Modeling a planar perovskite solar cell with SolarPVsoft

Here we show how you can use **SolarPVsoft**, to simulate/replicate the current-voltage (JV) curve of a solar cell. We focus on a perovskite solar cell with a mixed composition (RbCsMAFAPbIBr) in planar configuration:¹



The experimental device used as target has an active layer thickness of approximately 500 nm and an optical band gap of 1.62 eV. Under simulated sunlight (AM1.5G) at 100 mW/cm² it yields a short-circuit photocurrent of 19.14 mA/cm² and an open-circuit photovoltage of 1.07 V. The JV curve shown above was measured with a mask of 0.14 cm² (the geometrical active area is 0.16 cm²)

We first use the **diode equation functionality**. Check out the <u>theoretical background</u> and the <u>application help</u> for more information.

We start with a simple calculation without using parasitic resistances:

| Dark Saturation Current (A/cm ²) | Light Generated Current (A/cm ²) | Ideality Factor | Temperature (K) |
|--|--|---|---------------------|
| 2e-11 | 0.019 | 2 | 300 |
| Regular calculation or Resistances | Series Resistance (Ohm*cm ²) | Shunt Resistance (Ohm/cm ²) | Initial voltage (V) |
| NORMAL | 0 | 1e6 | 0.0 |
| Final voltage (V) | Step voltage (V) | Captcha | |
| 1.1 | 0.01 | IDPY | |
| | | | |
| | | | |
| Calculate Cancel | | | |
| | | | |

Calculation results

Jsc: 18.99 mA/cm2 Max. Power: 16.453 mW/cm2 at 0.920 V, 17.88 mA/cm Efficiency: 16.4 %

Please click on the following link if you would like to know more about the physics applied to this functionality: Theoretical Background



Note that we have fixed the ideality factor to 2 (a typical value for perovskite solar cells in that configuration)^{2–4} and adjusted the saturation current to fit the experimental open-circuit photovoltage (the lower this parameter the larger the V_{oc} , because the recombination rate is lower)

The predicted curve has a fill factor much larger than in the experiment. This is because parasitic resistances are not considered. We can go back in the simulation (press the "keep the same values button") and use consecutively different values of the series and shunt resistances until you get a good match with the experiment. Note that now the input fields of series and Shunt resistance are not blocked/shadowed anymore, and it is possible to change the numerical values. Here the final result of that search:

| Park Saturation Current (A/cm ²) | Light Generated Current (A/cm ²) | Ideality Factor | Temperature (K) |
|--|--|---|---------------------|
| 2e-11 | 0.019 | 2 | 300 |
| | | | |
| legular calculation or Resistances | Series Resistance (Ohm*cm ²) | Shunt Resistance (Ohm/cm ²) | Initial voltage (V) |
| RESISTANCES | 7 | 500 | 0.0 |
| inal voltage (V) | Step voltage (V) | Captcha SDPY | |
| 1.1 | 0.01 | 1000-1-200 | |
| | | | |
| | | | |
| Calculate Cancel | | | |
| Galealate | | | |



In this graph, there is a summary of several simulations, together with the experimental results:



We now move on to the **drift-diffusion simulation** functionality. Check out the <u>theoretical</u> <u>background</u> and the <u>application help</u> for more information.

We start with the "basic form". First, we need to input known values such as the thickness, the band gap and the dielectric constant. We also need to specify the absorption coefficient file and the illumination intensity. The file should be provided by the user with the format specified in the <u>application help</u>.

In this particular example we used the datafile that comes as an example and that can be straightforwardly downloaded from the app website. This is the result for the time-dependent photocurrent for an applied voltage of 0 V:

| kness in microns | Eg in eV | Illumination intensity in Suns | WHITE-light or MONOCHROMATIC? |
|--|---|--|---|
| | 1.62 | 0.86 | WHITE |
| | | | |
| le | Abs coeff 1/m | Dielectric constant | External voltage (V) - "Initial value" |
| ninar Abs_example.txt | 5.7e6 | 24.1 | 0.0 |
| | | | 1011000000 |
| | External voltage (V) - "Final value" | External voltage (V) - "Step value" | Captcha basic 2002 |
| t one value of voltage | 1.0 | 0.1 | |
| | | | |
| ulate Cancel | | | |
| | | | |
| Calculation | n results | | |
| | | | |
| | | | |
| Final current Jn = 19.18 mA/ | cm2; for bias = 0.0 V | | |
| | | | |
| Final current Jp = 19.18 mA/ | cm2; for bias = 0.0 V | | |
| | 'cm2; for bias = 0.0 V | | |
| ECCE = 99.8 % | icm2; for bias = 0.0 V | | |
| | cm2; for bias = 0.0 V | | |
| ECCE = 99.8 % | cm2; for bias = 0.0 V | | |
| ECCE = 99.8 % IPCE = 71.4 % | cm2; for bias = 0.0 V wing link if you would like to know more | e about the physics applied to this fu | inctionality: <u>Theoretical Background</u> |
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| ECCE = 99.8 % IPCE = 71.4 % Please click on the follo | | e about the physics applied to this fι | inctionality: <u>Theoretical Background</u> |
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| ECCE = 99.8 % IPCE = 71.4 % Please click on the follow Chart Chart Curvey of the follow Chart Curvey of the follow Curvey of | wing link if you would like to know mor | | Inctionality: <u>Theoretical Background</u> |

