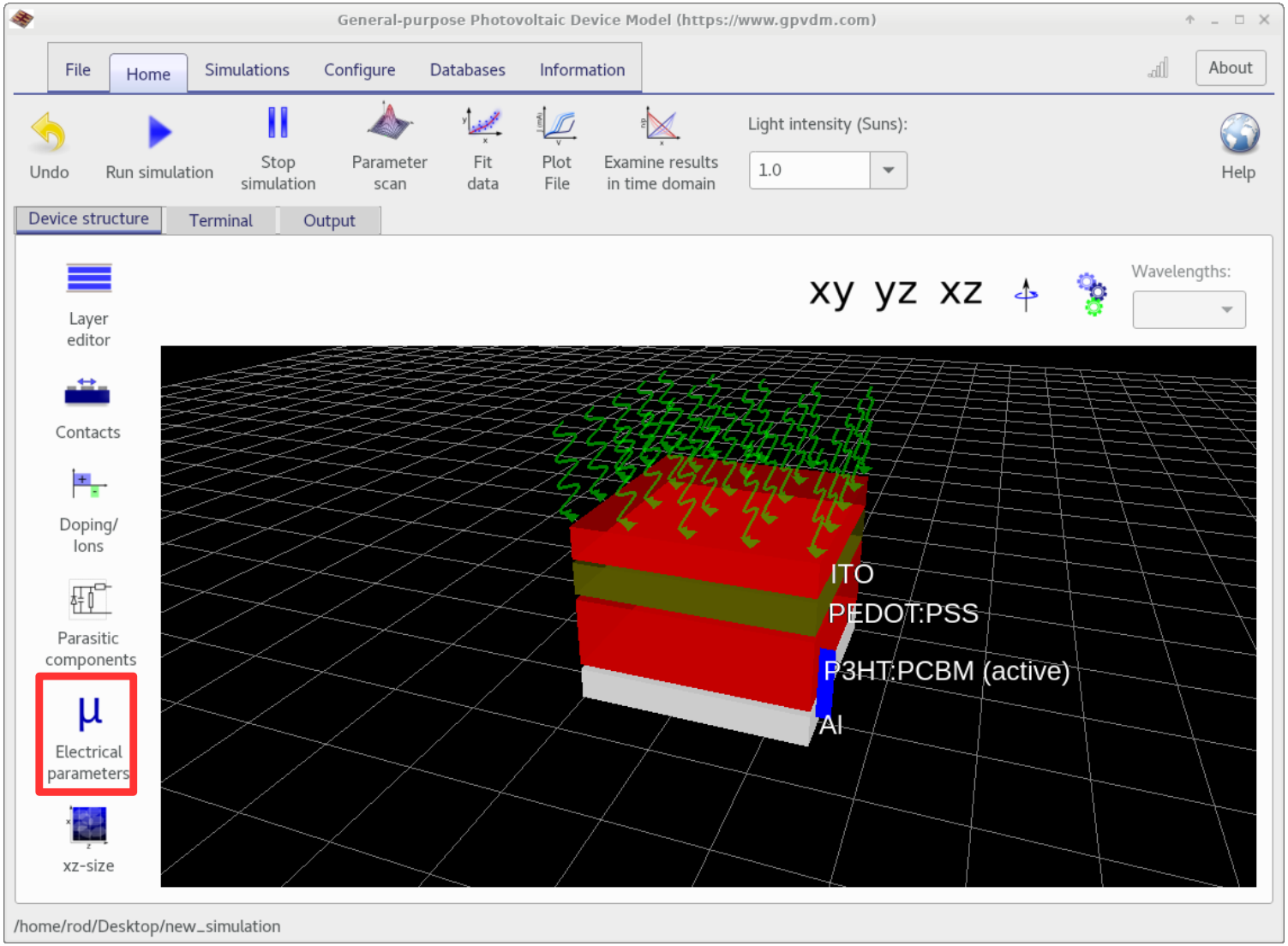
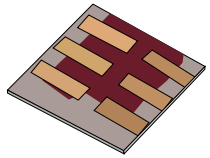
