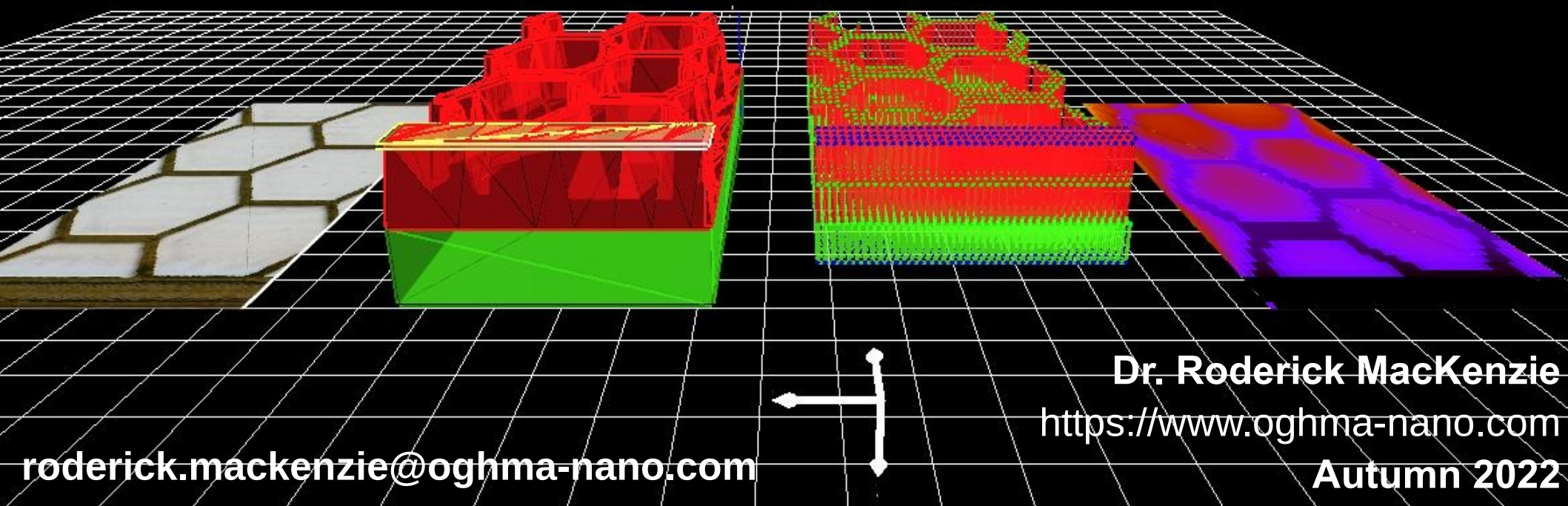
Editing and scanning electrical parameters in *OghmaNano*



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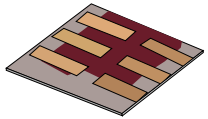
https://www.oghma-nano.com
roderick.mackenzie@oghma-nano.com

Autumn 2022

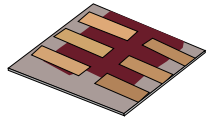
Download the software:



- Download all the software used in this talk from:
  - http://www.oghma-nano.com/download.php

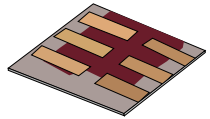
- Please report bugs to:
  - roderick.mackenzie@durham.ac.uk

Overview

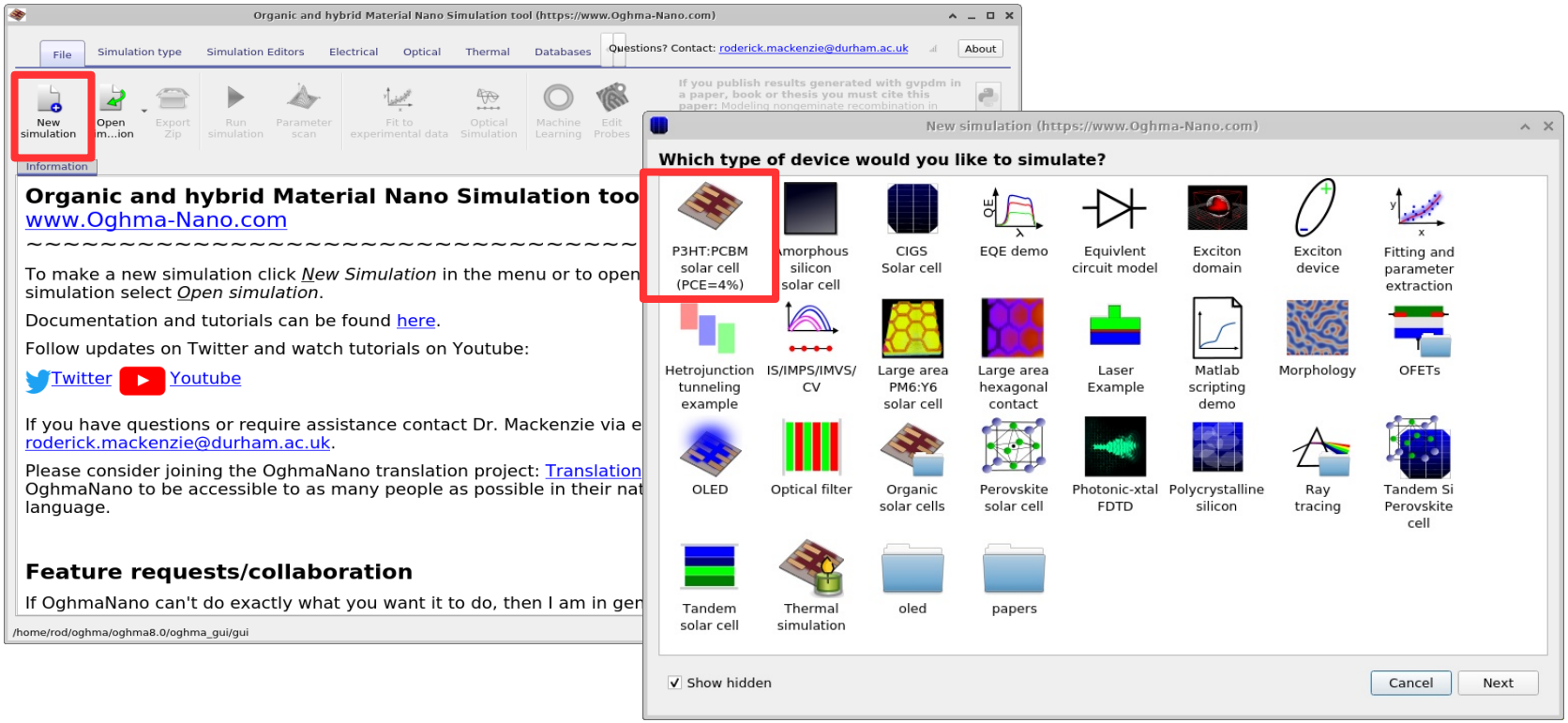


- **Making a new simulation**
- Defining device layers
- Editing the electrical parameters of a material
- Systematically varying electrical parameters over a range and plotting the results.

