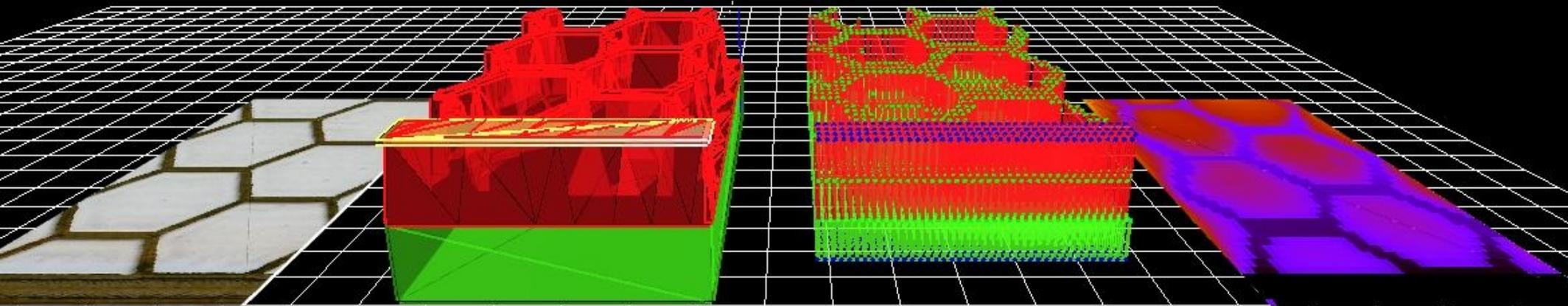
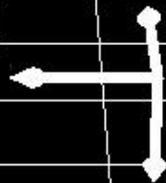


Editing and scanning electrical parameters in *OghmaNano*



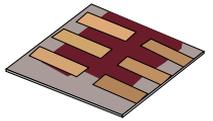
roderick.mackenzie@oghma-nano.com



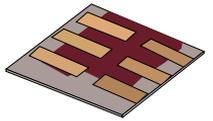
Dr. Roderick MacKenzie
<https://www.oghma-nano.com>

Autumn 2022

Download the software:

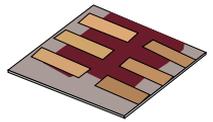


- Download all the software used in this talk from:
 - <http://www.oghma-nano.com/download.php>
- Please report bugs to:
 - roderick.mackenzie@durham.ac.uk



- **Making a new simulation**
- Defining device layers
- Editing the electrical parameters of a material
- Systematically varying electrical parameters over a range and plotting the results.

Your first OghmaNano simulation

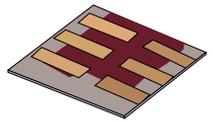


- Click on *New simulation*, in the file menu.

The screenshot shows the main application window titled "Organic and hybrid Material Nano Simulation tool" with a menu bar including File, Simulation type, Simulation Editors, Electrical, Optical, Thermal, Databases, and About. The "File" menu is open, and the "New simulation" option is highlighted with a red box. A dialog box titled "New simulation" is overlaid, asking "Which type of device would you like to simulate?". The dialog contains a grid of 28 device options, each with a small icon and a text label. The "P3HT:PCBM solar cell (PCE=4%)" option is highlighted with a red box. Other options include amorphous silicon solar cell, CIGS Solar cell, EQE demo, Equivalent circuit model, Exciton domain, Exciton device, Fitting and parameter extraction, Hetrojunction tunneling example, IS/IMPS/IMVS/ CV, Large area PM6:Y6 solar cell, Large area hexagonal contact, Laser Example, Matlab scripting demo, Morphology, OFETs, OLED, Optical filter, Organic solar cells, Perovskite solar cell, Photonic-xtal FDTD, Polycrystalline silicon, Ray tracing, Tandem Si Perovskite cell, Tandem solar cell, Thermal simulation, oled, and papers. At the bottom of the dialog, there is a "Show hidden" checkbox and "Cancel" and "Next" buttons.

- Save it somewhere but **not** in the install directory.

You should get this window.



Organic and hybrid Material Nano Simulation tool (<https://www.Oghma-Nano.com>)

File Simulation type Simulation Editors Electrical Optical Thermal Databases Information Questions? Contact: roderick.mackenzie@durham.ac.uk About

New simulation Open simulation Export Zip **Run simulation** Parameter scan Fit to experimental data Optical Simulation Machine Learning Edit Probes

If you publish results generated with ogpdm in a paper, book or thesis you must cite this paper: Modeling nongeminate recombination in P3HT: PCBM solar cells, The Journal of Physical Chemistry C, 115, 9806–9813, 2011 and along with these [two papers](#) in your work. Script Editor

Device structure Terminal Output Tutorials/Documentation

Layer editor Contacts Electrical parameters Emission parameters Substrate xz-size XY YZ XZ

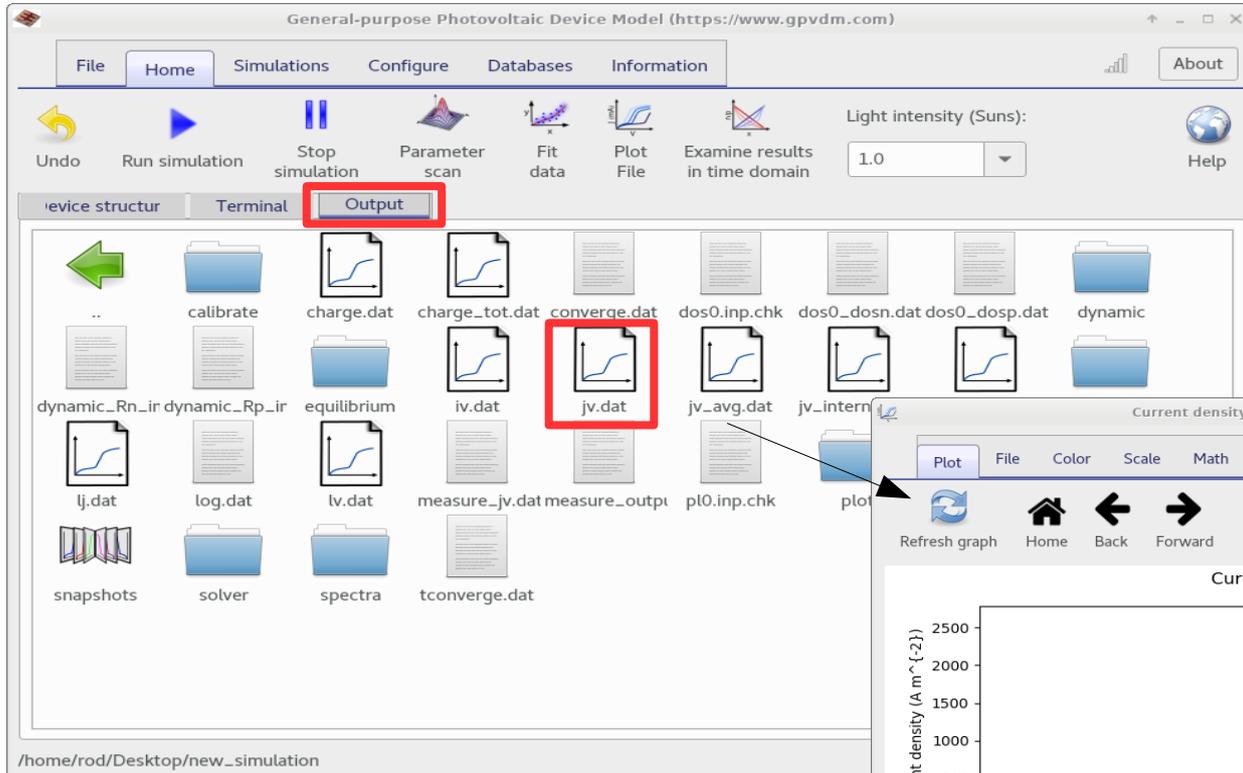
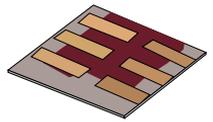
ITO
PEDOT:PSS
P3HT:PCBM (active)
Al