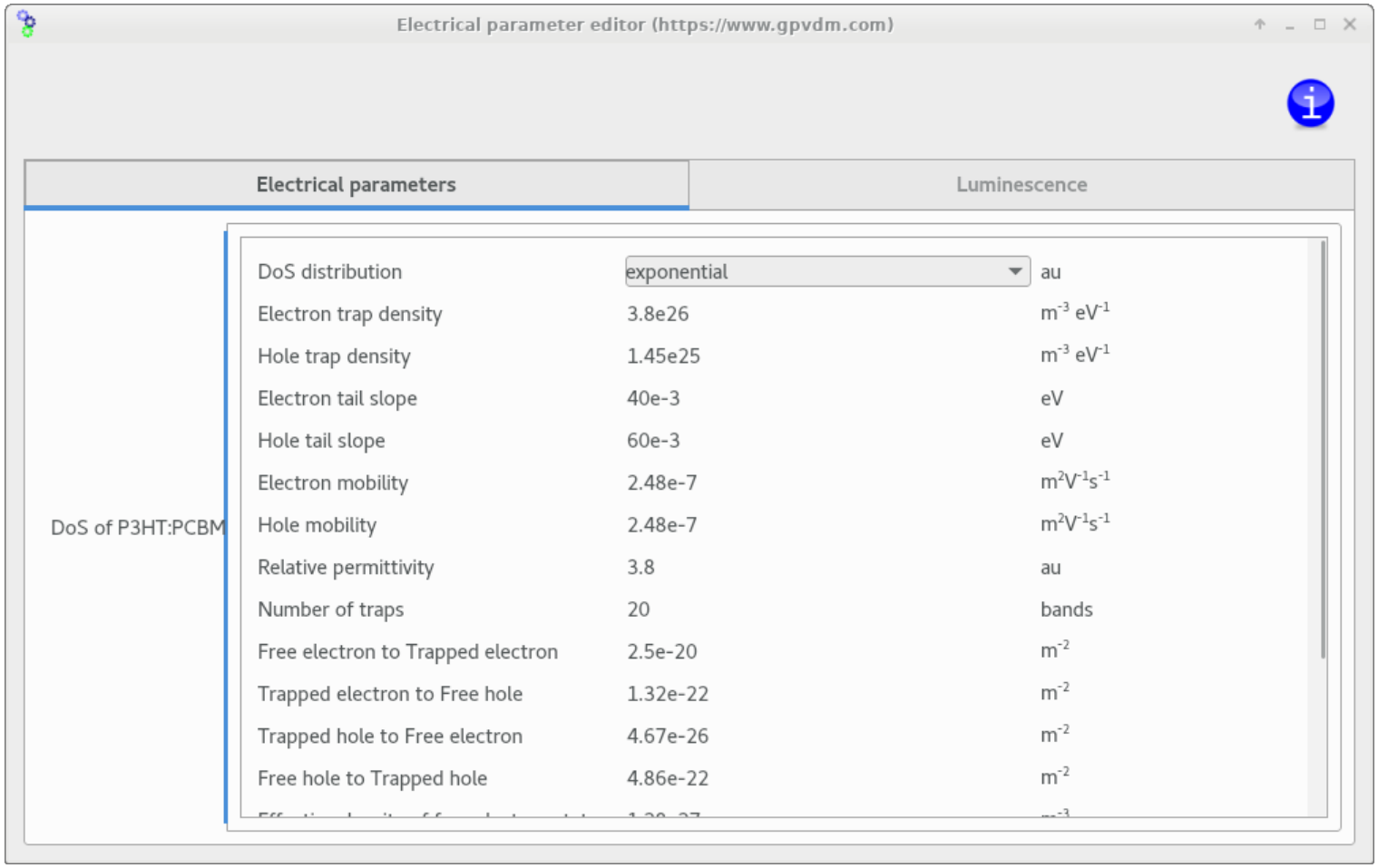
Editing the electrical parameters of a material