Your first OghmaNano simulation

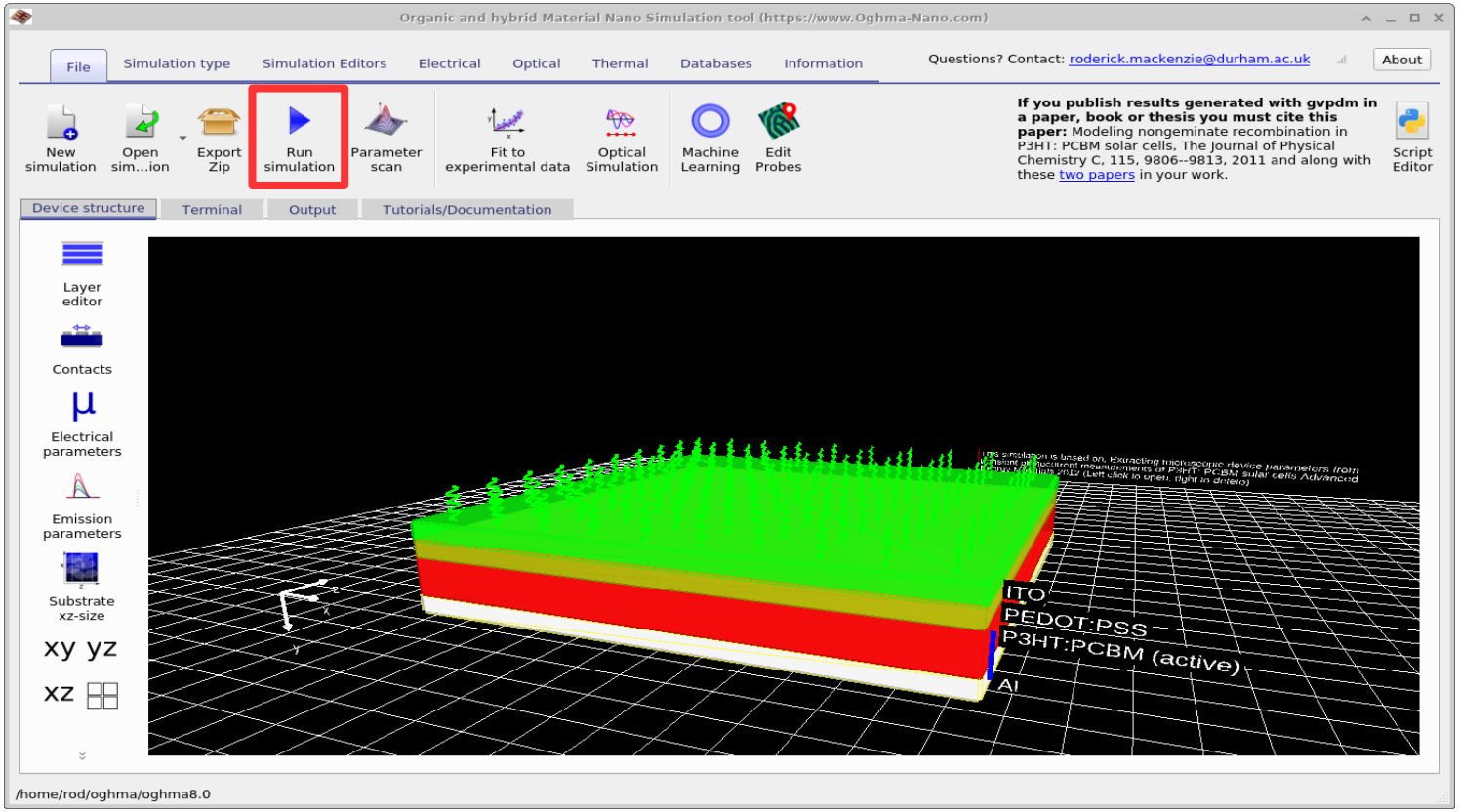


- Click on *New simulation*, in the file menu.



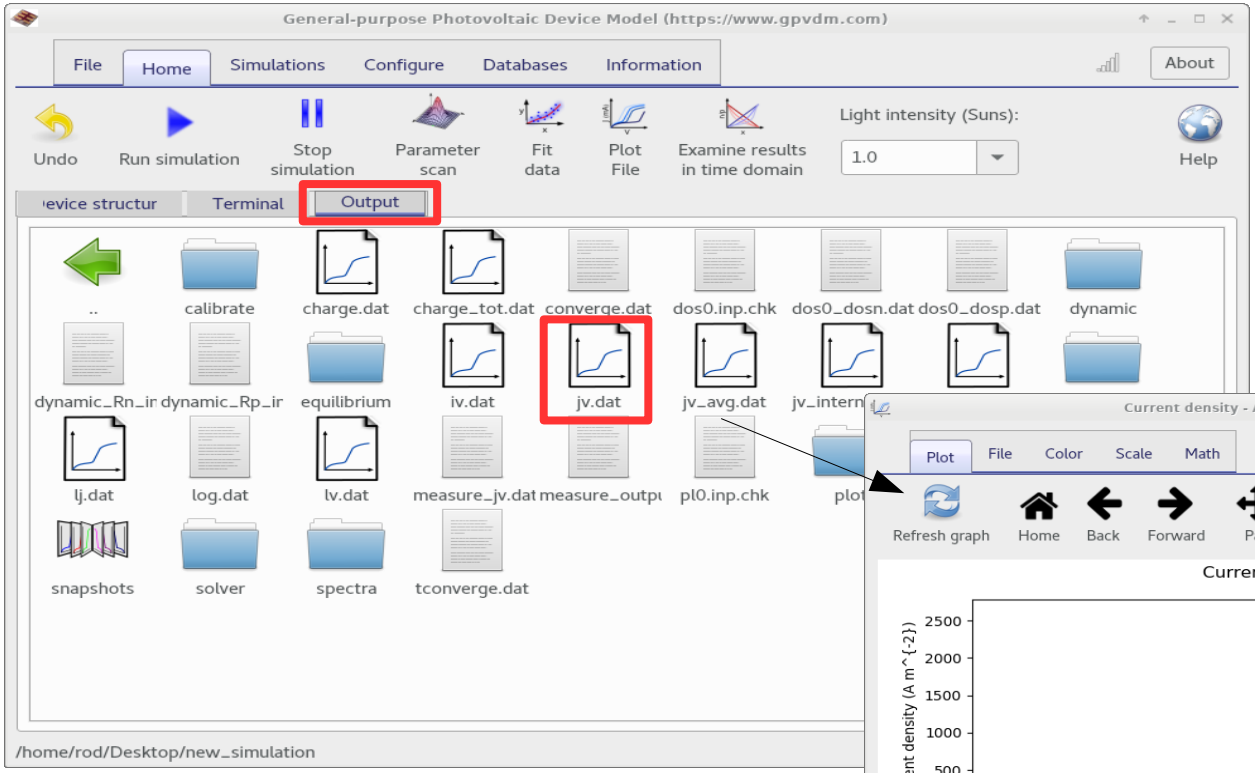
- Save it somewhere but ***not*** in the install directory.

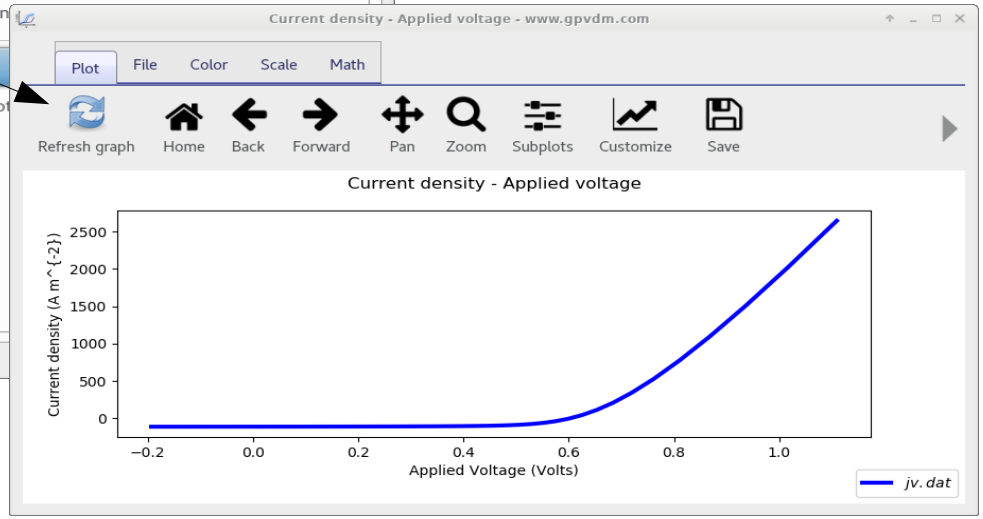
You should get this window.