This simulation is based on: Extracting microscopic device parameters from transient photocurrent measurements of P3HT:PCBM solar cells. *Advanced Energy Materials*, 2012 (see link in upper right in article)

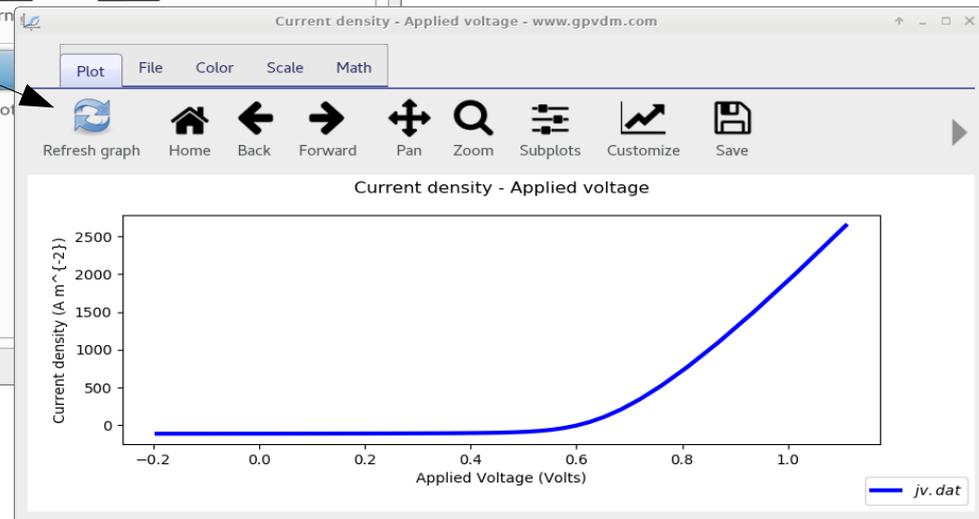
/home/rod/oghma/oghma8.0

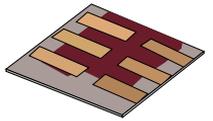
Click the play button

Examining the results



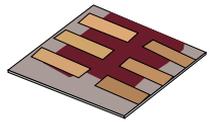
Double click on `jv.dat` to view J-V curve generated by the model.





- Making a new simulation
- **Defining device layers**
- Editing the electrical parameters of a material
- Systematically varying electrical parameters over a range and plotting the results.

The layer editor to change the structure of the cell

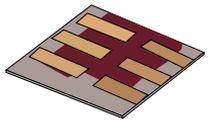


The screenshot shows the 'Layer editor' window of the Organic and hybrid Material Nano Simulation tool. The window title is 'Layer editor (https://www.Oghma-Nano.com)'. It features a toolbar with icons for adding (+), removing (-), moving down (down arrow), and moving up (up arrow) layers. Below the toolbar is a table with the following columns: Layer name, Thickness (m), Optical material, Layer type, Solve optical problem, Solve thermal problem, and ID.

Layer name	Thickness (m)	Optical material	Layer type	Solve optical problem	Solve thermal problem	ID
ITO	1e-07	oxides/ito	contact	Yes	Yes	e...
PEDOT:PSS	1e-07	polymers/pedotpss	other	Yes	Yes	...
P3HT:PCBM	2.2e-07	blends/p3htpcbm	active layer	Yes	Yes	...
Al	1e-07	metal/al	contact	Yes	Yes	...

Below the table is a 3D visualization of the cell structure, showing layers labeled ITO, PEDOT:PSS, P3HT:PCBM (active), and Al. The layers are colored in a stack: red (ITO), yellow (PEDOT:PSS), green (P3HT:PCBM), and blue (Al). The simulation tool interface also includes a menu bar (File, Simulation type, Simulation Editors, Electrical, Optical, Thermal, Databases, Info, Questions? Contact: ro) and a toolbar with icons for New simulation, Open simulation, Export Zip, Run simulation, Parameter scan, Fit to experimental data, Optical Simulation, Machine Learning, and Edit Probes. The 'Layer editor' icon is highlighted with a red box in the left sidebar.

The layer editor



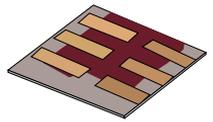
Layer editor (<https://www.Oghma-Nano.com>)

+ - ↓ ↑

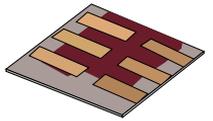
Layer name	Thicknes (m)	Optical material	Layer type	Solve optical problem	Solve therma problem	ID
ITO	1e-07	... oxides/ito	contact	Yes	Yes	e...
PEDOT:PSS	1e-07	... polymers/pedotpss	other	Yes	Yes	...
P3HT:PCBM	2.2e-07	... blends/p3htpcbm	active layer	Yes	Yes	...
Al	1e-07	... metal/al	contact	Yes	Yes	...

- **Layer name:** An English name for the layer, this has no technical significance (Tip: It might not like names with non English characters, i.e. Chinese characters)
- **Thickness of the layer:** The thickness of the layer in meters.
- **Optical material:** This points to the n/k data in the materials database. Use the “...” button to select a new material.
- **Layer type:** Can be **contact**, **other** or **active**.

The layer editor

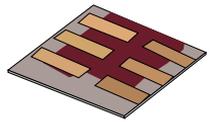


Layer type	Description	Electrical Equations solved	Optical Equations solved.
active	The electrical model is solved over these layers, each layer gets it's own set of electrical parameters.	Yes	Yes
other	No electrical equations are solved in these layers.	No	Yes
contact	These layers are used to define the electrical contacts, no electrical equations are solved in the layers.	No	Yes



- Making a new simulation
- Defining device layers
- **Editing the electrical parameters of a material**
- Systematically varying electrical parameters over a range and plotting the results.