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

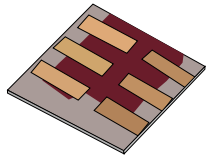
This is the electrical parameter window





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

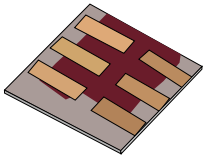
Types of layers in gpvdm:

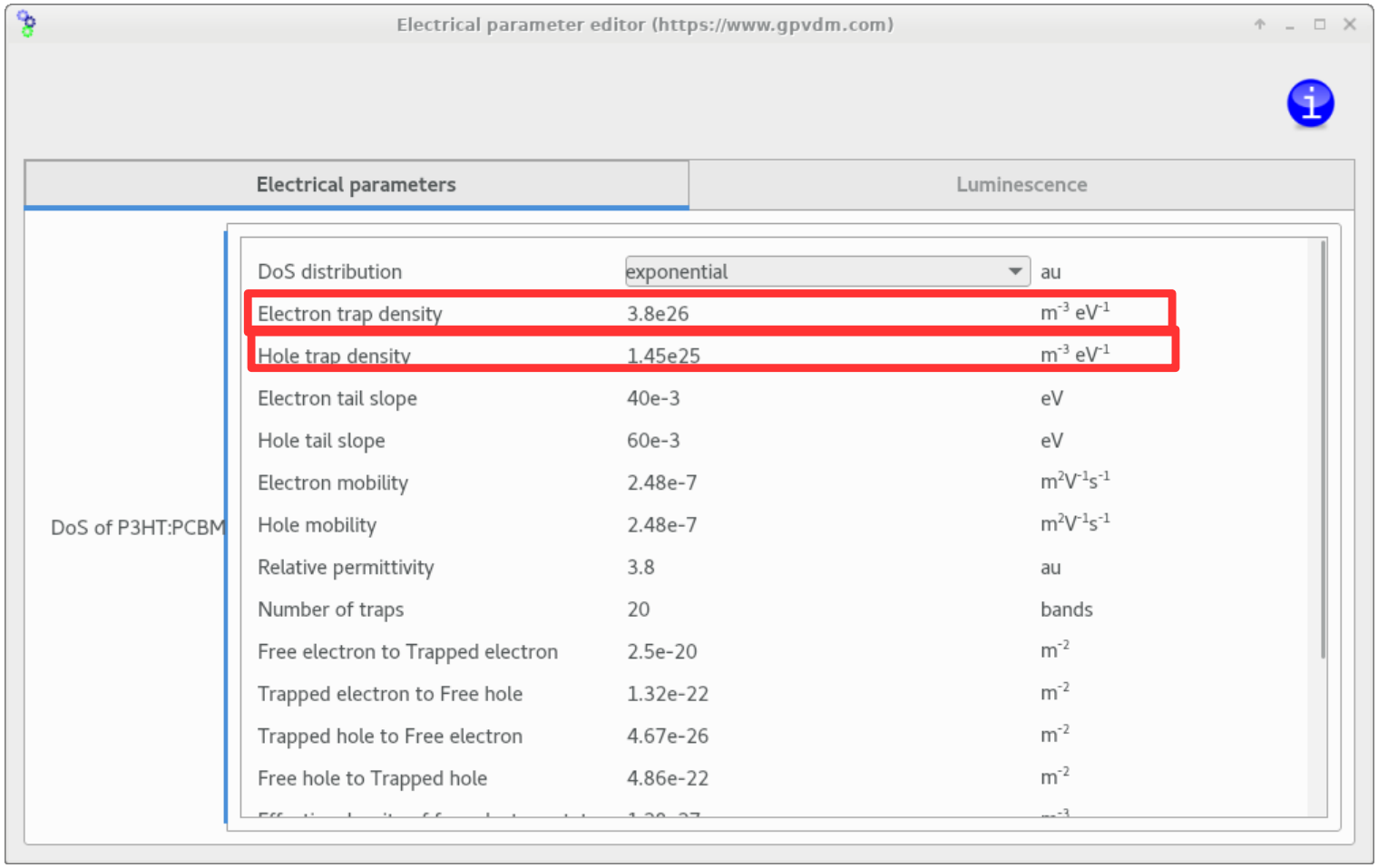


Layer type	Description	Electrical Equations solved	Optical Equations solved.
active	The electrical model is solved over these layers, each layer gets it's own set of electrical parameters.	Yes	Yes
other	No electrical equations are solved in these layers.	No	Yes
contact	These layers are used to define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

- The layer type can be changed using the layer editor…. more on this later.