Click the play button

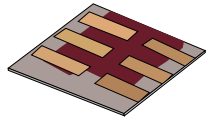
Examining the results





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

Overview



- Making a new simulation
- **Defining device layers**
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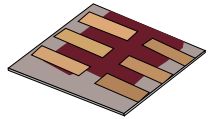
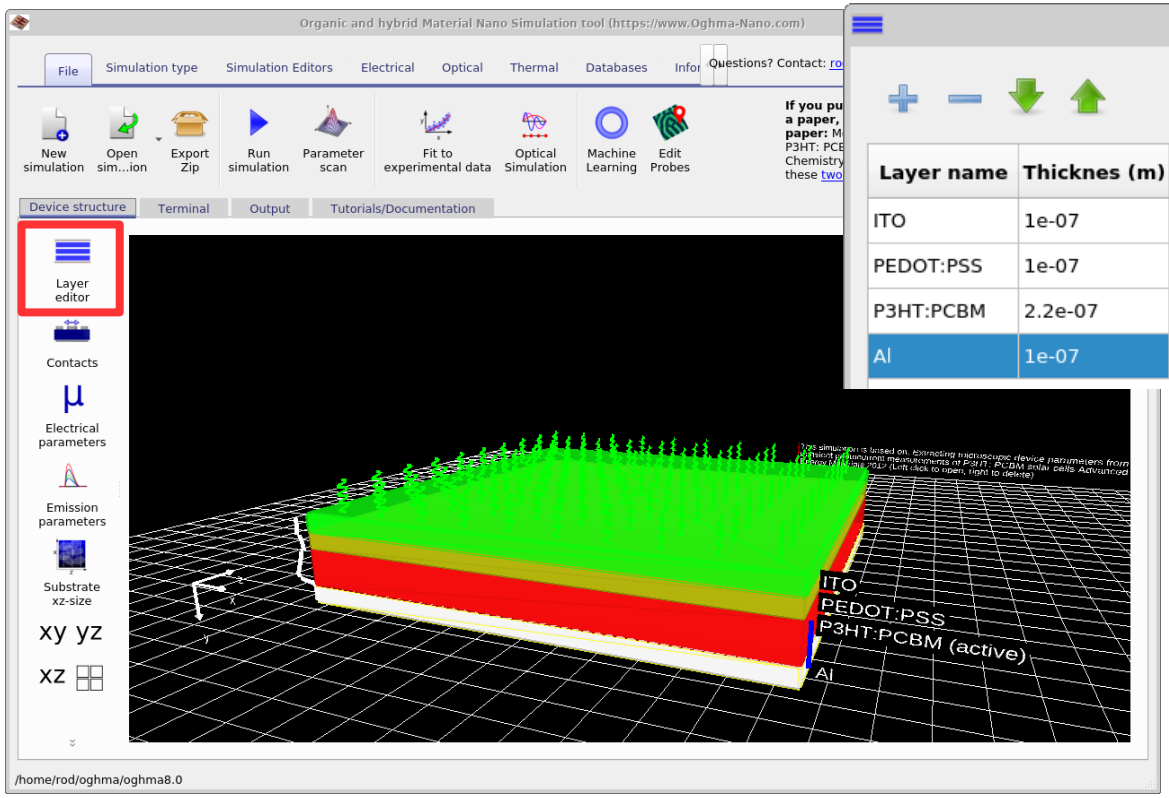
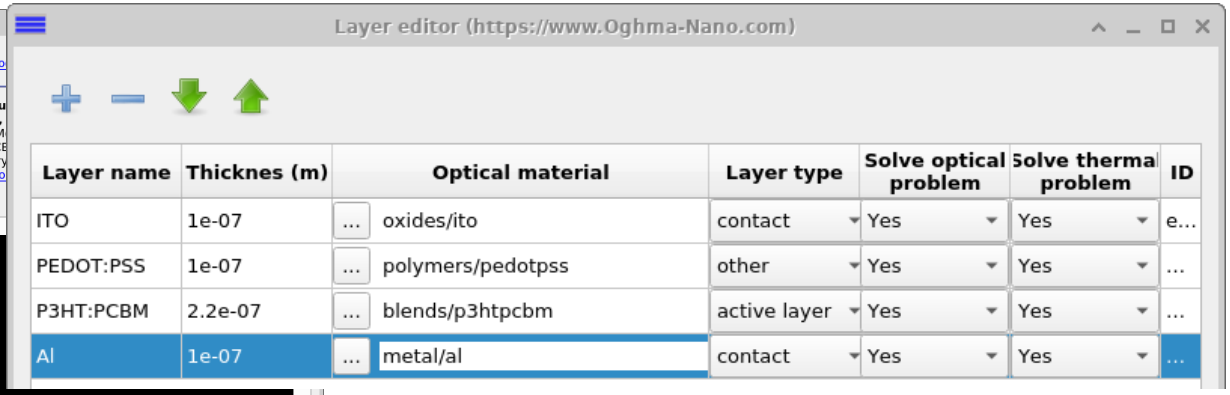
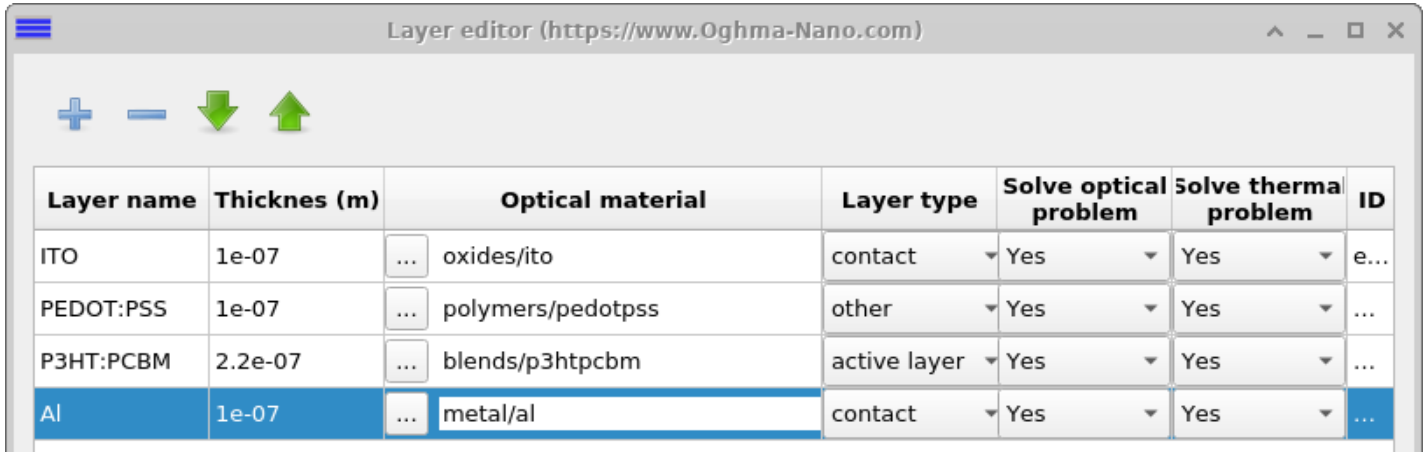
The layer editor to change the structure of the cell





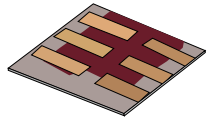


The layer editor



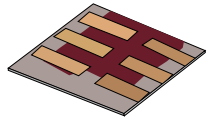
- **Layer name:** An English name for the layer, this has no technical significance (Tip: It might not like names with non English characters, i.e. Chinese characters)
- **Thickness of the layer:** The thickness of the layer in meters.
- **Optical material:** This points to the n/k data in the materials 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

