Supporting information

Gate Tunable Photovoltaic Effect in MoS_2 vertical P-N Homostructures

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p-n junction (MoS_2:Nb – MoS_2:Fe): Gate dependent *J*-V_{SD} characteristics in the dark

The device shows gate-tunable rectification in the dark, see Figure S1. Since V_G acts similar to an effective bias voltage in respect to the modulation of the barrier height and the extent of the space charge region, the device is closer to breakdown at high V_G. The breakdown voltage is therefore reduced by a positive V_G. The Shockley model equations do not model the reverse breakdown which accounts for the deviation of the model from the data in reverse bias.

The inset shows the gate leakage-current for this particular device. The leakage current has been determined for all devices. Devices with leakage currents above 150 pA at V_G = 30 V or V_{SD}-dependent leakage were discarded.

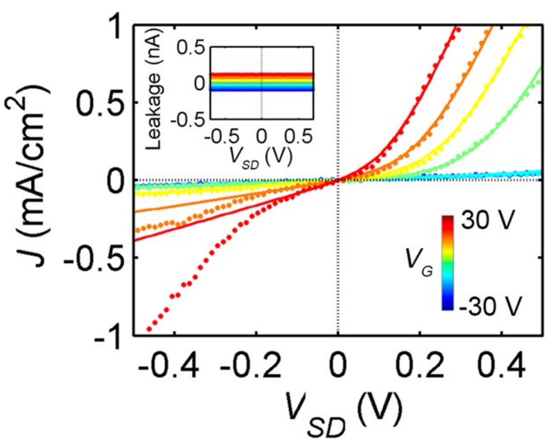

Figure S1. *J*-V_{SD} curves taken in the dark at V_G from +30 V to -30 V in 10-V steps. Experimental data is depicted as points and a Shockley-model-fit is overlaid. The inset shows the leakage-current to the gate electrode.

p-n junction (MoS_2:Nb – MoS_2:Fe): *J-V_{SD}* characteristics under illumination at high *V_{SD}*

Figure S2 shows *J*-V_{SD} curves at high V_{SD}. The current density *J* saturates at high positive bias V_{SD}. We attribute this to either Schottky barriers formed at the interface between the flakes and the metal leads or barriers forming in the direction parallel to the flake when moving away from the junction area toward the electrode contacting the MoS_2.[1] However, most relevant for photovoltaic applications is quadrant IV in which the effects of the leads are small, as discussed in the main text regarding Figure 3(c).

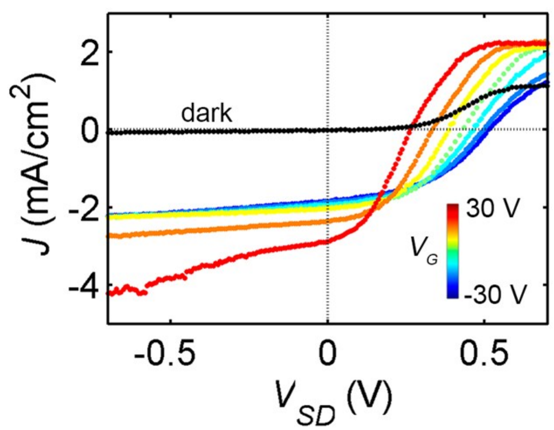

Figure S2. *J*-V_{SD} curves taken under illumination with 660 nm at 80 mW/cm² at gate voltages from +30 V to -30 V in 10-V steps (black: *J*-V_{SD} in the dark at V_G = 0 V).