Editing the electrical parameters of a material



Organic and hybrid Material Nano Simulation tool (<https://www.Oghma-Nano.com>)

File Simulation type Simulation Editors Electrical Optical Thermal Databases Info Questions? Contact: roderick.mackenzie@durham.ac.uk About

New simulation Open simulation Export Zip Run simulation Parameter scan Fit to experimental data Optical Simulation Machine Learning Edit Probes

If you publish results generated with gvpdm in a paper, book or thesis you must cite this paper: Modeling nongeminate recombination in P3HT:PCBM solar cells. The Journal of Physical Chemistry C, 115, 9806--9813, 2011 and along with these [two papers](#) in your work.

Script Editor

Device structure Terminal Output Tutorials/Documentation

Layer editor

Contacts

Electrical parameters

Emission parameters

Substrate xz-size

xy yz

XZ

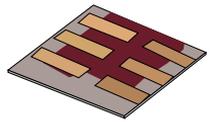
ITO
PEDOT:PSS
P3HT:PCBM (active)
Al

The simulation is based on extracting microscopic device parameters from contact photocurrent measurements on P3HT:PCBM solar cells. Advanced Energy Materials 2012 (left click to open link to website)

/home/rod/oghma/oghma8.0

- Click on the Electrical parameter editor, under the device structure tab.

This is the electrical parameter window



Electrical parameter editor (https://www.Oghma-Nano.com)

Enable Drift Diff. Enable Auger Dynamic SRH traps Equilibrium SRH traps Excitons Excited states Configure Help

P3HT:PCBM

Free carriers

Electron mobility	2.48e-07	Symmetric	$\text{m}^2\text{V}^{-1}\text{s}^{-1}$
Hole mobility	2.48e-07	Symmetric	$\text{m}^2\text{V}^{-1}\text{s}^{-1}$
Effective density of free electron states (@300K)	1.28e27		m^{-3}
Effective density of free hole states (@300K)	2.86e25		m^{-3}
n_{free} to p_{free} Recombination rate constant	0.0		m^3s^{-1}
Free carrier statistics	Maxwell Boltzmann - analytic		type

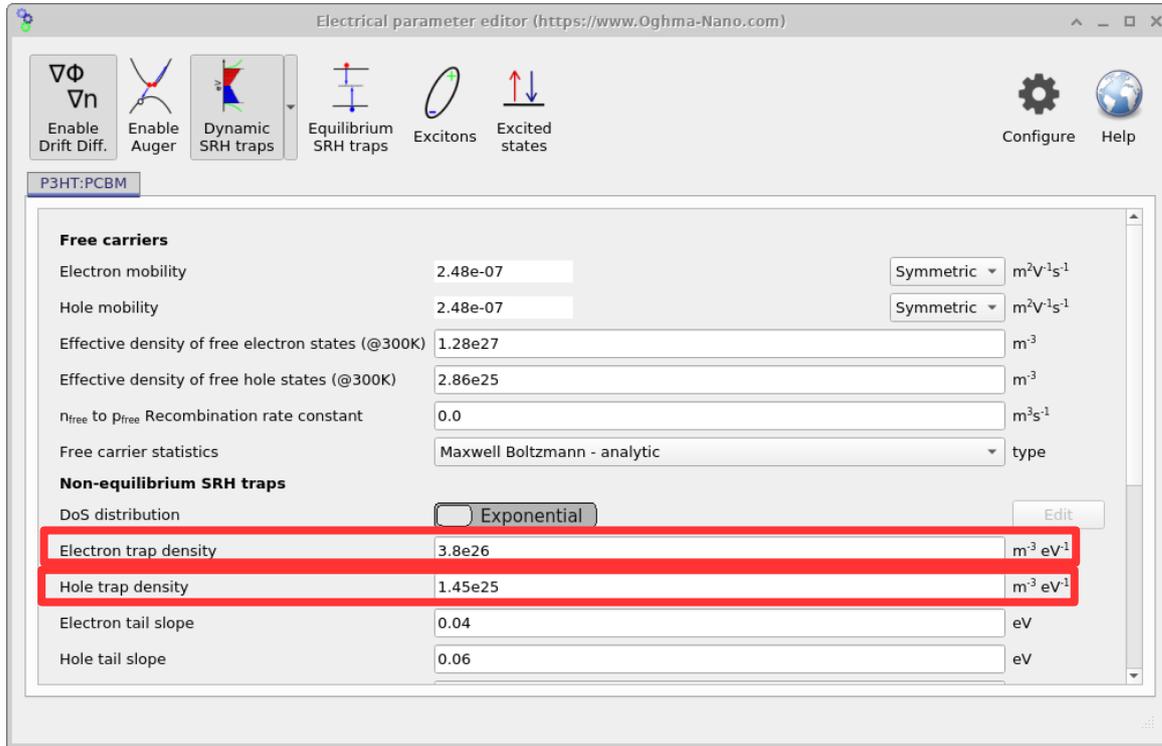
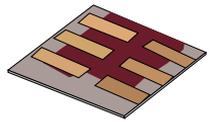
Non-equilibrium SRH traps

DoS distribution Exponential Edit

Electron trap density	3.8e26	$\text{m}^{-3}\text{eV}^{-1}$
Hole trap density	1.45e25	$\text{m}^{-3}\text{eV}^{-1}$
Electron tail slope	0.04	eV
Hole tail slope	0.06	eV

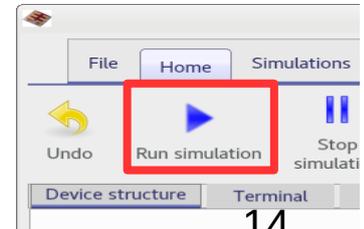
• Here you can edit the electrical parameters of the electrically active layers. Each **electrically active** layer will get a new tab here.

Editing an electrical parameter...the trap density....

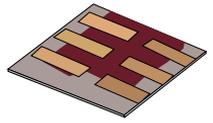


a) Make the density of trap state symmetric at $1 \times 10^{24} \text{ m}^{-3}$, and rerun the simulation.

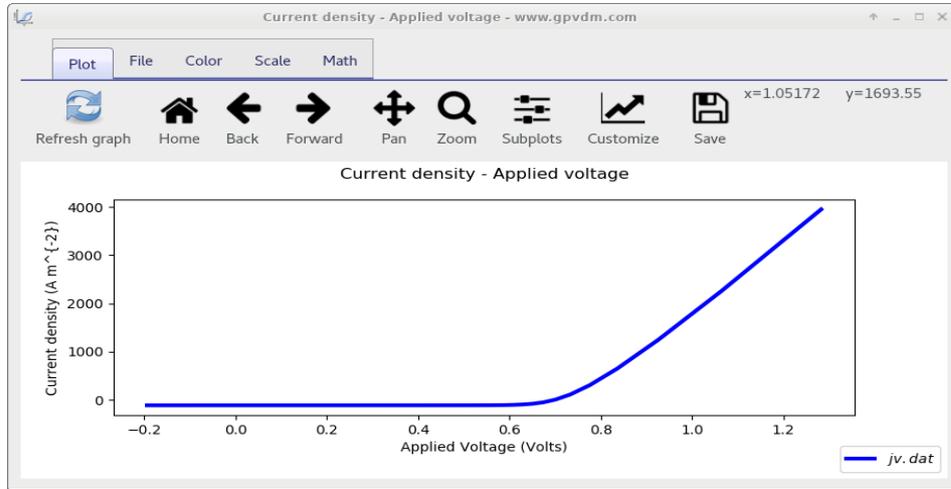
b) Now re-plot the JV curve (**ju.dat**), also find the (**sim_info.dat**) file, double click on it and find the power conversion efficiency.