Overview



- Making a new simulation
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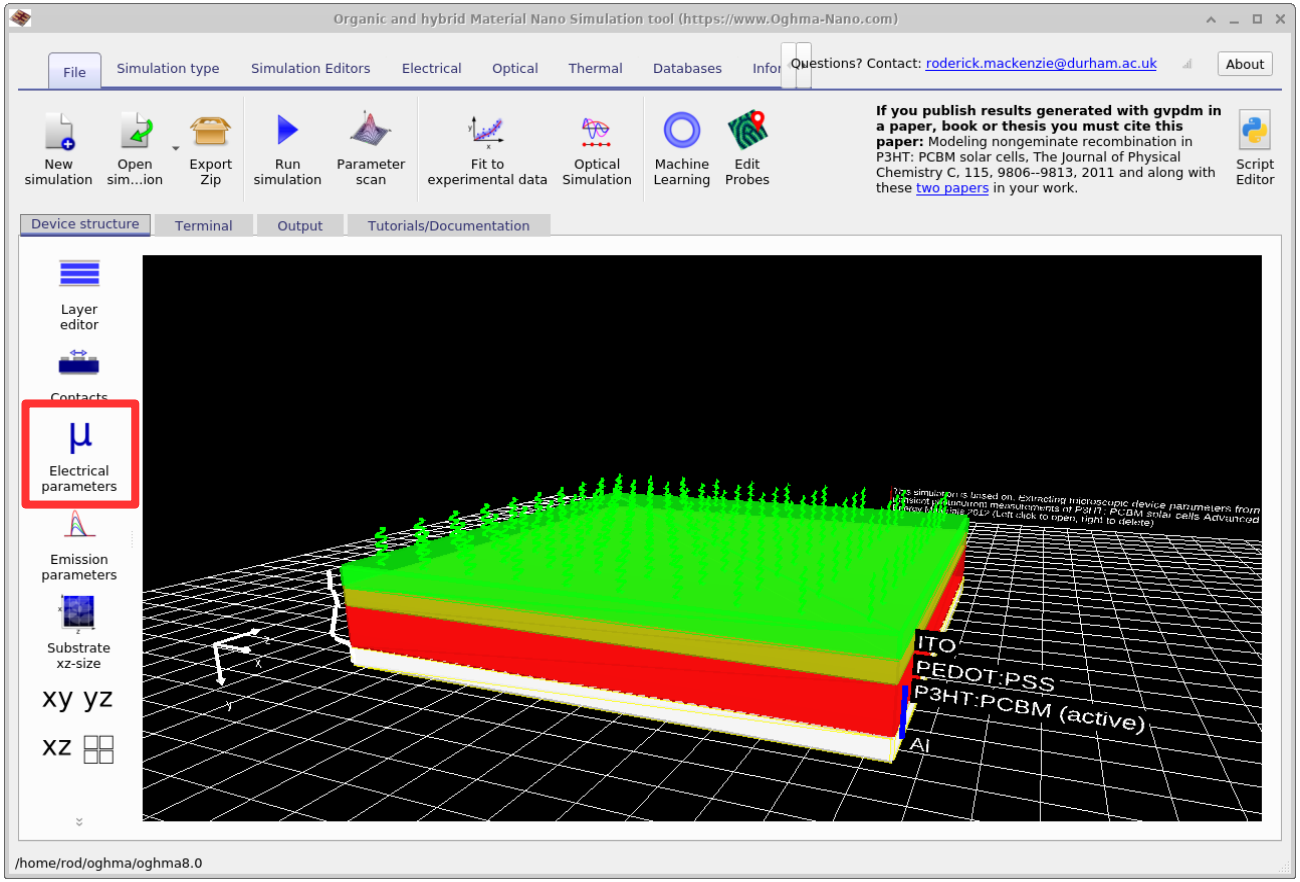
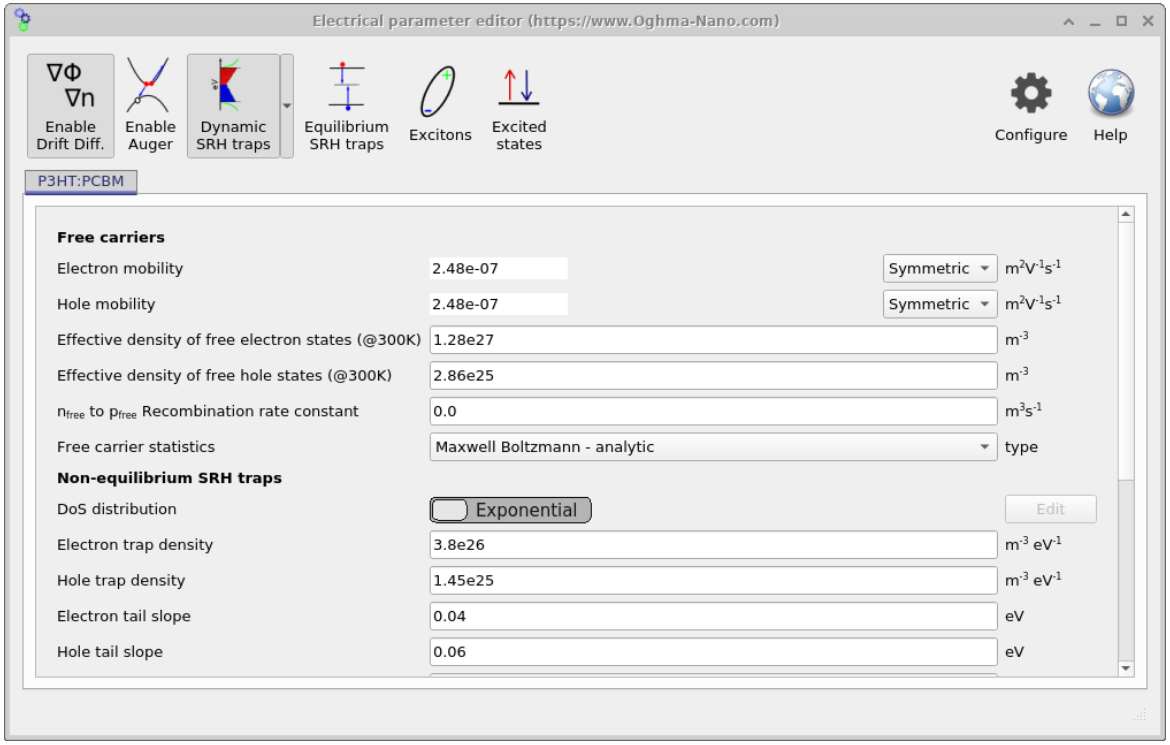
Editing the electrical parameters of a material



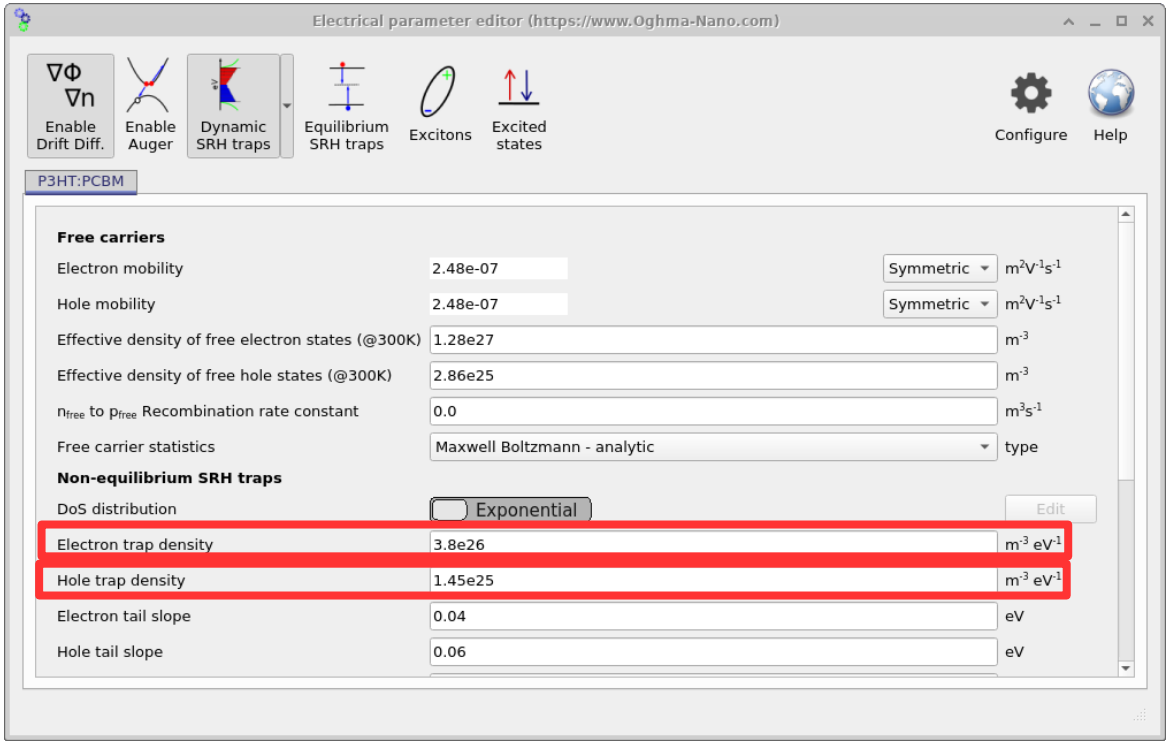
- Click on the Electrical parameter editor, under the device structure tab.

This is the electrical parameter window



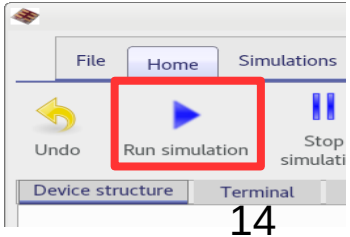
•Here you can edit the electrical parameters of the electrically active layers. Each ***electrically active*** layer will get a new tab here.

