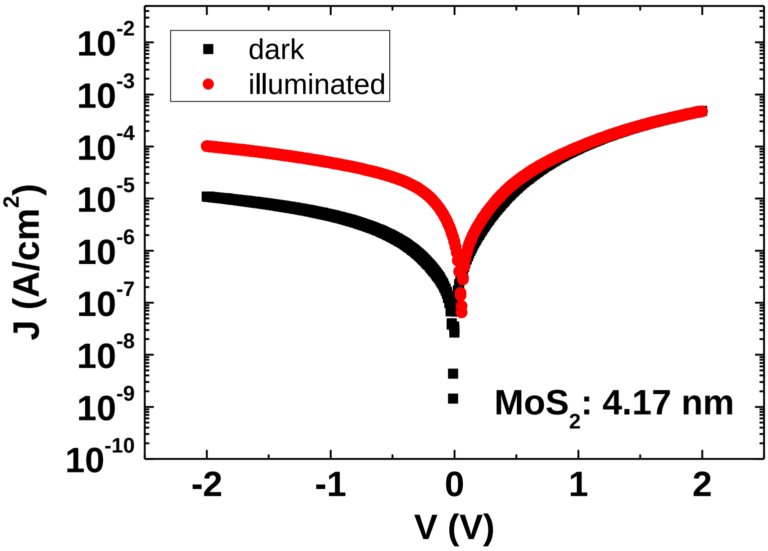


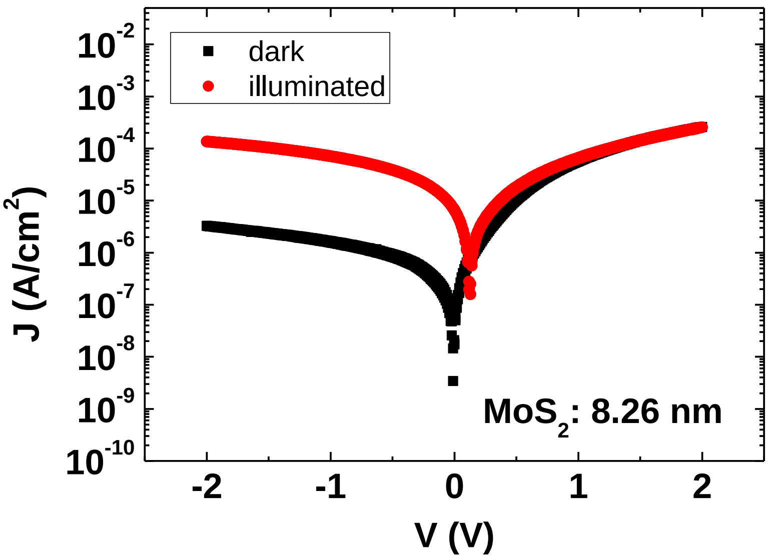
Figure S4. Plot of *dV/dJ* vs. *1/J* extracted from the *J-V* data of the diode with 12.52 nm thick MoS_2, giving a series resistance value of 7.3 kΩ and an ideality factor value of 1.68.

Additional *J-V* plots of the MoS_2/p-Si diode devices

(a)



(b)



(c)

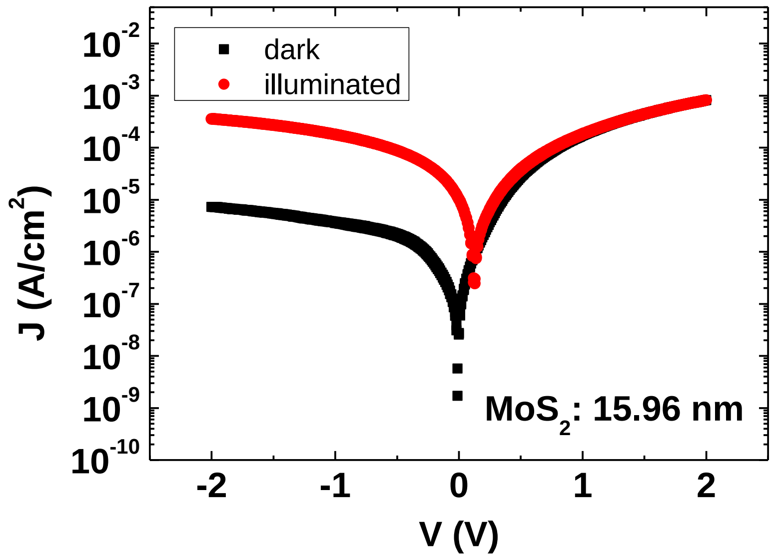


Figure S5. Semi-logarithmic *J*-*V* plots of the MoS_2/p-Si diode devices with MoS_2 film thickness of (a) 4.17 nm, (b) 8.26 nm, and (c) 15.96 nm in the dark and illumination (50 % of full intensity).