You should have results which look a bit like this:



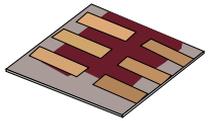
ju.dat:



sim_info.dat:

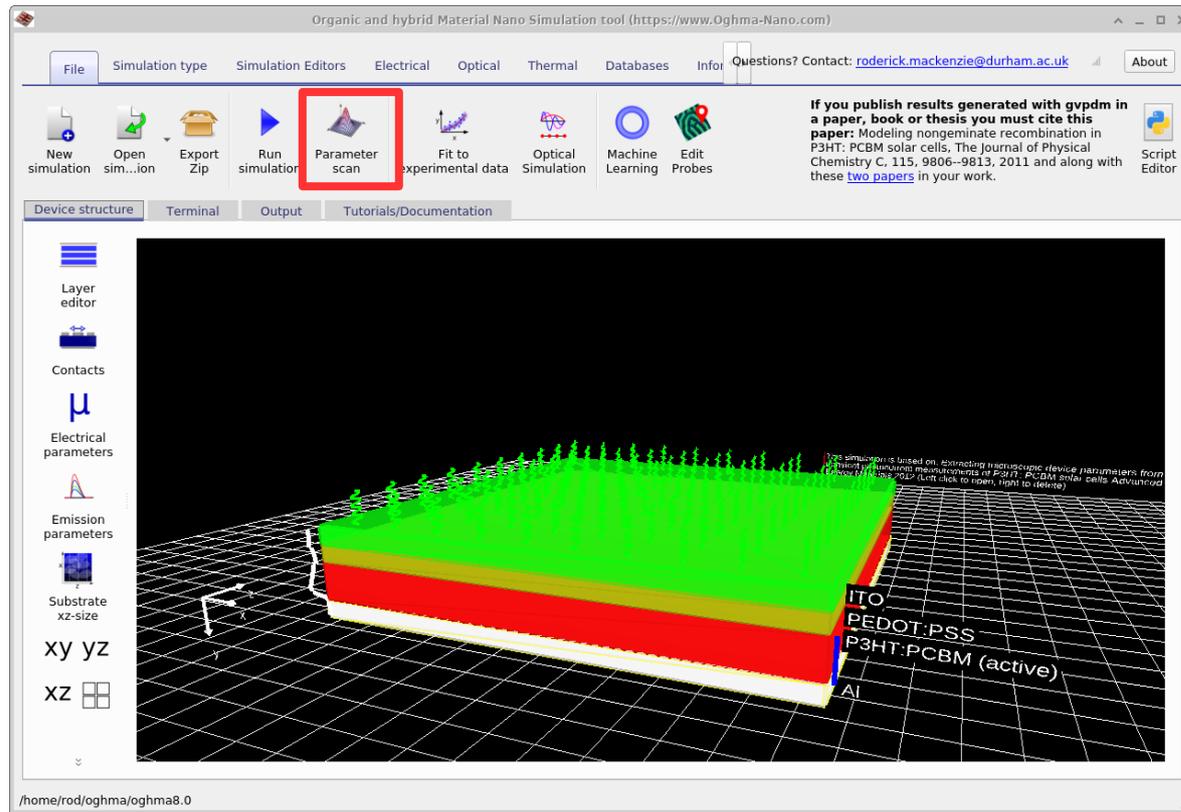
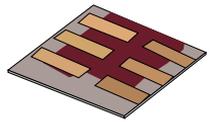
Simulation information (www.gpvdm.com)

Simulation Information		
Fill factor	0.801681	a.u.
Power conversion efficiency	6.317818	Percent
Max power	63.178183	Watts
V_{oc}	0.697817	V
Recombination time constant at V_{oc}	6.033818e-04	s
Recombination rate at V_{oc}	2.053384e+26	$\text{m}^{-3}\text{s}^{-1}$
Average carrier density at P_{max}	2.597280e+22	m^{-3}
Recombination time constant	1.782948e-03	m^{-1}
Trapped electrons at V_{oc}	1.868796e+20	m^{-3}
Trapped holes at V_{oc}	6.739736e+21	m^{-3}
Free electrons at V_{oc}	9.096213e+22	m^{-3}
Free holes at V_{oc}	9.051892e+22	m^{-3}
J_{sc}	-1.129337e+02	A m^{-2}
Total carriers (n+p)/2 at V_{oc}	1.817027e+23	m^{-3}



- Making a new simulation
- Defining device layers
- Editing the electrical parameters of a material
- **Systematically varying electrical parameters over a range and plotting the results.**

Varying a parameter many times using the Parameter Scan, window.

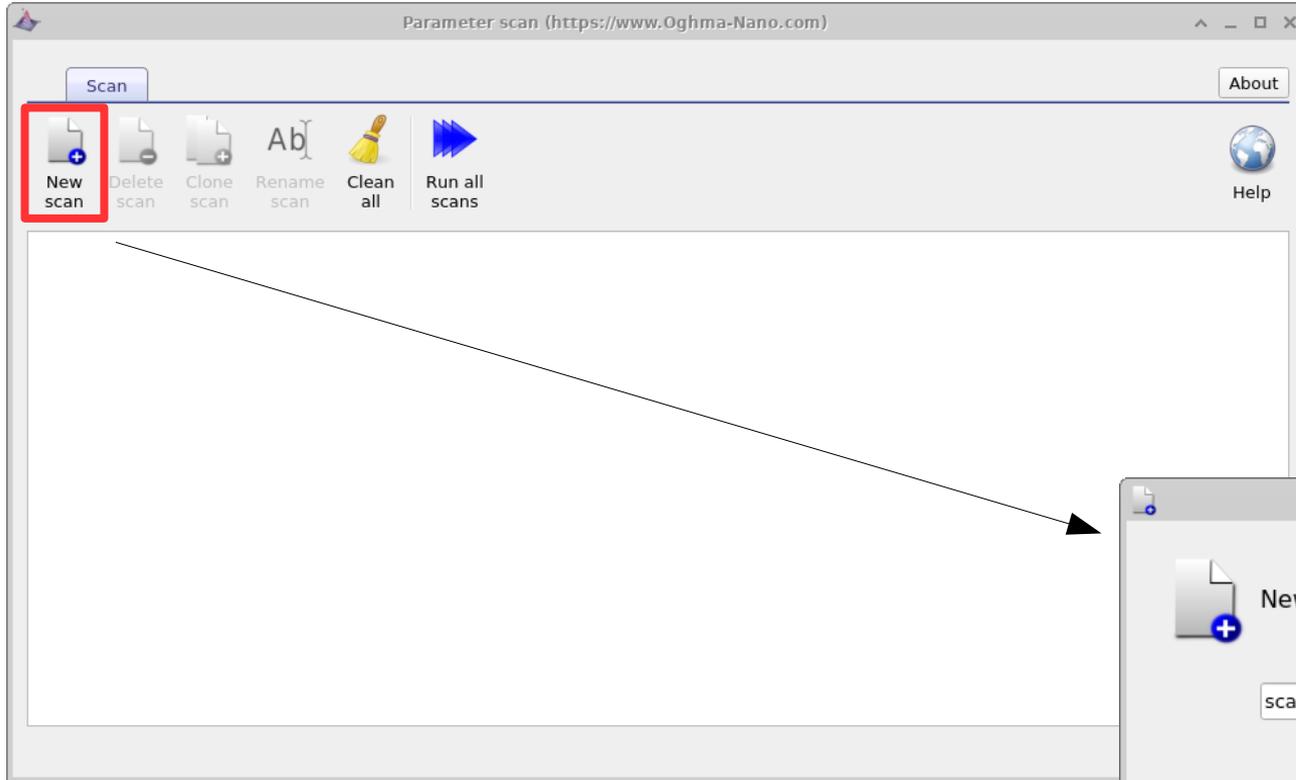
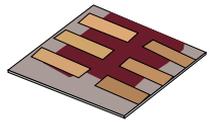