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

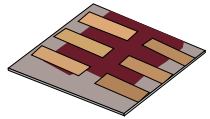


a) Make the density of trap state symmetric at $1x10^{24}$ m^{-3}, and rerun the simulation.

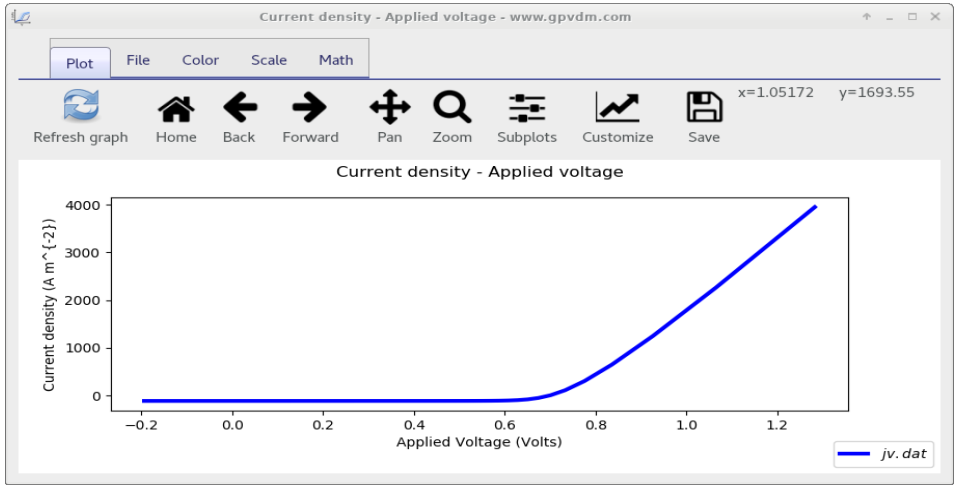
b) Now re-plot the JV curve (**jv.dat**), also find the (**sim_info.dat)** file, double click on it and find the power conversion efficiency.



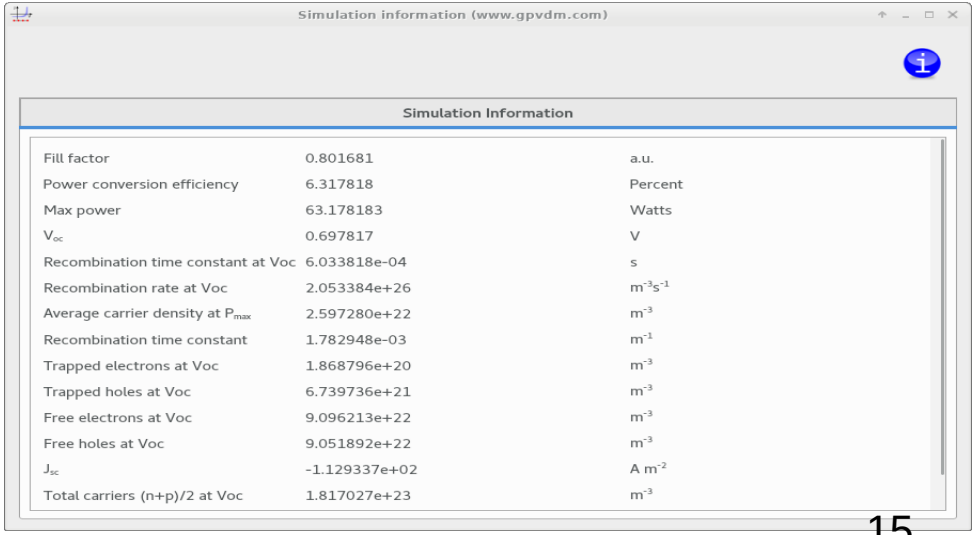
You should have results which look a bit like this:



jv.dat:

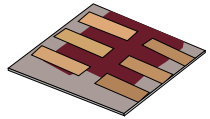


sim_info.dat:



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 Voc	6.033818e-04	s
Recombination rate at Voc	2.053384e+26	$m^{-3}s^{-1}$
Average carrier density at P_{max}	2.597280e+22	m^{-3}
Recombination time constant	1.782948e-03	m^{-1}
Trapped electrons at Voc	1.868796e+20	m^{-3}
Trapped holes at Voc	6.739736e+21	m^{-3}
Free electrons at Voc	9.096213e+22	m^{-3}
Free holes at Voc	9.051892e+22	m^{-3}
J_{sc}	-1.129337e+02	A m^{-2}
Total carriers (n+p)/2 at Voc	1.817027e+23	m^{-3}

Overview



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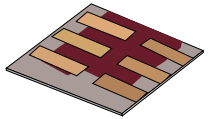
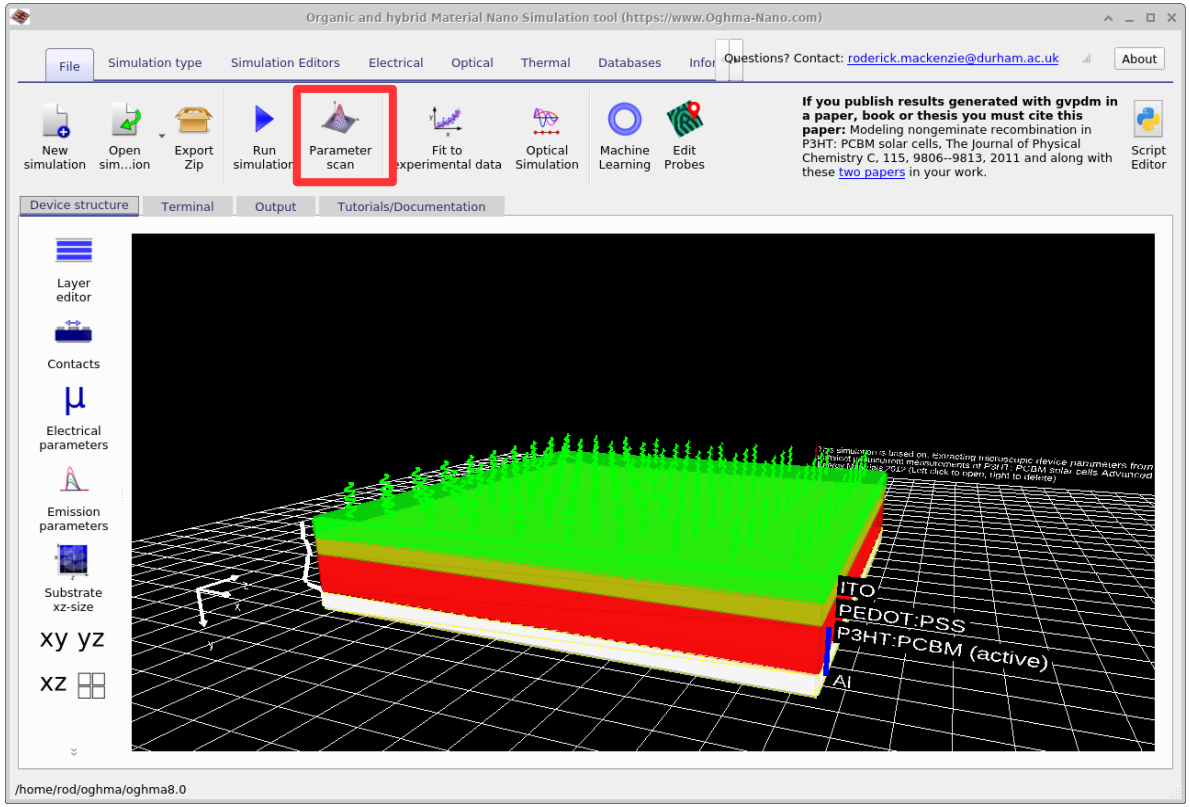
Varying a parameter many times using the Parameter Scan, window.



