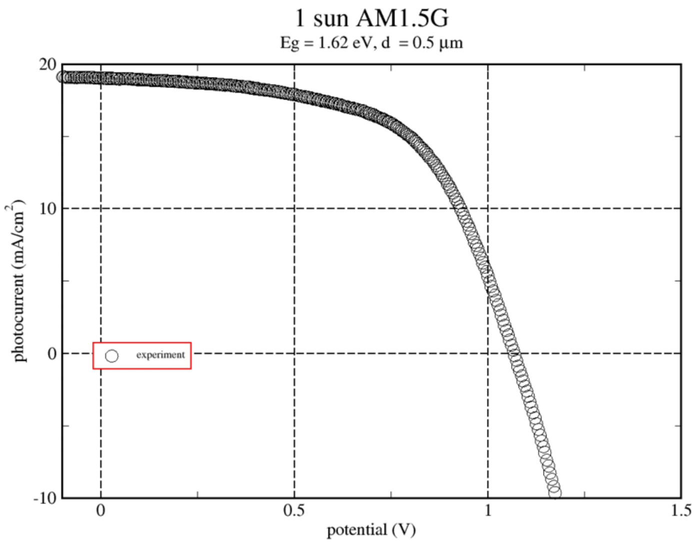
Modeling a planar perovskite solar cell with SolarPVsoft

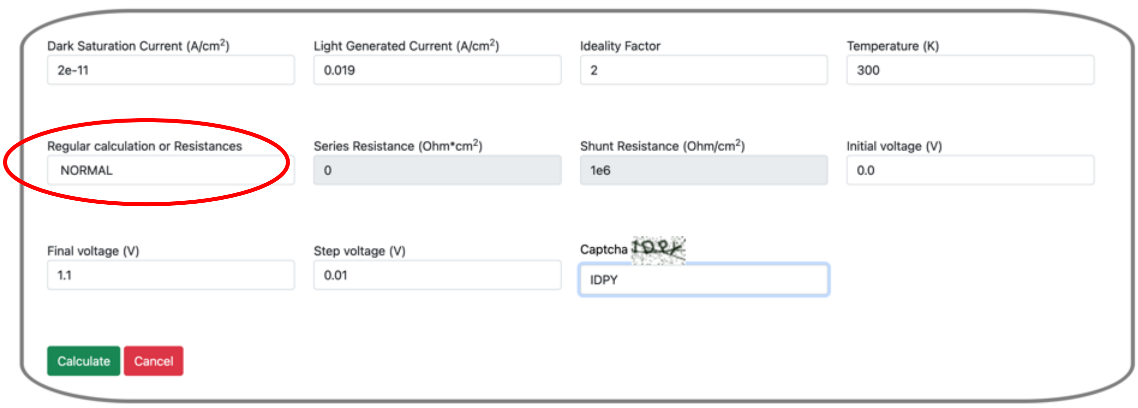
Here we show how you can use **SolarPVsoft**, to simulate/replicate the current-voltage (JV) curve of a solar cell. We focus on a perovskite solar cell with a mixed composition (RbCsMAFAPbIBr) in planar configuration:[1]



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/cm^2 it yields a short-circuit photocurrent of 19.14 mA/cm^2 and an open-circuit photovoltage of 1.07 V. The JV curve shown above was measured with a mask of 0.14 cm^2 (the geometrical active area is 0.16 cm^2)

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

We start with a simple calculation without using parasitic resistances:



Calculation results

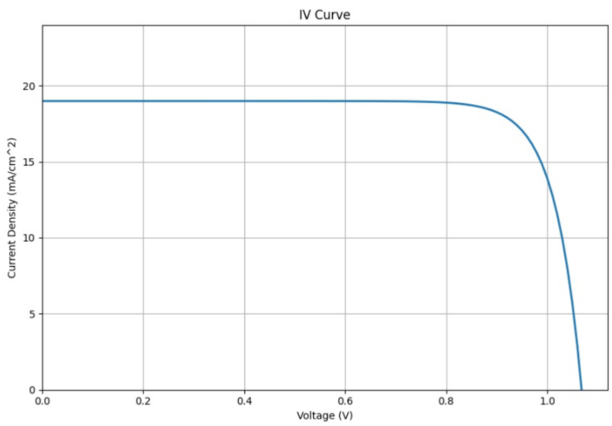
Jsc: 18.99 mA/cm2

Max. Power: 16.453 mW/cm2 at 0.920 V, 17.88 mA/cm²

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

Chart

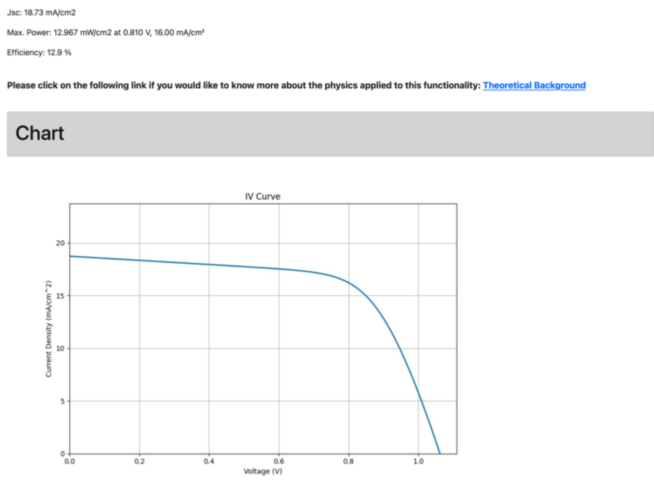


Note that we have fixed the ideality factor to 2 (a typical value for perovskite solar cells in that configuration)[2–4] and adjusted the saturation current to fit the experimental open-circuit photovoltage (the lower this parameter the larger the V_{oc}, because the recombination rate is lower)

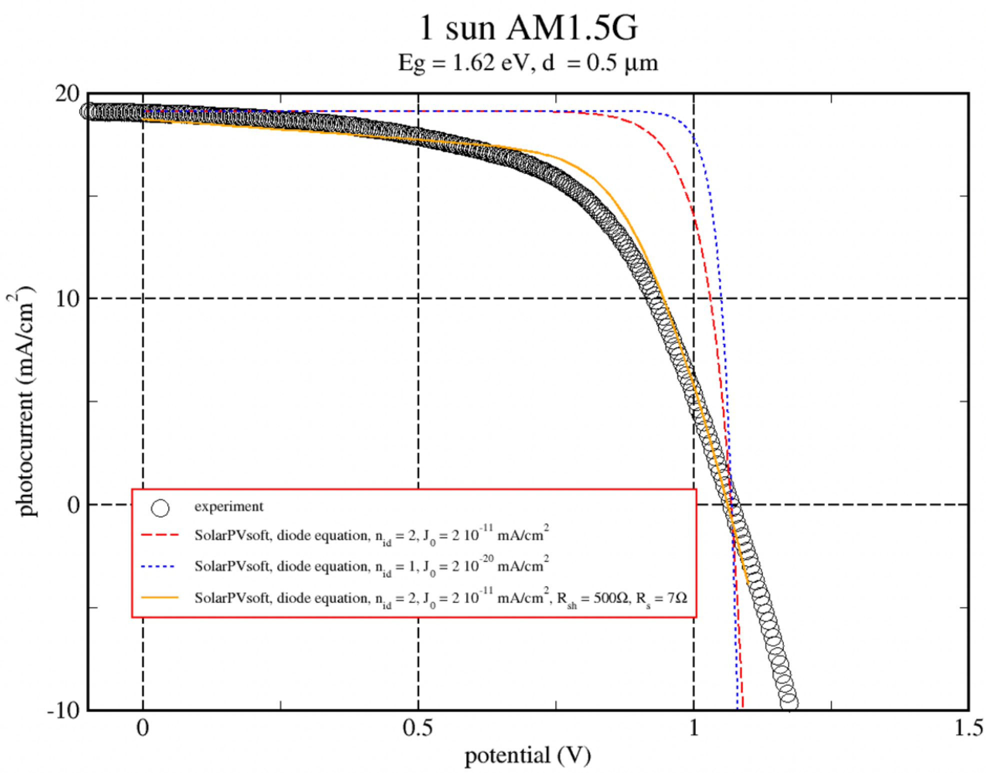
The predicted curve has a fill factor much larger than in the experiment. This is because parasitic resistances are not considered. We can go back in the simulation (press the "keep the same values button") and use consecutively different values of the series and shunt resistances until you get a good 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:


Dark Saturation Current (A/cm²): 2e-11
Light Generated Current (A/cm²): 0.019
Ideality Factor: 2
Temperature (K): 300
Regular calculation or Resistances: RESISTANCES
Series Resistance (Ohm*cm²): 7
Shunt Resistance (Ohm/cm²): 500
Initial voltage (V): 0.0
Final voltage (V): 1.1
Step voltage (V): 0.01
Captcha

Calculate Cancel



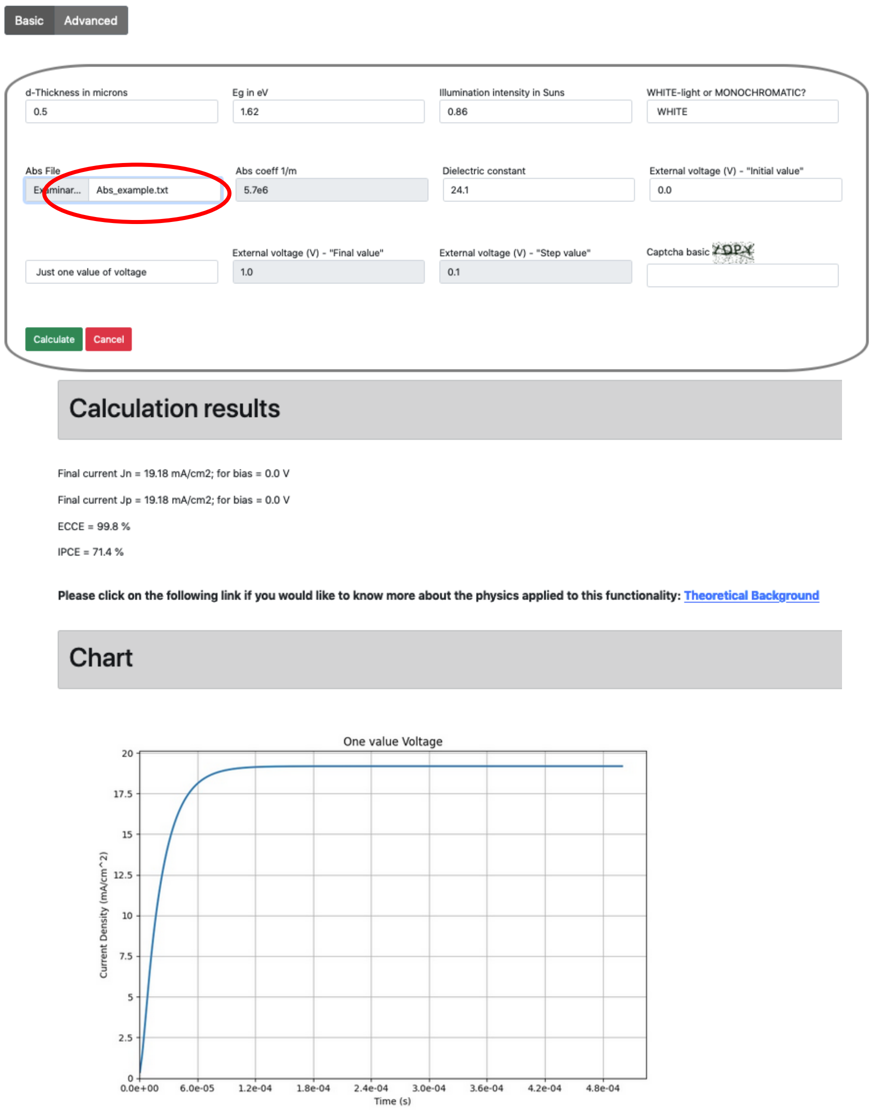
In this graph, there is a summary of several simulations, together with the experimental results:



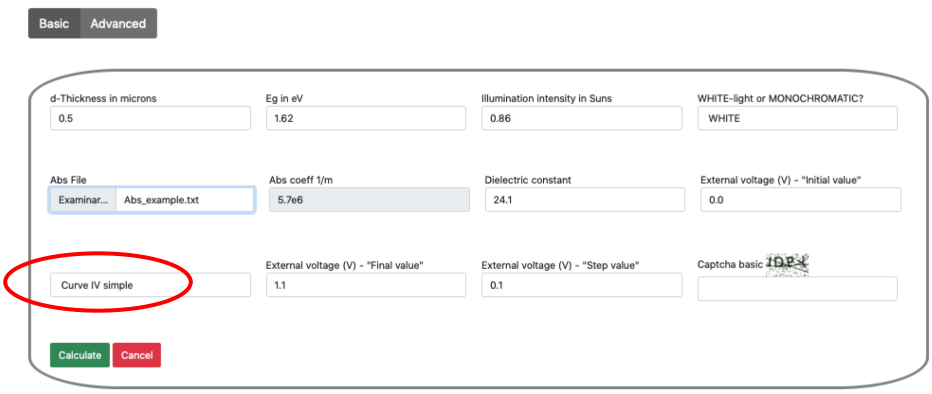
We now move on to the **drift-diffusion simulation** functionality. Check out the theoretical background and the application help for more information.

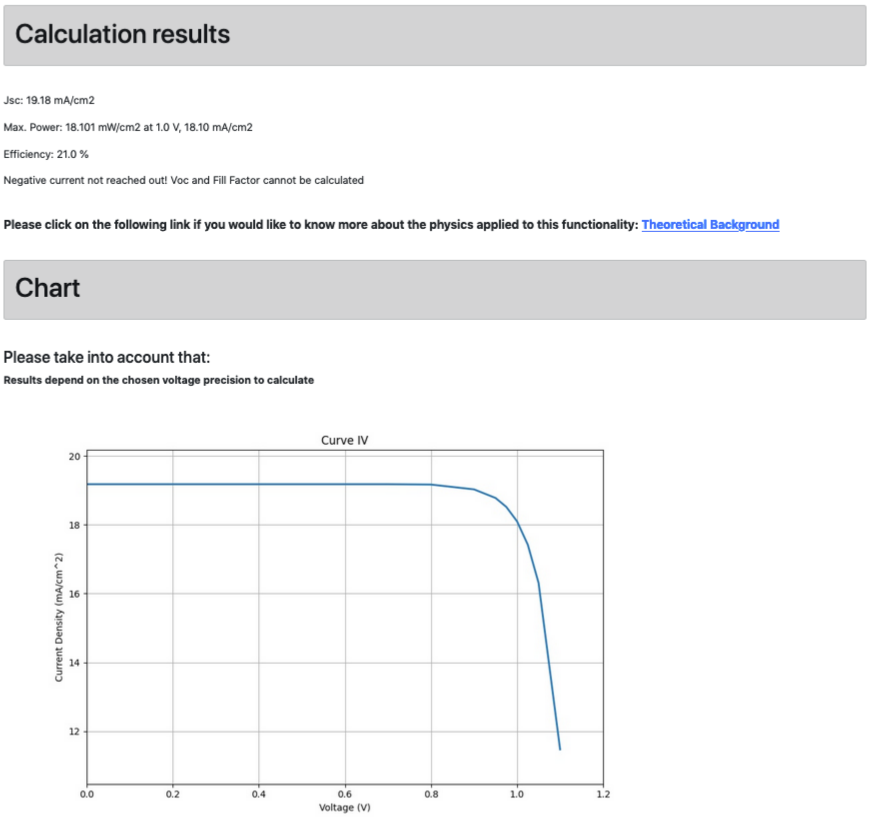
We start with the "basic form". First, we need to input known values such as the thickness, the band gap and the dielectric constant. We also need to specify the absorption coefficient file and the illumination intensity. The file should be provided by the user with the format specified in the application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