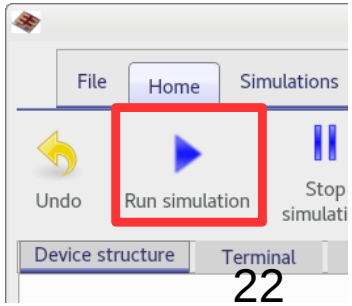
Editing an electrical parameter...the trap density….



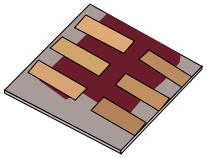


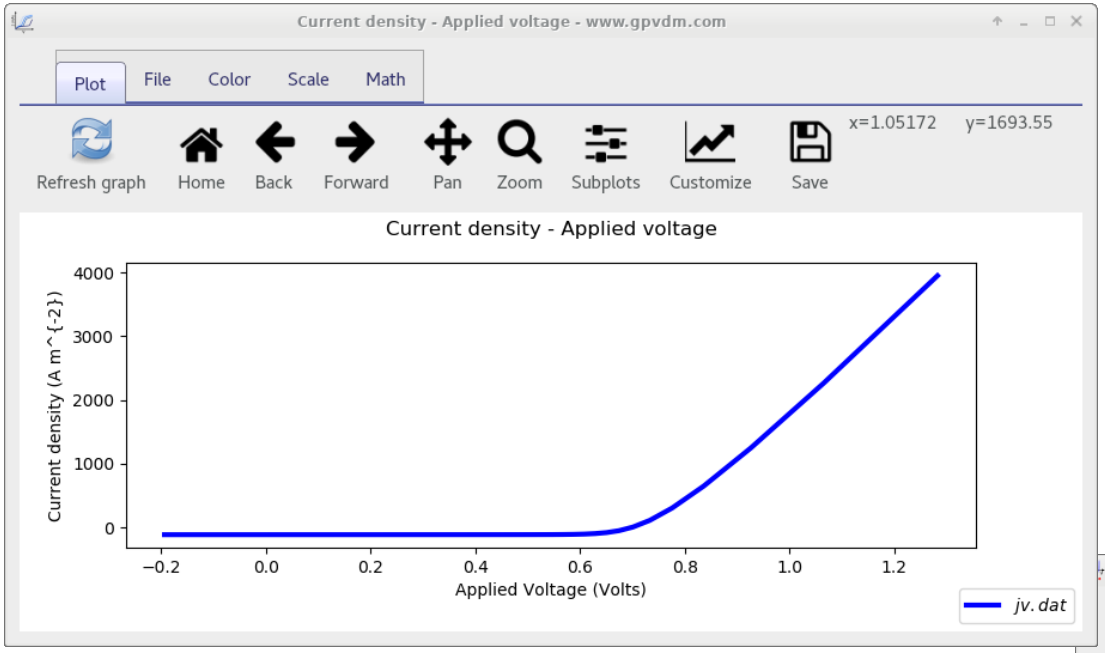
a) Make the density of trap state symetric at $1x10^{24}$ $m^{-3,}$ and rerun the simulation.