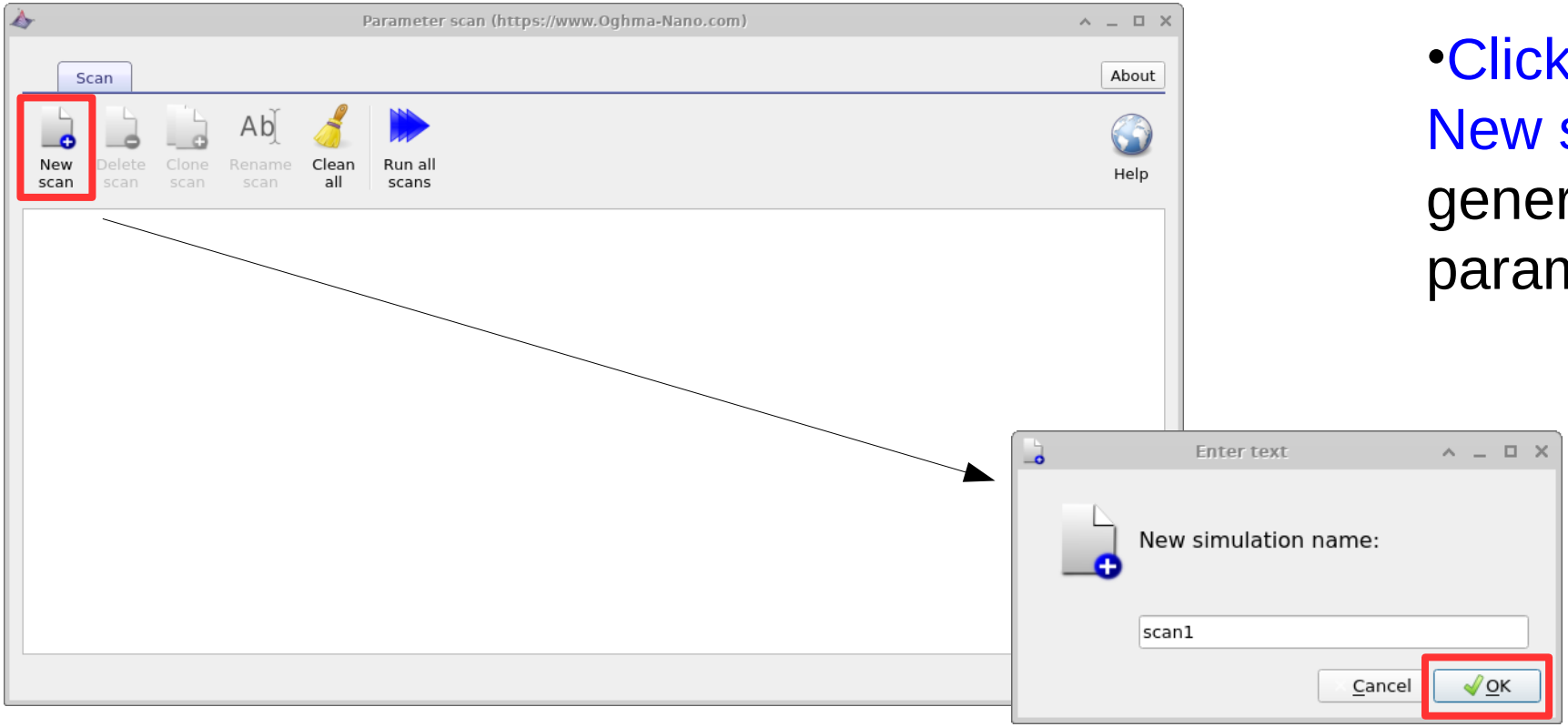


- Often we want to change a simulation parameter several times to understand how a parameter affects a device.