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:



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:



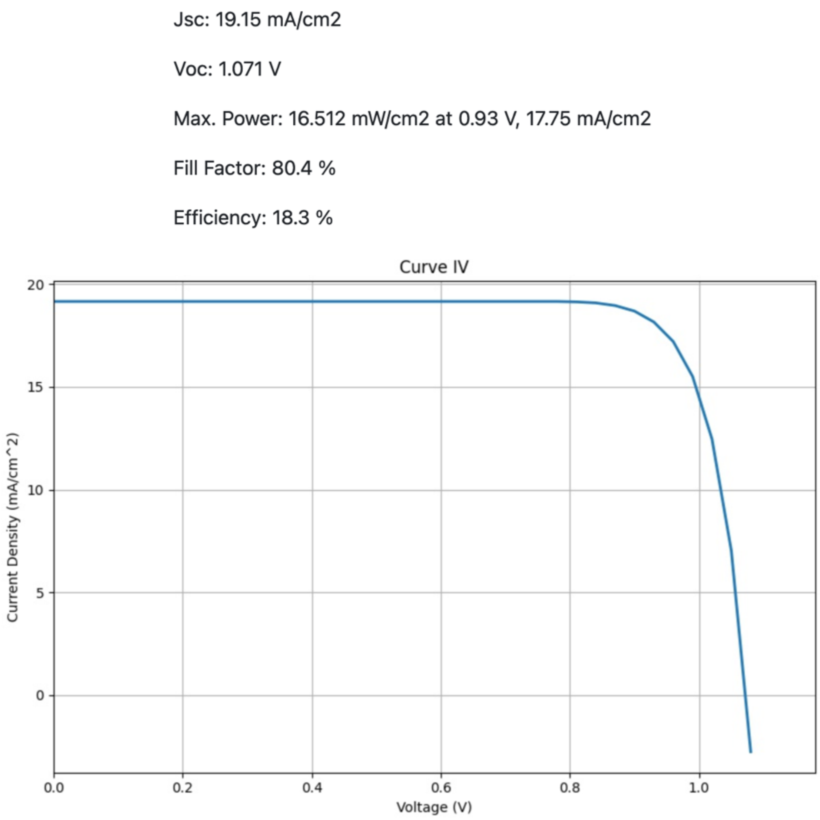


Note that the current parameters predict a too high value of the V_{oc} (even beyond the selected voltage range). This is because the default values of the drift-diffusion model are not adequate in this case.