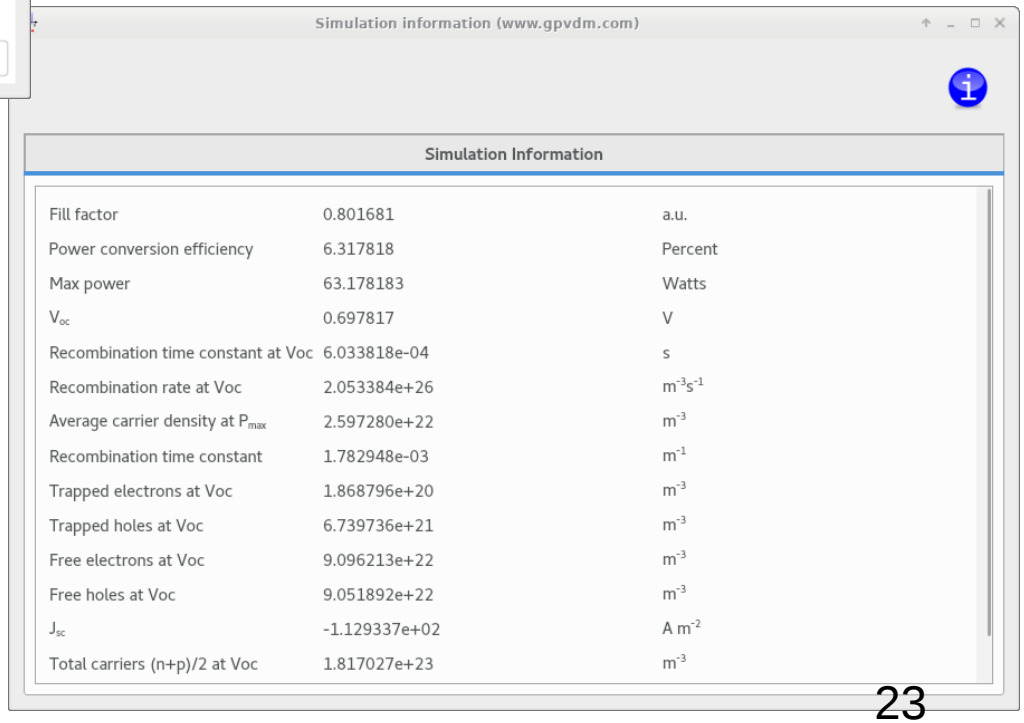
b) Now re-plot the JV curve (**jv.dat**), also find the (**sim_info.dat)** file, double click on it and find the power conversion efficiency.



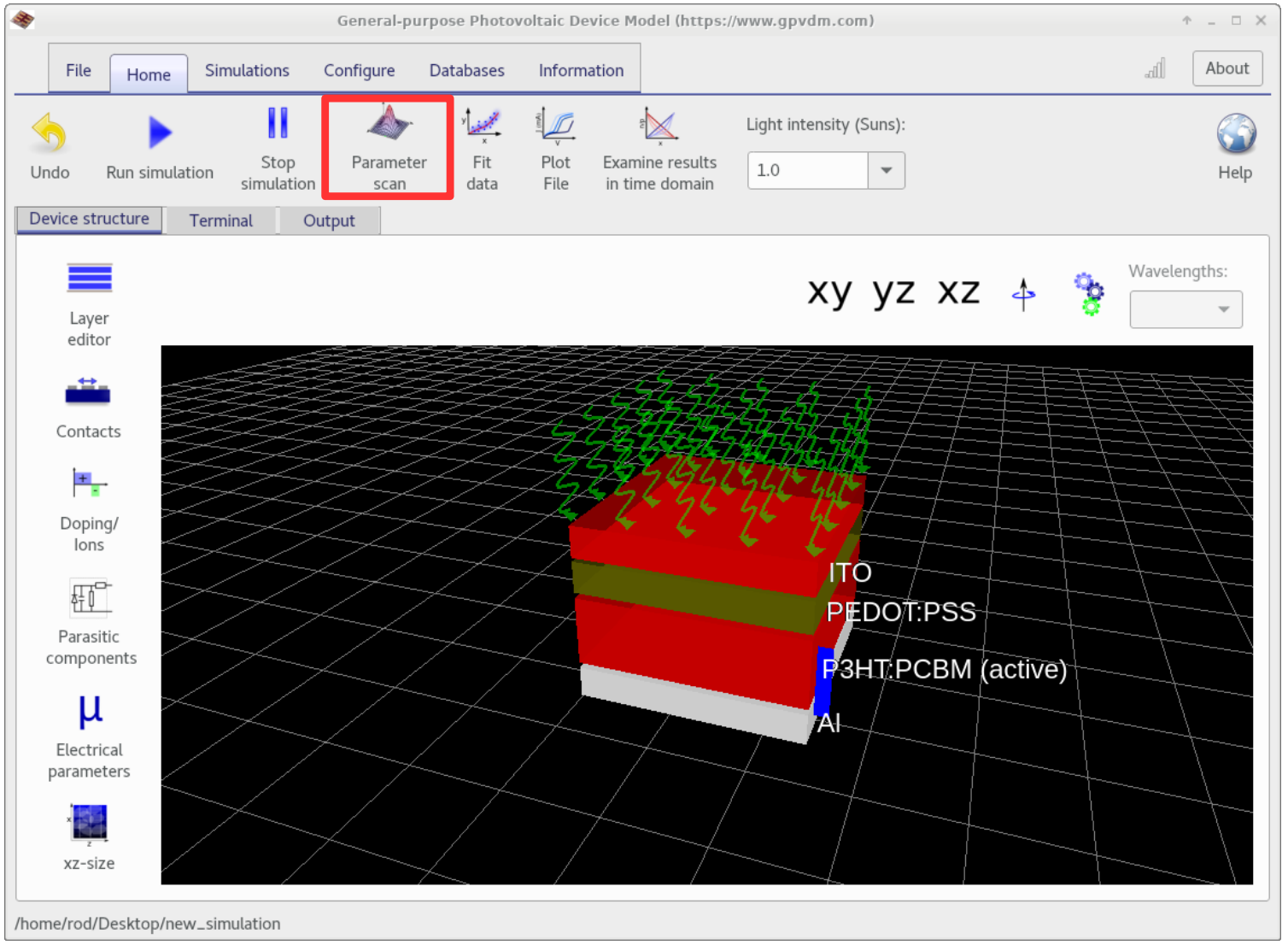
You should have results which look a bit like this:







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

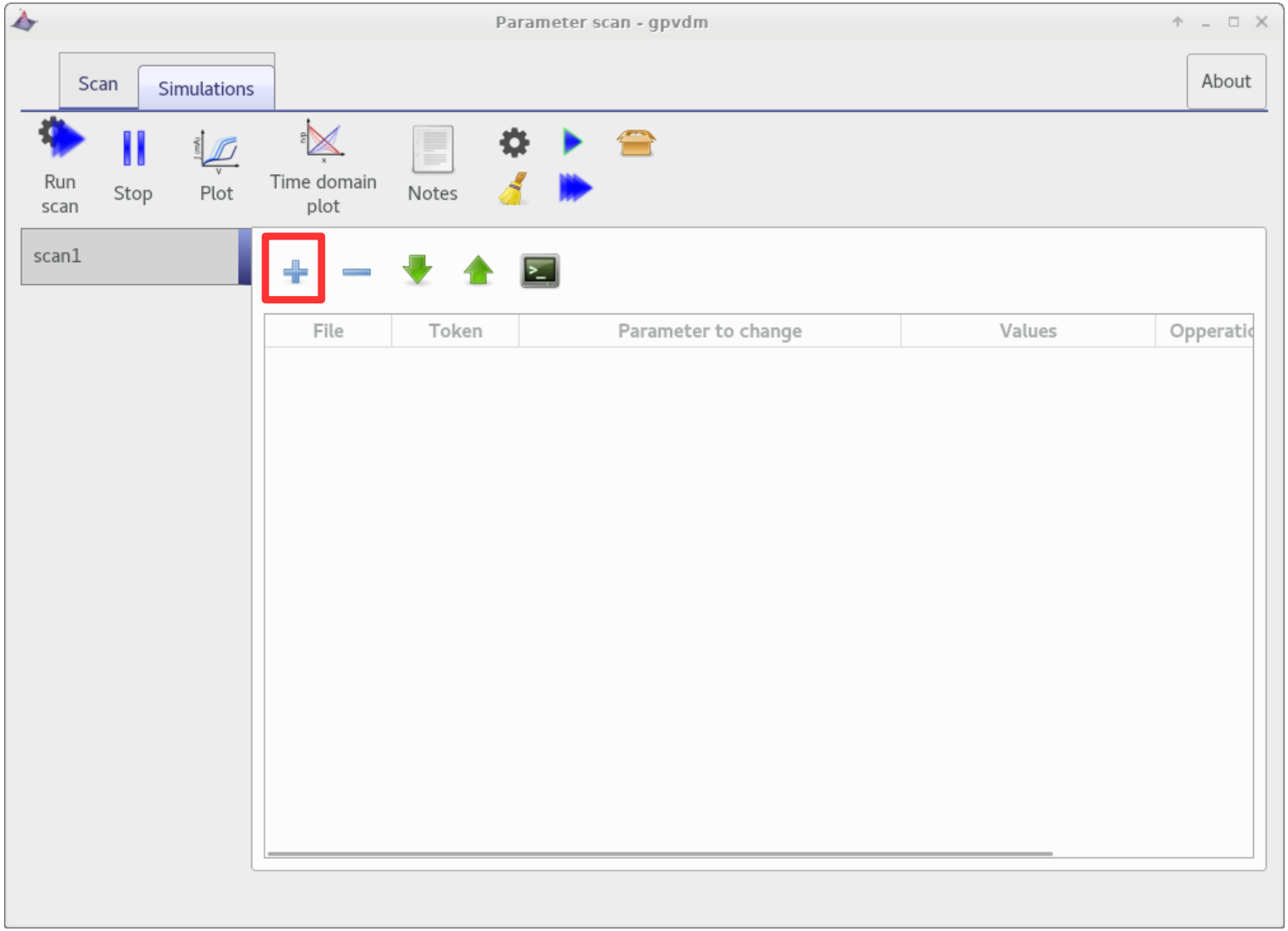


- Often we want to change a simulation parameter several times to understand how a parameter affects a device.