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

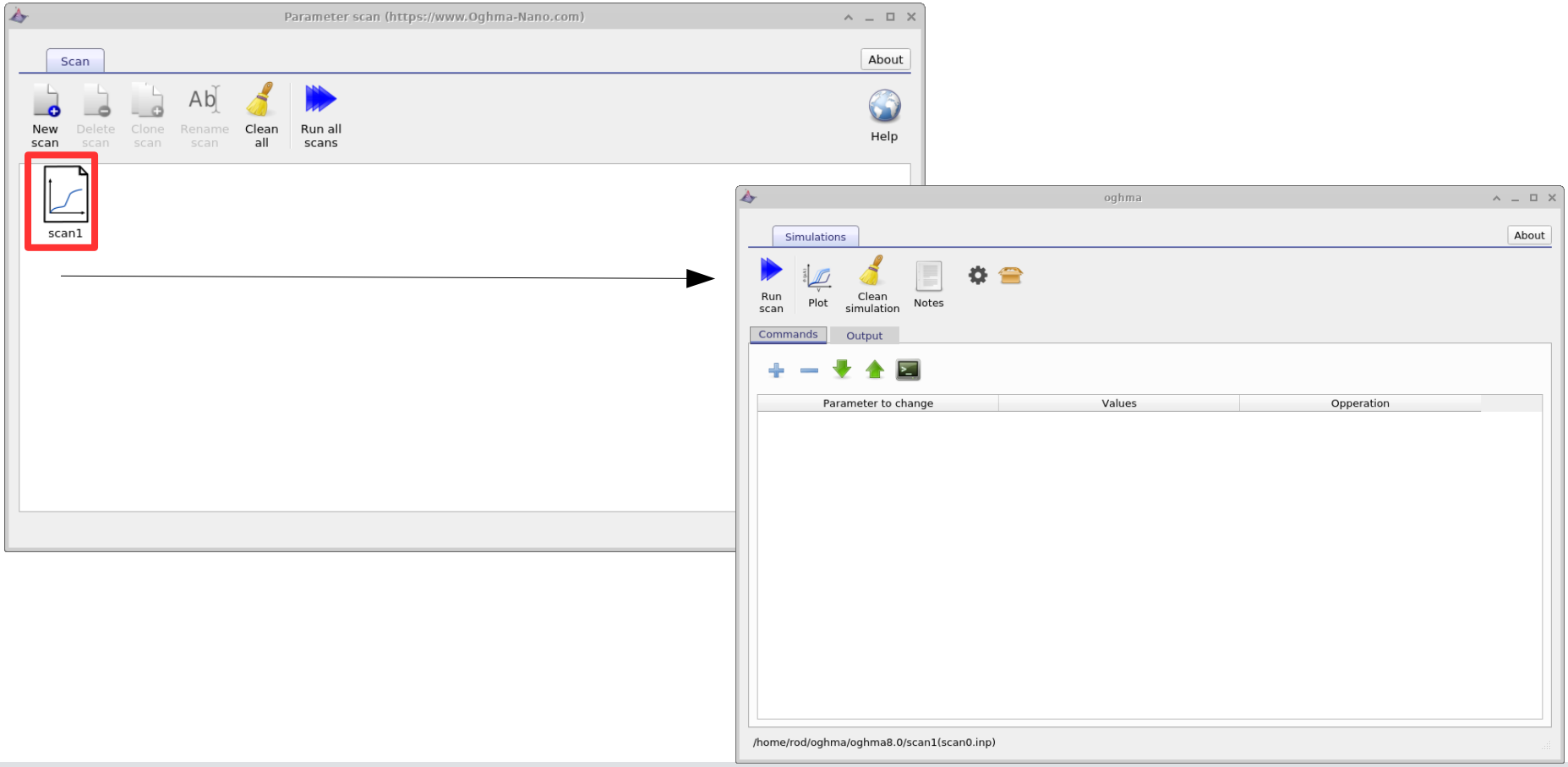
- **Click on the parameter scan tool**

The parameter scan window

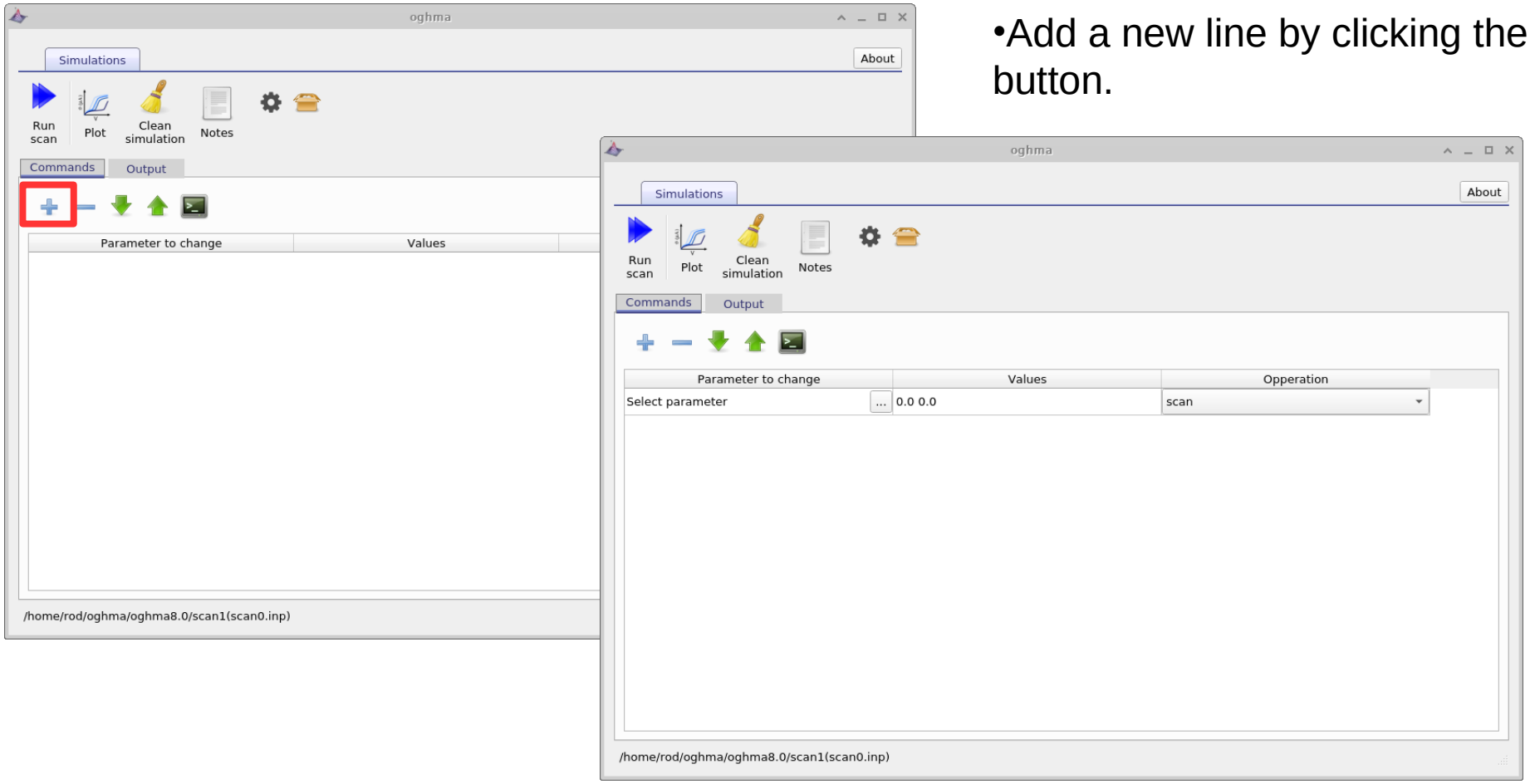


- Click on the New scan to generate a new parameter scan.

The parameter scan window

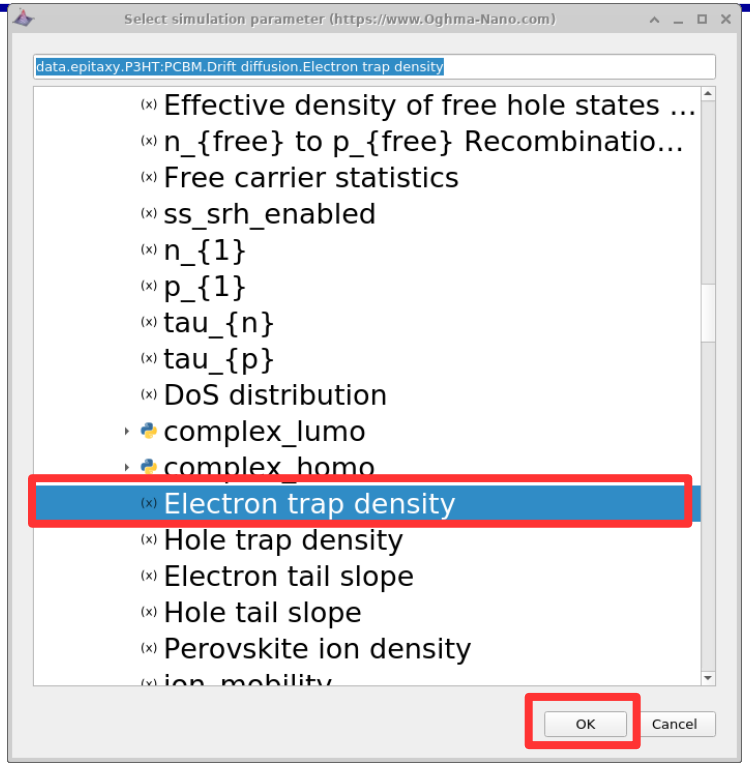


A new line should appear...



- Add a new line by clicking the + button.

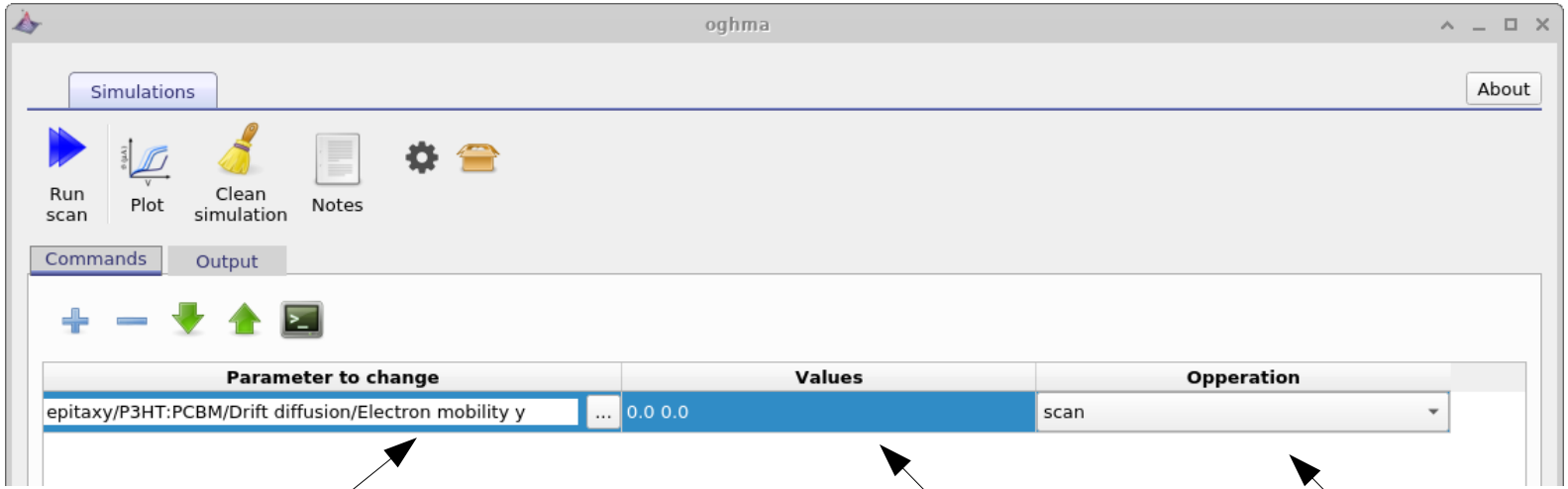
A new line should appear...



•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...