- Often we want to change a simulation parameter several times to understand how a parameter affects a device.

- To do this, use the ***Parameter Scan tool***

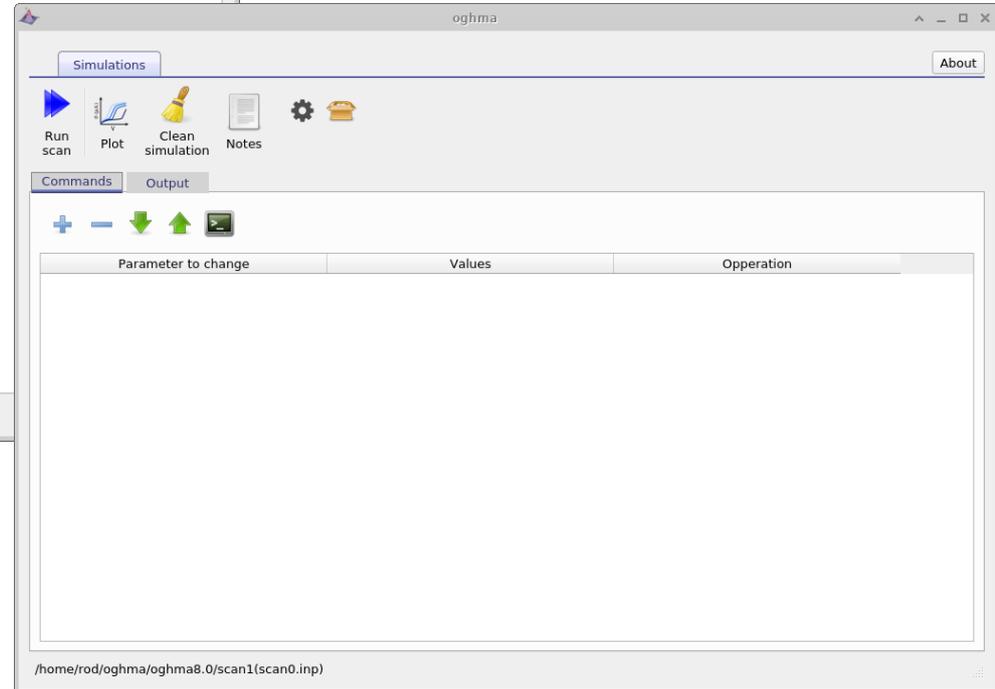
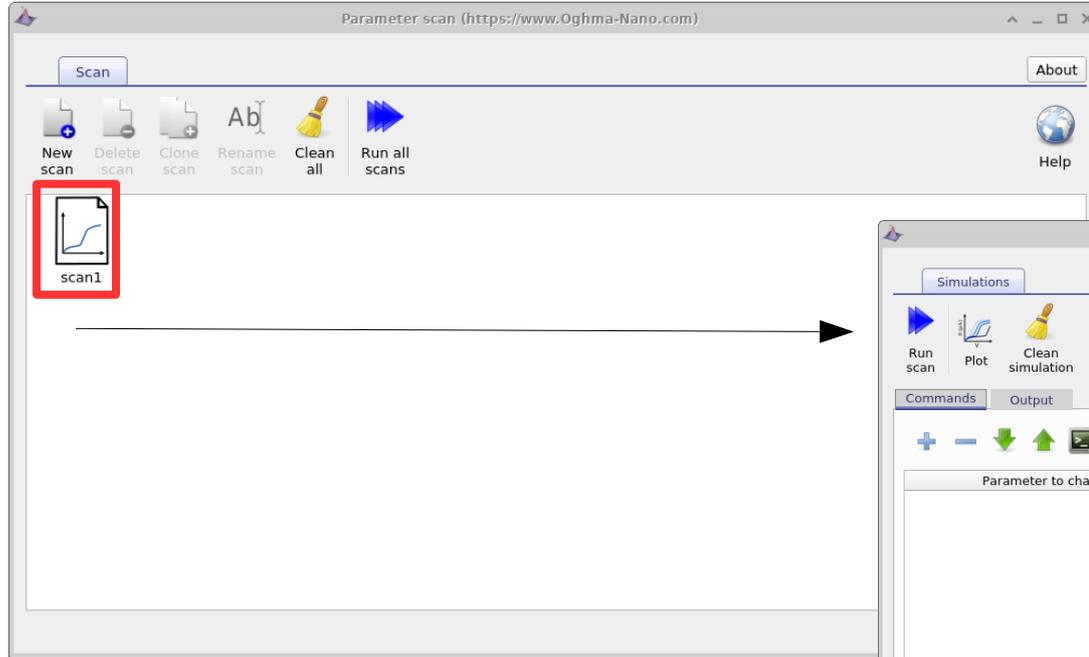
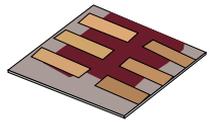
- **Click on the parameter scan tool**