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

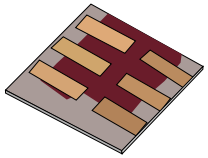
- **Click on the parameter scan tool**

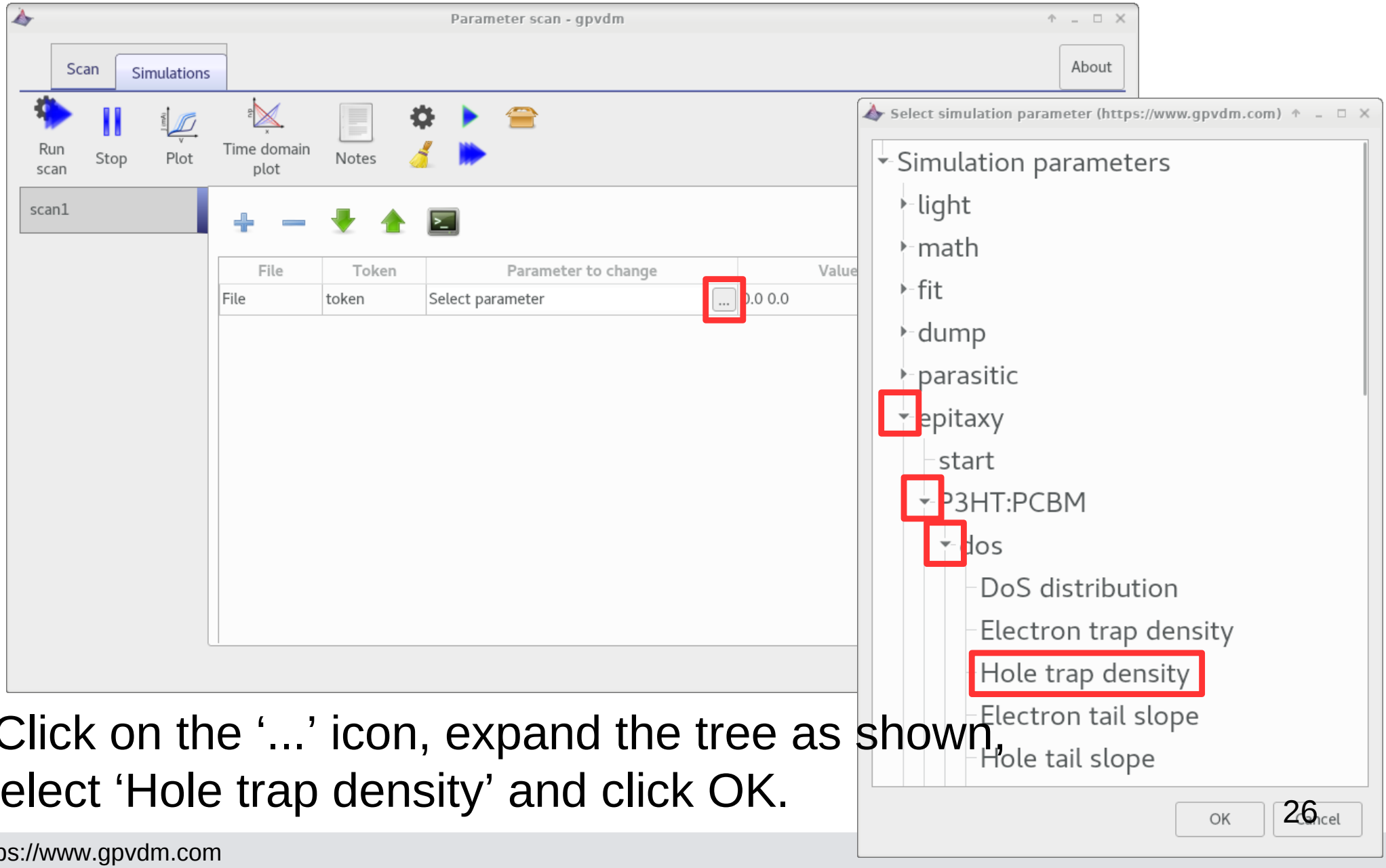
The parameter scan window