Additional data for the spectral response measurements

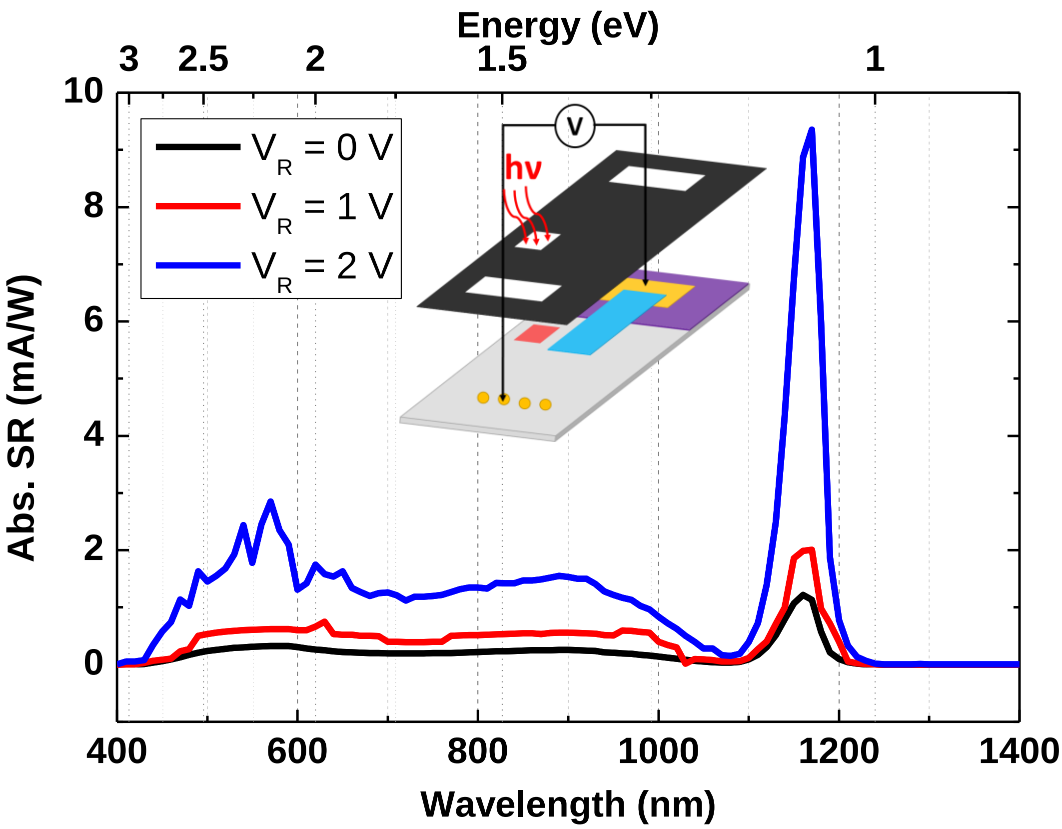


Figure S6. Absolute spectral response vs. wavelength (lower x-axis) and energy (upper x-axis) related to the diode device with an 8.26 nm thick MoS_2 film at zero bias and reverse bias (V_R) of 1 and 2 V with the mask opening on p-Si. The inner picture is a schematic diagram of the n-type MoS_2/p-Si heterojunction diode device with mask opening on p-Si.

References

1 Fujiwara, H. *Spectroscopic ellipsometry : principles and applications*. 81-87 (John Wiley & Sons Ltd, 2007).

2 Jellison, G. E. & Modine, F. A. Parameterization of the optical functions of amorphous materials in the interband region. *Appl. Phys. Lett.* **69**, 371 (1996).