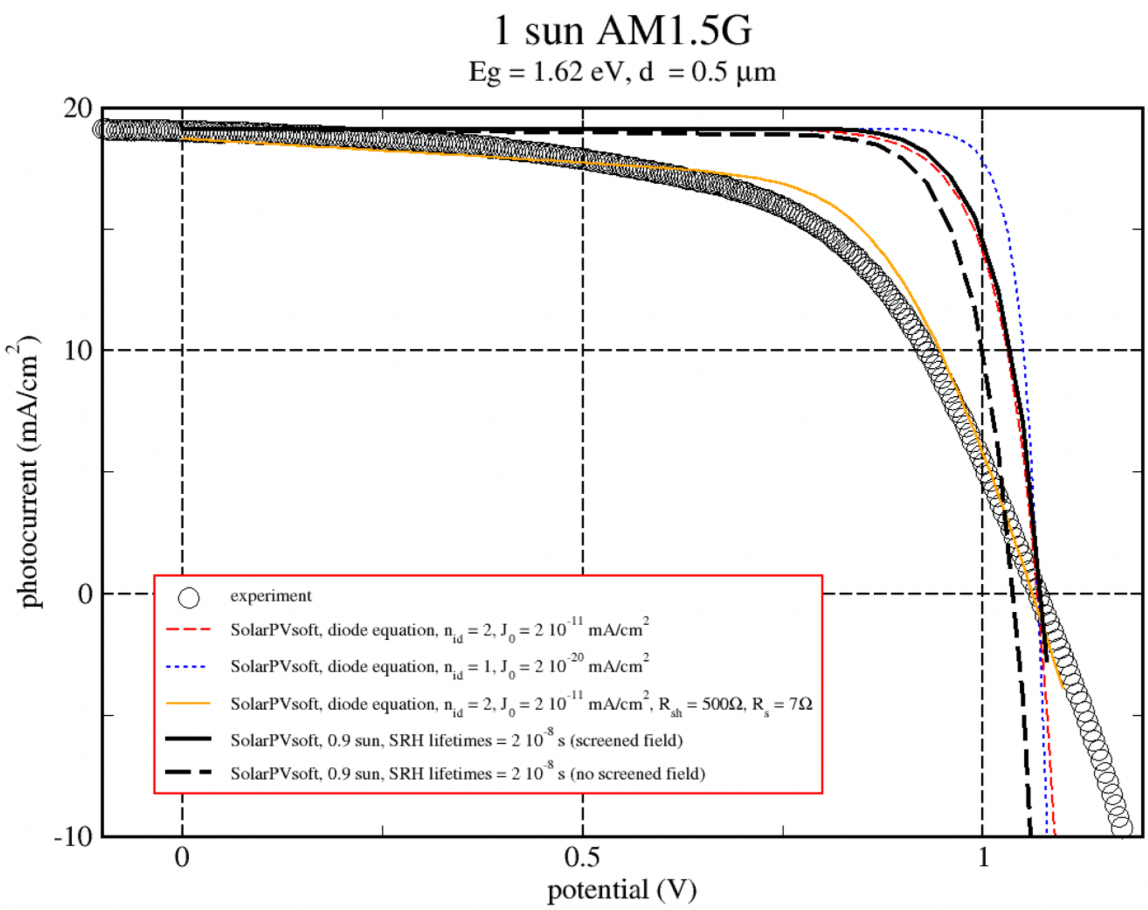
To correct that we can move to the “advanced” form. Using previous published work[5] we can work with more “realistic” parameters for diffusion coefficients and lifetimes. Here a set that works pretty well:

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 surprising[4] as the dominant recombination mechanism in the model is SRH recombination (see the theoretical background)
- 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

(1) Saliba, M.; Matsui, T.; Domanski, K.; Seo, J.-Y.; Ummadisingu, A.; Zakeeruddin, S. M.; Correa-Baena, J.-P.; Tress, W. R.; Abate, A.; Hagfeldt, A.; Grätzel, M. Incorporation of Rubidium Cations into Perovskite Solar Cells Improves Photovoltaic Performance. *Science* **2016**, aah5557. https://doi.org/10.1126/science.aah5557.

(2) Contreras-Bernal, L.; Salado, M.; Todinova, A.; Calio, L.; Ahmad, S.; Idígoras, J.; Anta, J. A. Origin and Whereabouts of Recombination in Perovskite Solar Cells. *J. Phys. Chem. C* **2017**, *121* (18), 9705–9713. https://doi.org/10.1021/acs.jpcc.7b01206.

(3) Contreras-Bernal, L.; Ramos-Terrón, S.; Riquelme, A.; Boix, P. P.; Idígoras, J.; Mora-Seró, I.; Anta, J. A. Impedance Analysis of Perovskite Solar Cells: A Case Study. *J. Mater. Chem. A* **2019**, *7* (19), 12191–12200. https://doi.org/10.1039/C9TA02808K.

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(5) Riquelme, A.; Bennett, L. J.; Courtier, N. E.; Wolf, M. J.; Contreras-Bernal, L.; Walker, A. B.; Richardson, G.; Anta, J. A. Identification of Recombination Losses and Charge Collection Efficiency in a Perovskite Solar Cell by Comparing Impedance Response to a Drift-Diffusion Model. *Nanoscale* **2020**, *12* (33), 17385–17398. https://doi.org/10.1039/D0NR03058A.