The parameter scan window

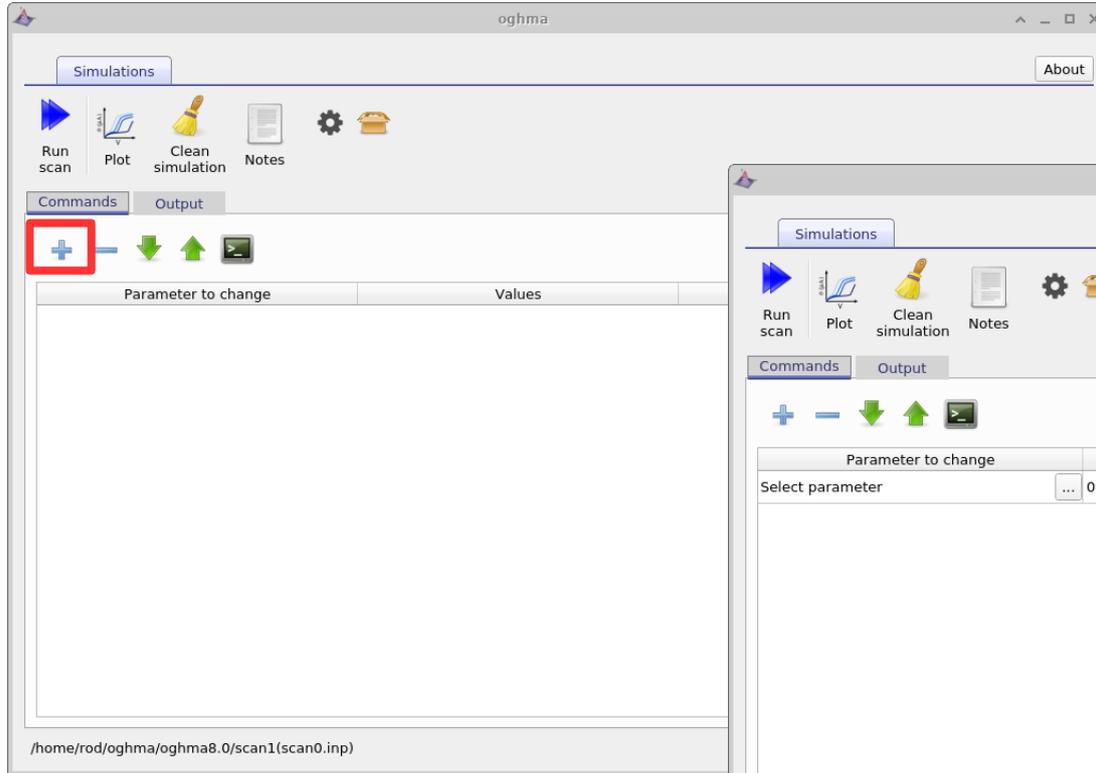
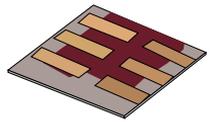


- Click on the **New scan** to generate a new parameter scan.

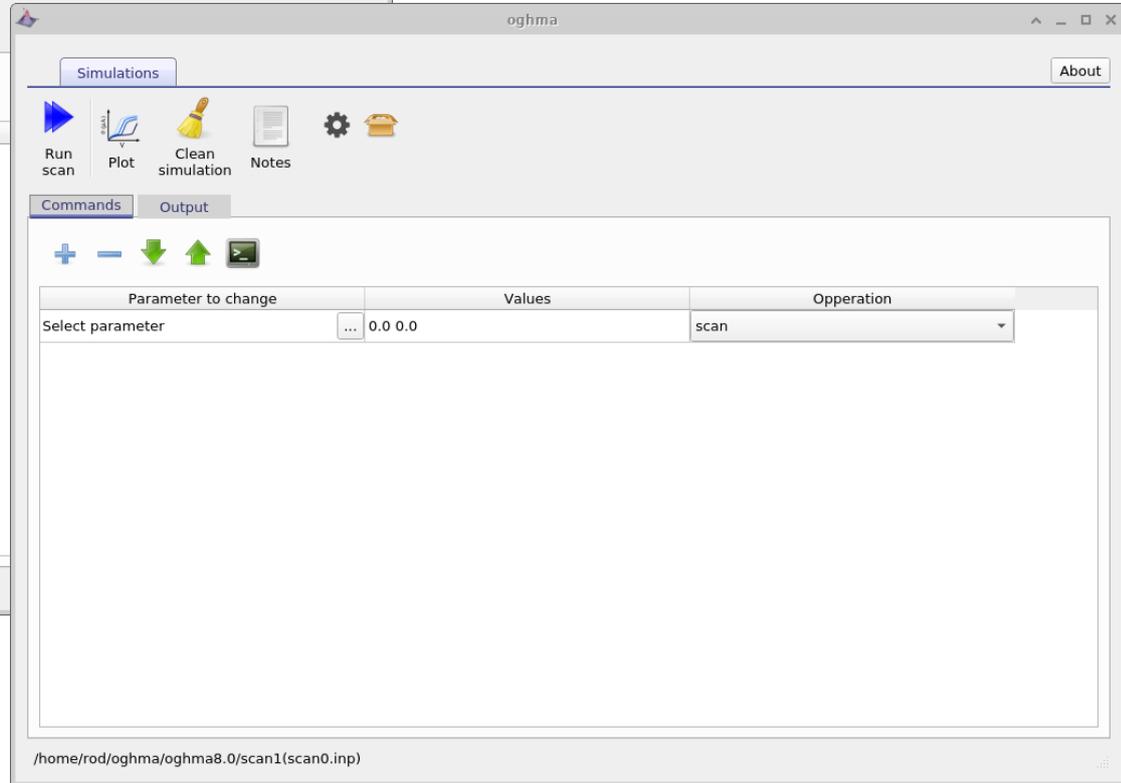
The parameter scan window



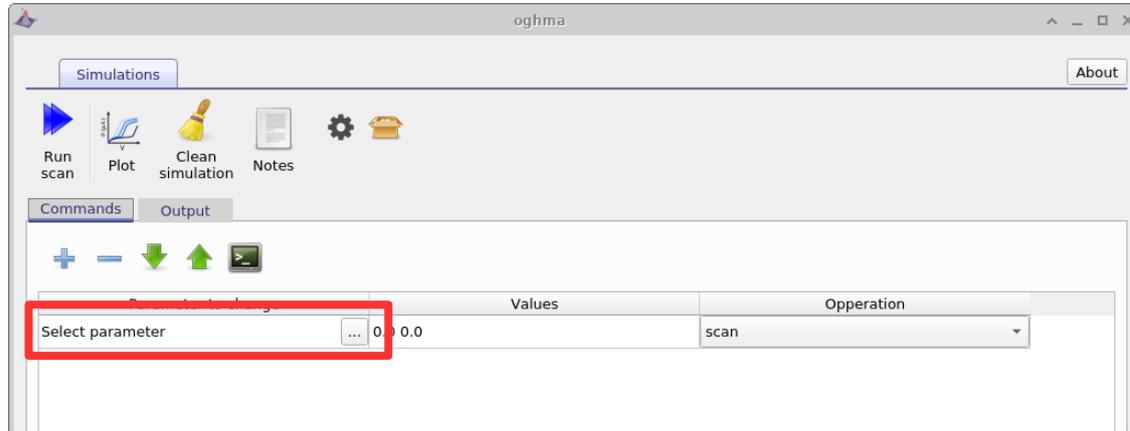
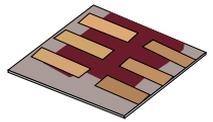
A new line should appear...