The extent of the space charge region

In order to estimate the potential of substitutional Nb doping to generate ultra-thin MoS2 homojunctions we can calculate the extent of the space charge region for the doping level achieved. The nominal doping level of the p-MoS2 is 0.5% Nb. The actual concentration of dopant atoms has been estimated to be 0.4% from electron spectroscopy for chemical analysis (ESCA) measurements. The bulk electrical doping extracted from sheet resistance measurements is 3.0 x 10^{19}cm^{-3}. Using the total depletion approximation[2] the thickness x_p of the p-side of the p-n junction under equilibrium is given by

$$x_p = \sqrt{\frac{2\,\varepsilon_{MoS2}\varepsilon_0 V_{built-in} N_D}{q\,N_A\,(N_A + N_D)}}$$

where ε_{MoS2} is the relative permittivity of MoS_2 (11 from X. Chen et al.[3]), ε_0 is the permittivity of vacuum, q is the electron charge and N_A (N_D) is the acceptor (donor) density in the p (n) flake. $V_{built-in}$ is the built-in potential which can be calculated as $V_{built-in} = kT\,Ln(N_A N_D/n_i^2)$ where n_i is the intrinsic concentration (1.6 × 10^8 cm^{-3}, from S. Kim et al.[4]). As a limit, assuming that $N_D = N_A$, we obtain x_p = 5 nm.

p-n junction (MoS_2:Nb – native MoS_2)

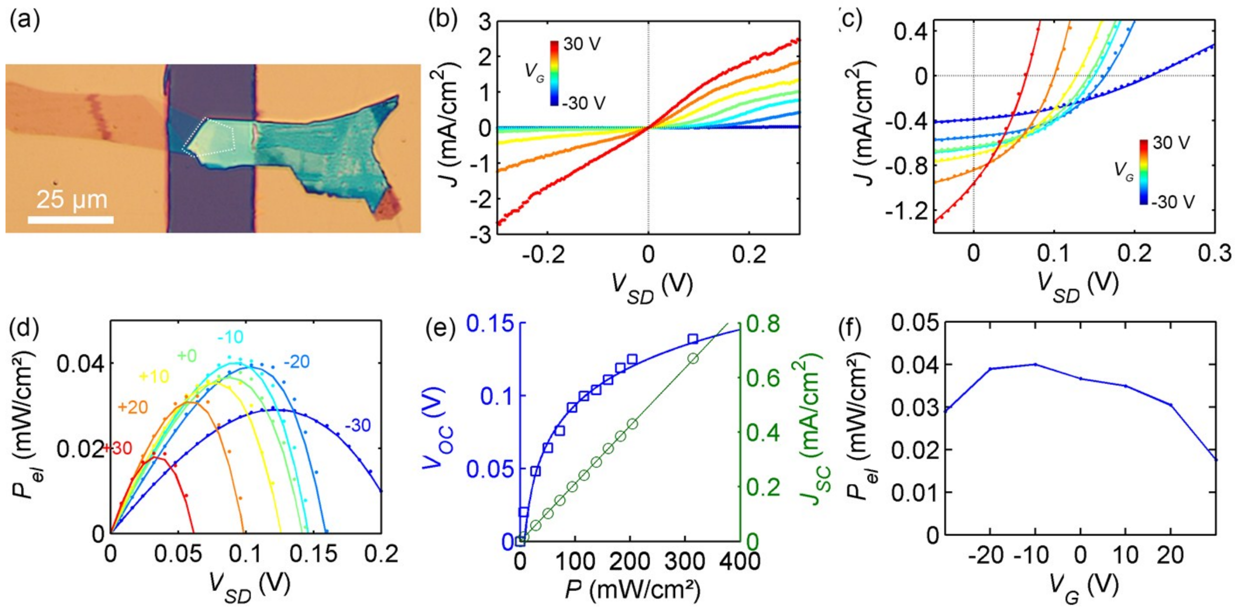

Figure S3. a) Optical image of the device. The dotted line indicates the junction area. b) J-V_{SD} curves taken in the dark and c) under illumination (λ = 660 nm, intensity 80 mW/cm²) with various V_G. Fits assuming a Shockley-diode are overlaid. d) Electrical power density P_{el} as a function of V_G. e) Logarithmic (and linear) power-dependence of V_{OC} (and I_{SC}) extracted from illumination power-dependent measurements. f) Gate-dependence of the electrical power P_{el}.

Gate dependence of dark current. Comparison to flakes

We have fabricated devices consisting of flakes of each of the three materials on 295 nm SiO_2/Si substrates with Au/Ti contacts. None of these devices exhibit a photovoltaic response. Therefore the photovoltaic response discussed in the main text originates indeed at the p-n junction and not at any other barrier, such as Schottky barriers at the contacts.