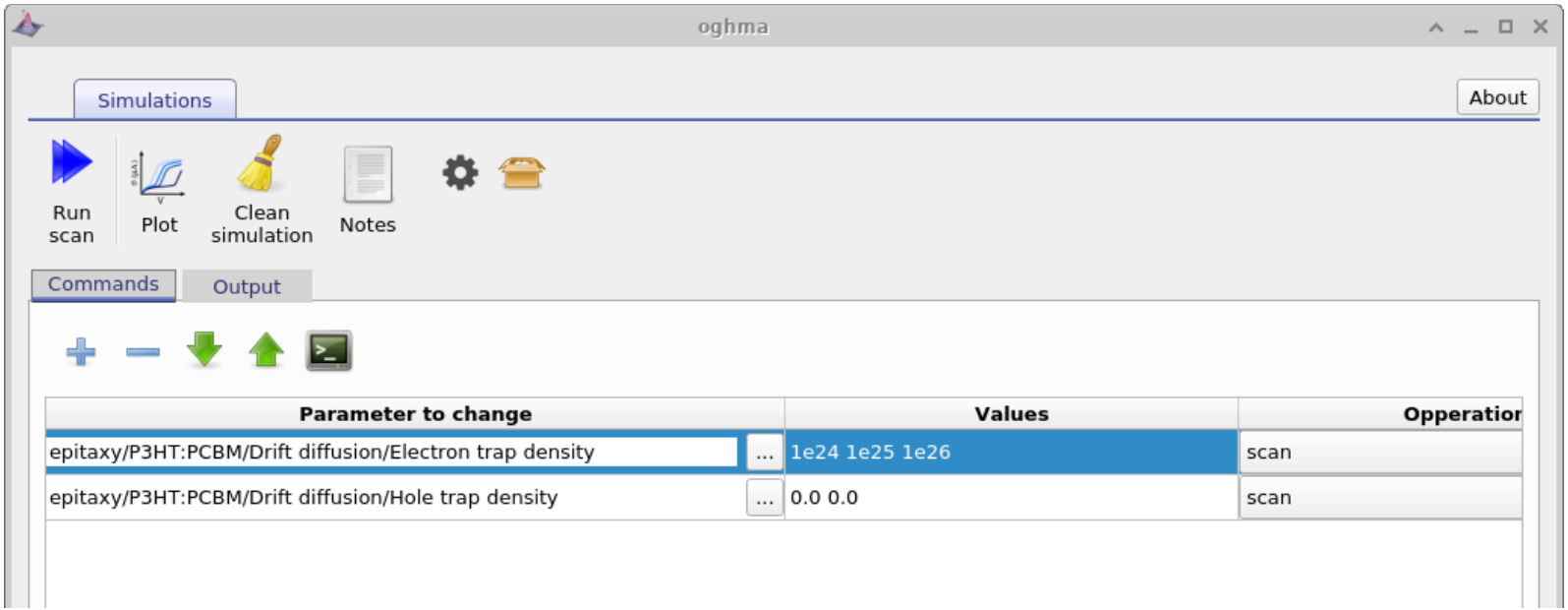


This shows the parameter which will be edited.

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})

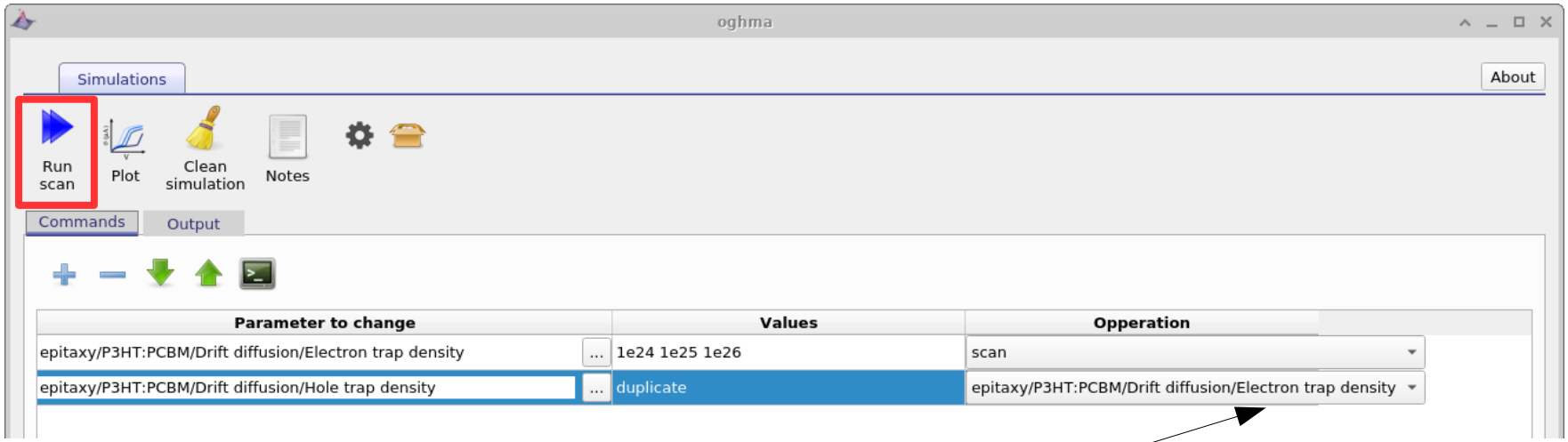
This selects the operation which will be performed. (more explained later)

But we want to simulate a symmetric device (where Ntraph=Ntrape)...



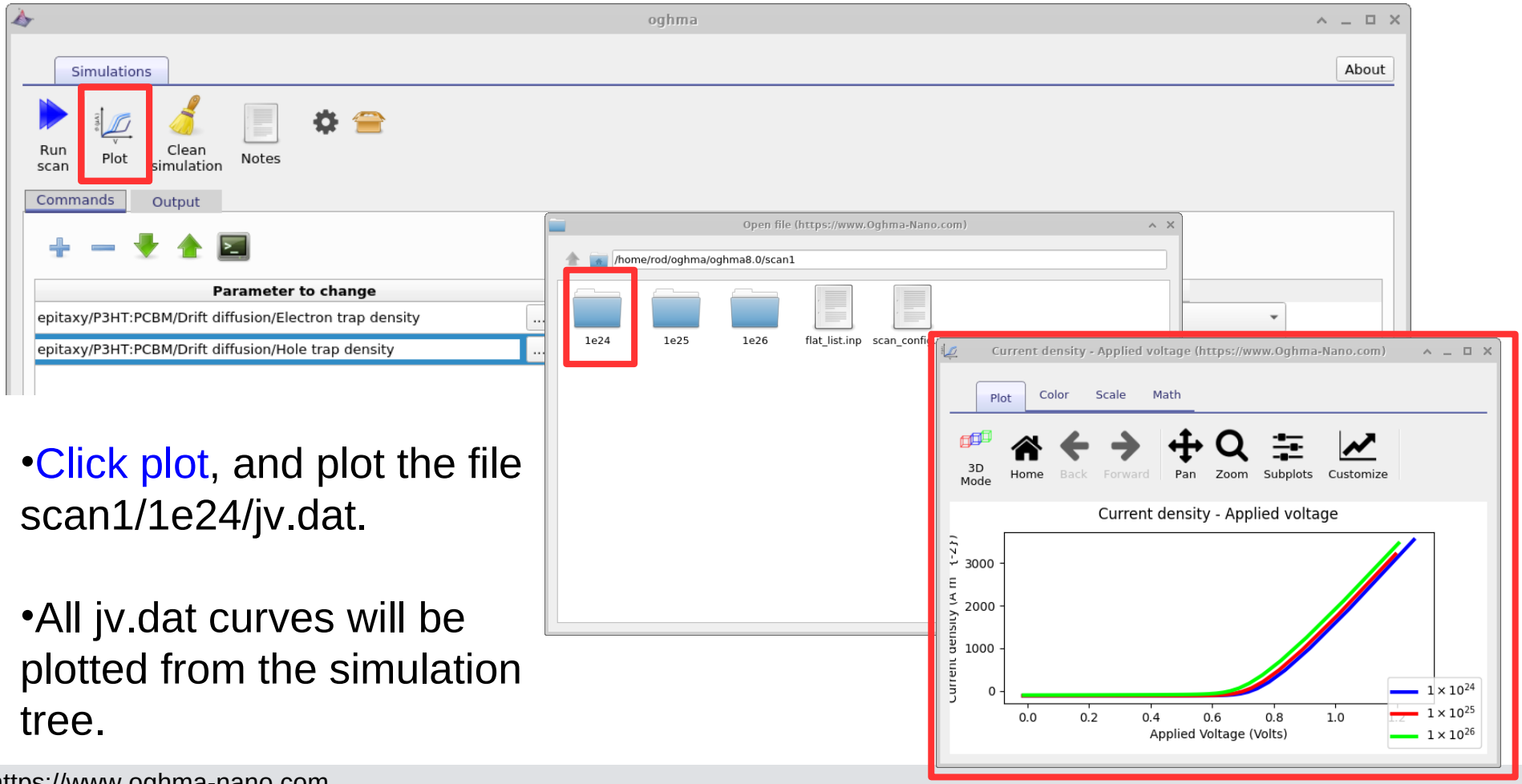
So using the '+' button add another row and then using the '...' buttons make it look like the above..

But we want to simulate a symmetric device (where Ntraph=Ntrape)...



- 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.

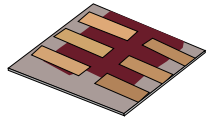
Plotting the results.



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

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

Overview



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