- Add a new line by clicking the + button.

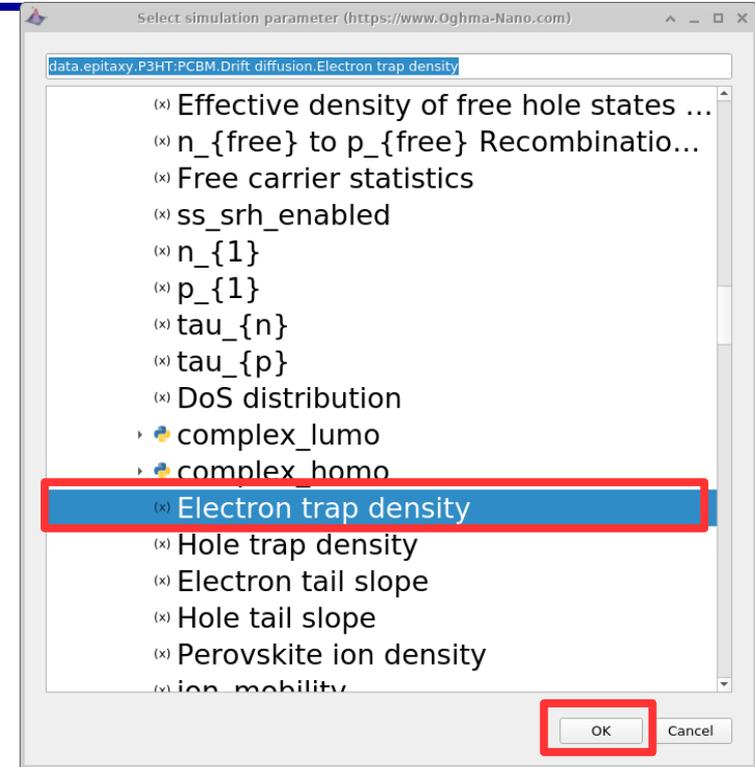


A new line should appear...

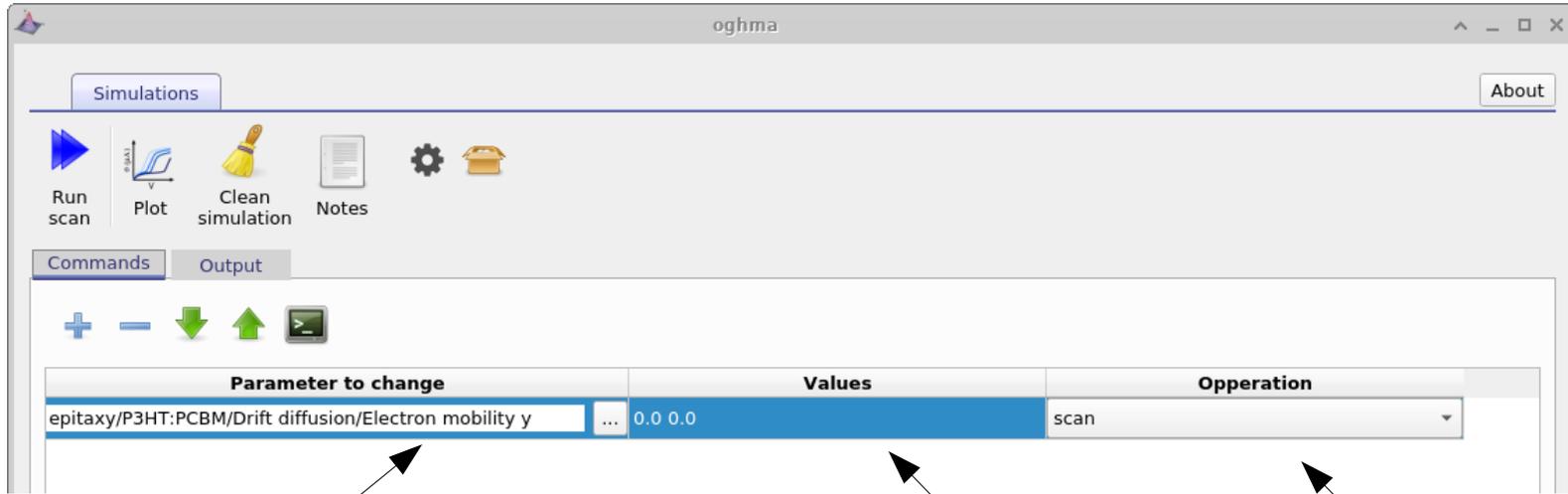
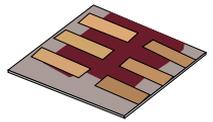


• Click on the '...' icon, expand the tree as shown, select 'Hole trap density' and click OK.

• Then select *epitaxy/P3HT:PCBM/Drift diffusion/Electron trap density*



The parameter scan window...

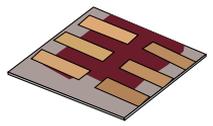


This shows the parameter which will be edited.

Enter these ($1e24$ $1e25$ $1e26$) values in here. They are the trap densities we are going to scan over (units are $m^{-3} eV^{-1}$)

This selects the operation which will be performed. (more explained later)

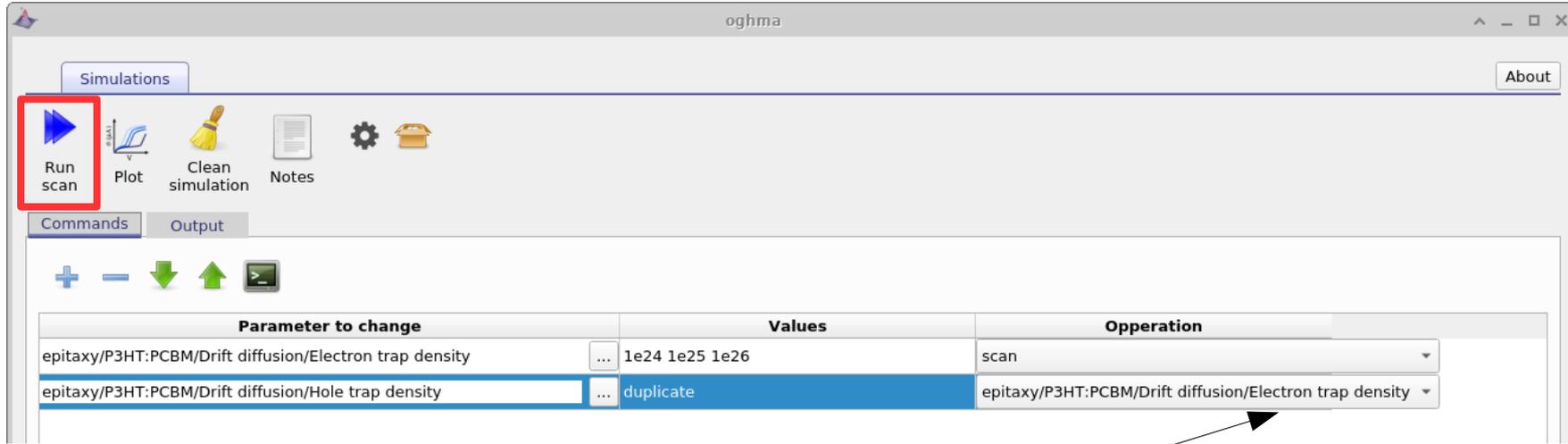
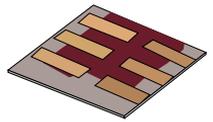
But we want to simulate a symmetric device (where $N_{traph}=N_{trape}$)...