The gate dependences of the dark current in forward bias for single-flake devices are shown in figure S4. We find that the dark current across MoS_2:Nb decreases with V_G and it increases across the MoS_2:Fe and the native MoS_2 with V_G, confirming p- and n-doping. In our p-n junctions, we find the same qualitative gate dependence as in the n-type flakes. This indicates that the total conductance of the p-n junction is mostly influenced by the n-type flakes presumably due to their lower thickness.

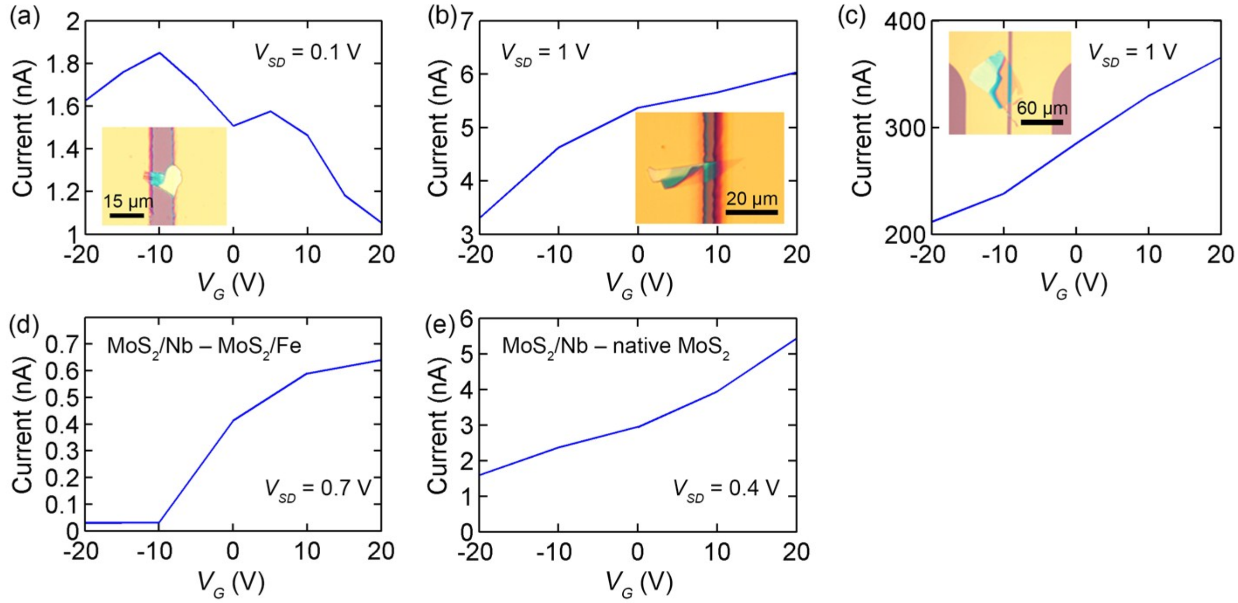

Figure S4. Gate dependence of dark current in forward bias conditions. a) MoS_2:Nb. b) MoS_2:Fe. c) Natural MoS_2. d) p-n junction, MoS_2:Nb.-MoS_2:Fe. e) p-n junction, MoS_2:Nb-natural MoS_2. The insets show optical images of the devices.

Additional IV-curve

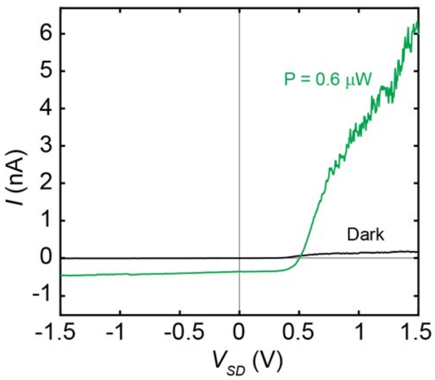

Figure S5. *I*-V_{SD} curves taken in the dark and under illumination (λ = 530 nm, intensity 6 μW) of device in Figure 6.

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