Solar-energy conversion and light emission in an atomic monolayer p–n diode

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1. I-V characteristic of WSe\(_2\) p–n junction diode in the dark

The Shockley diode equation relates the current \(I\) of a p–n junction to the bias voltage \(V\),

\[
I = I_s (e^{V/nV_T} - 1),
\]

where \(I_s\) is the saturation current, \(V_T\) is the thermal voltage (\(\approx 26\) mV at \(T = 300\) K), and \(n\) is the ideality factor. A more realistic diode model has to take a series resistance \(R_s\) – which in our device is associated with the metal/WSe\(_2\) contacts and the p- and n-doping regions – into account. An explicit equation for the diode current can then be obtained\(^1\) by using the Lambert \(W\)-function

\[
I = \frac{nV_T}{R_s} W\left(\frac{I_S R_s}{nV_T} e^{(V+I_S R_s)/nV_T}\right) - I_S.
\]

The model can reproduce our measurement \((V_{G1} = -40\) V, \(V_{G2} = 40\) V, blue line in Supplementary Figure 1a) over several orders of magnitude (solid black line), and we extract \(I_s = 0.02\) fA, \(n = 2.6\), and \(R_s = 95\) M\(\Omega\). For bias voltages below \(\approx 0.5\) V, the current falls below the noise floor of our measurement equipment (100 fA). For opposite gate biases \((V_{G1} = 40\) V, \(V_{G2} = -40\) V; Supplementary Figure 1b), we find a much larger resistance of \(R_s = 8\) G\(\Omega\). The diode parameters \(I_s\) and \(n\), however, are essentially the same \((I_s = 0.03\) fA, \(n = 2.6\)).

2. I-V characteristic of WSe\(_2\) p–n junction diode under optical illumination

Supplementary Figure 2a shows I-V characteristics of the p–n junction diode \((V_{G1} = -40\) V, \(V_{G2} = 40\) V) under optical illumination with power densities varied between 0 and 3000 W/m\(^2\). As described in the main text, a slope of the curves at short circuit is observed that can be modelled by a shunt resistance \(R_{SH}\). The I-Vs under optical illumination can be obtained from the equivalent circuit in the inset of Supplementary Figure 2a,

\[
I = I_S (e^{(V-I_S R_S)/nV_T} - 1) + \frac{V-I_S R_S}{R_{SH}} I_L,
\]

where \(I_L\) is the photocurrent, and \(R_s = 95\) M\(\Omega\), \(n = 2.6\), and \(I_s = 0.02\) fA, as deduced above.

**Supplementary Figure 1.** I-V characteristic of p-n junction diode under forward bias. Solid blue line: experimental data; solid black line: fit of diode equation with $R_S \neq 0$; dashed black line: fit of diode equation with $R_S = 0$. $R_S$ denotes the diode serial resistance. The noise floor of the measurement instrument is 100 fA (green dashed line). (a) $V_{G1} = -40$ V, $V_{G2} = 40$ V. (b) $V_{G1} = 40$ V, $V_{G2} = -40$ V.

By using the Lambert $W$-function, $I$ can again be written as an analytical expression of $V$

$$I = \frac{nV_T}{R_S} W\left(\frac{I_SM_R S}{R_S} e^{rac{I_S R_S (V+I_S R_S+I_M R_S) + nV_T (R_S+R_S)}} + \frac{V-I_S R_S - I_M R_S}{R_S+R_S}\right).$$

We fit this equation to the measurement data in Supplementary Figure 2a (dashed lines), extract $R_{SH}$, and plot the results in Supplementary Figure 2b (green symbols). In the same figure we plot the quantity $R_{CH} = V_m/I_m \approx V_{OC}/I_{SC}$, which is the characteristic resistance of the solar cell (blue symbols). The influence of the shunt on electrical output power can be determined by calculating the power in the absence of $R_{SH}$ minus the power loss in the shunt,

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\( P_{el} \approx V_m I_m - \frac{V_m^2}{R_{SH}} \). A similar analysis for \( R_S \) yields \( P_{el} \approx V_m I_m - I_m^2 R_S \). In the presence of both series and shunt resistance, we thus obtain for the fill factor of the solar cell

\[
FF \approx FF_{ideal} \left(1 - \frac{R_{CH}}{R_{SH}}\right) \left(1 - \frac{R_S}{R_{CH}}\right).
\]

From Supplementary Figure 2c, in which we plot the quantities \( R_S/R_{CH} \) and \( R_{CH}/R_{SH} \), it becomes apparent that recombination losses (described by \( R_{SH} \)) severely reduce the fill factor by \( \approx 40 \% \), whereas resistive losses (\( R_S \)) at the contacts are negligible (< 0.5 %).

Supplementary Figure 2. (a) I-V characteristic of p-n junction diode (\( V_{G1} = -40 \) V, \( V_{G2} = 40 \) V) under optical illumination. Solid blue lines: experimental data; dashed green lines: theoretical fits. Inset: Equivalent circuit model of a photovoltaic solar cell. (b) Optical power dependence of characteristic resistance \( R_{CH} \) and shunt resistance \( R_{SH} \) (extracted from (a)). (c) Normalized series (\( R_S/R_{CH} \)) and shunt (\( R_{CH}/R_{SH} \)) resistances, describing dissipation and recombination losses, respectively.
3. Device operation as photoconductor

When operated as n- or p-type resistor (see Supplementary Figures 3a and b, respectively), the device shows a photoconductive response. We find responsivities $R_V = \Delta V / P_{opt}$ of $>10^7$ V/W for both n- and p-type conduction. In accordance with previous work\(^3\) on MoS\(_2\), we attribute the optical response to photoexcited carriers, trapped in the WSe\(_2\) or the WSe\(_2/\)Si\(_3\)N\(_4\)-interface, that cause additional gating of the channel and thus influence the resistance of the device.

![Supplementary Figure 3](image-url)

Supplementary Figure 3. Device operation as (a) n-type ($V_{G1} = V_{G2} = 40$ V) and (b) p-type ($V_{G1} = V_{G2} = -40$ V) photoconductor ($P_{opt} = 9$ nW). Solid lines: in the dark; dashed lines: with illumination.

4. Estimation of optical absorption and collection efficiency

The optical absorption in monolayer WSe\(_2\) is estimated by integration of the absorption spectrum\(^4\) over the wavelength range of the halogen lamp in Supplementary Figure 4. Standing wave effects in the device are neglected. The so obtained absorption is $\approx 5\%$.


The electroluminescence collection efficiency $\eta_{\text{coll}}$ is estimated from the transmission $T$ of all optical components in the beam path (microscope objective, cryostat window, beamsplitter, fiber coupler, etc.) and the integral over the collection angle defined by the numerical aperture $NA$ of the objective lens

$$\eta_{\text{coll}} = \frac{T}{4\pi} \int_0^{2\pi} d\phi \int_0^{\arcsin(NA)} \sin(\Theta) d\Theta.$$ 

Modifications of the emission pattern due to the substrate and the electrodes are neglected.

5. **Emission spectrum of halogen lamp**

![Emission spectrum of halogen lamp](image)

*Supplementary Figure 4.* Emission spectrum of halogen lamp.