Parameter to change	Values	Operator
epitaxy/P3HT:PCBM/Drift diffusion/Electron trap density	1e24 1e25 1e26	scan
epitaxy/P3HT:PCBM/Drift diffusion/Hole trap density	0.0 0.0	scan

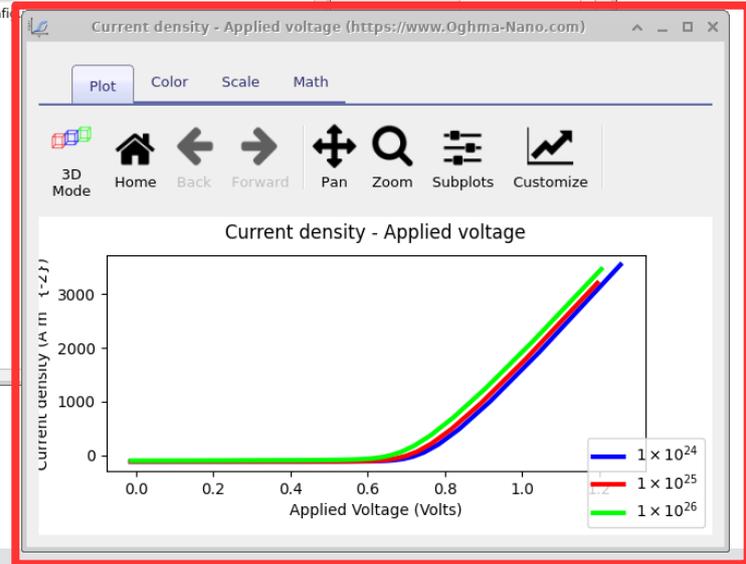
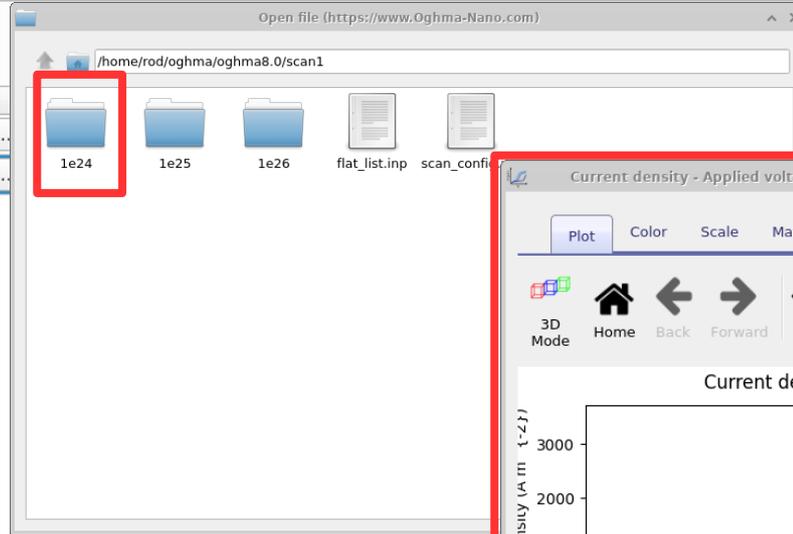
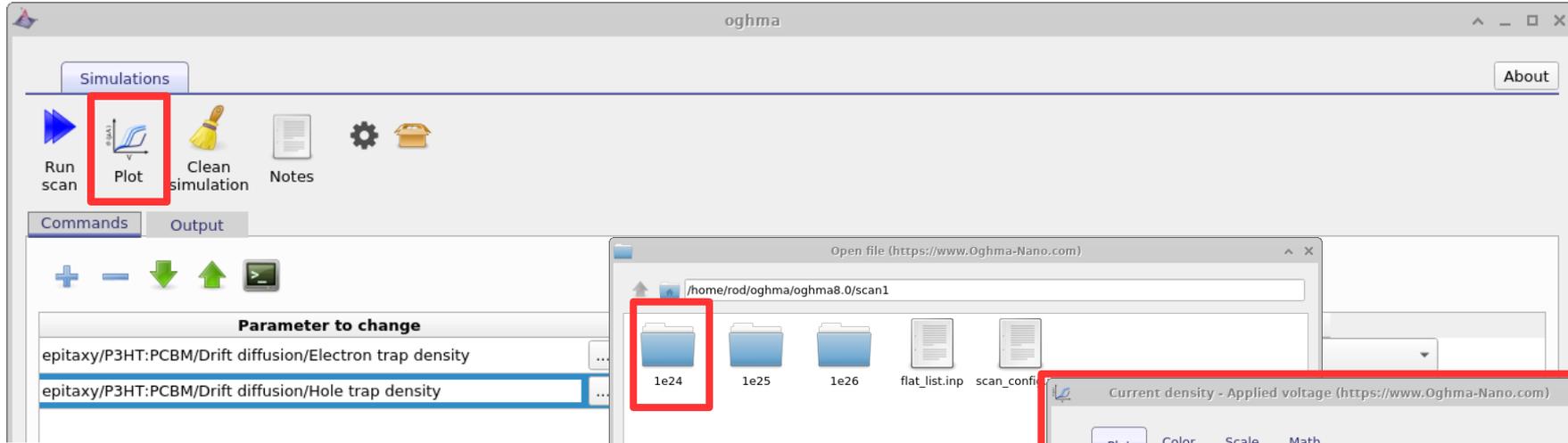
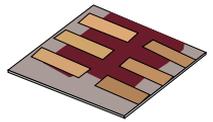
So using the '+' button **add another row** and then using the '...' buttons **make it look like the above..**

But we want to simulate a symmetric device (where $N_{traph}=N_{trape}$)...



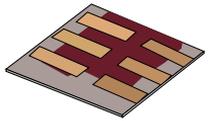
- Then from this menu select, 'epitaxy/P3HT:PCBM/dos/Electron trap density'.
- This means that the values for Hole trap density will follow that of the Electron trap density.
- Now click 'Run scan'...., it will run the simulations in parallel across all cores of your CPU.

Plotting the results.



- Click plot, and plot the file scan1/1e24/jv.dat.

- All jv.dat curves will be plotted from the simulation tree.



- Making a new simulation
- Defining device layers
- Editing the electrical parameters of a material
- Systematically varying electrical parameters over a range and plotting the results.