Note that the illumination intensity (0.86 suns in this case) was adjusted to match the experimental value. Once we have this, we can run the full IV curve by choosing "Curve IV simple" in the form:

| I-Thickness in microns | Eg in eV | Illumination intensity in Suns | WHITE-light or MONOCHROMATIC? |
|--------------------------|--------------------------------------|-------------------------------------|--|
| 0.5 | 1.62 | 0.86 | WHITE |
| Abs File | Abs coeff 1/m | Dielectric constant | External voltage (V) - "Initial value" |
| Examinar Abs_example.txt | 5.7e6 | 24.1 | 0.0 |
| \frown | External voltage (V) - "Final value" | External voltage (V) - "Step value" | Captcha basic 1924 |
| Curve IV simple | 1.1 | 0.1 | |

Calculation results

Jsc: 19.18 mA/cm2 Max. Power: 18.101 mW/cm2 at 1.0 V, 18.10 mA/cm2 Efficiency: 21.0 % Negative current not reached out! Voc and Fill Factor cannot be calculated

Please click on the following link if you would like to know more about the physics applied to this functionality: Theoretical Background

Chart

Please take into account that: Results depend on the chosen voltage precision to calcula



Note that the current parameters predict a too high value of the V_{oc} (even beyond the selected voltage range). This is because the default values of the drift-diffusion model are not adequate in this case.

To correct that we can move to the "advanced" form. Using previous published work⁵ we can work with more "realistic" parameters for diffusion coefficients and lifetimes. Here a set that works pretty well:

| d-Thickness in microns | nx-discretization points | nt-time steps (adim) | dt-time increment (adim) |
|-------------------------------------|---|-------------------------------|---|
| 0.5 | 100 | 1000000 | 1e-5 |
| nnc- states/m ³ | nnv- states/m ³ | Eg in eV | Electron diff cte m ² /s |
| 3.97e24 | 3.97e24 | 1.62 | 5e-5 |
| Holes diff cte m ² /s | Illumination intensity in Suns | WHITE-light or MONOCHROMATIC? | Abs File |
| 5e-5 | 0.9 | WHITE | Examinar Abs_example.txt |
| Holes lifetime in seconds | External voltage (V) - "Initial value" | | External voltage (V) - "Final value" |
| Poles lifetime in seconds 2e-8 | External voltage (V) - "Initial value" 0.0 | Curve IV simple | External voltage (V) - "Final value" 1.1 |
| External voltage (V) - "Step value" | Screened Field | Captcha advanced ZGQP | |
| 0.03 | Screened Field | -747.82% (A | |
| | | | |
| Calculate Cancel | | | |
| | | | |

This is the transient current a 0V:



Note that for this set of parameters the electron collection efficiency (ECCE) is close to 100%. This would be the internal quantum efficiency of the device if no other losses (apart from optical losses) are affecting the solar cell. This is the result for the full JV curve:



In the next graph we show a summary of all results obtained with **SolarPVsoft** for the modelling of this solar cell:



A few comments:

- The drift-diffusion model with electron/hole lifetimes that fit the experimental V_{oc} and effective illumination that fits the J_{sc} yields the same results as the diode equation with $n_{id} = 2$. This is not surprising⁴ as the dominant recombination mechanism in the model is SRH recombination (see the <u>theoretical background</u>)
- It is well-known that the ions determine the photovoltaic response of a perovskite solar cell. The model used in **SolarPVsoft** is very simple and only considers electrons and holes. However, one can analyze indirectly the effect of the ions via the boundary conditions. The default case is "screened field", meaning that there is concentration of ions which is high enough to cancel the electric field within the active layer. The opposite case if the "no screened field", where the electric field is only determined by the electronic properties of the material.
- Comparison of the "screened" and "no screened" results gives us an idea of how important the effect of the ions could be. Ions tend to accumulate at the interfaces and reduce the applied electric field.⁵ As observed, this is mainly affecting the *V*_{oc}.
- Finally, we notice that parasitic resistances are not considered in the drift-diffusion model in the current version of **SolarPVsoft**. You need to use the diode equation utility to estimate the impact of parasitic resistances in your device.

References

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