•Click on the + to add a new line to the scan.

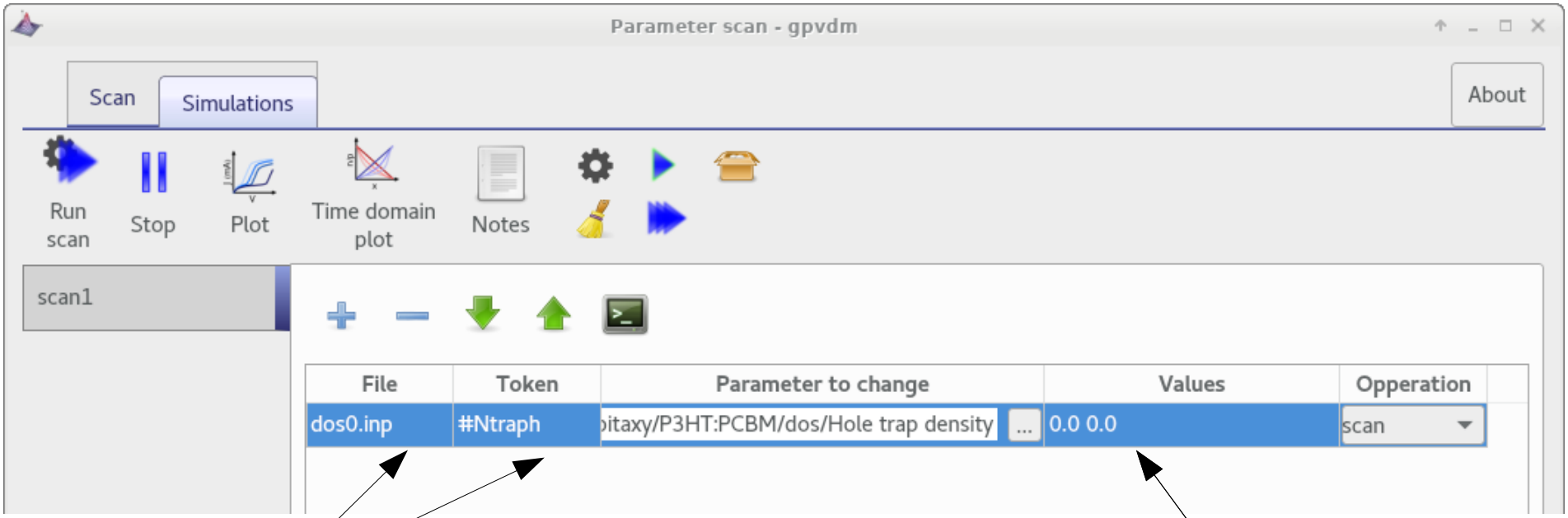
A new line should appear...





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

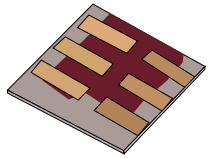
The parameter scan window...

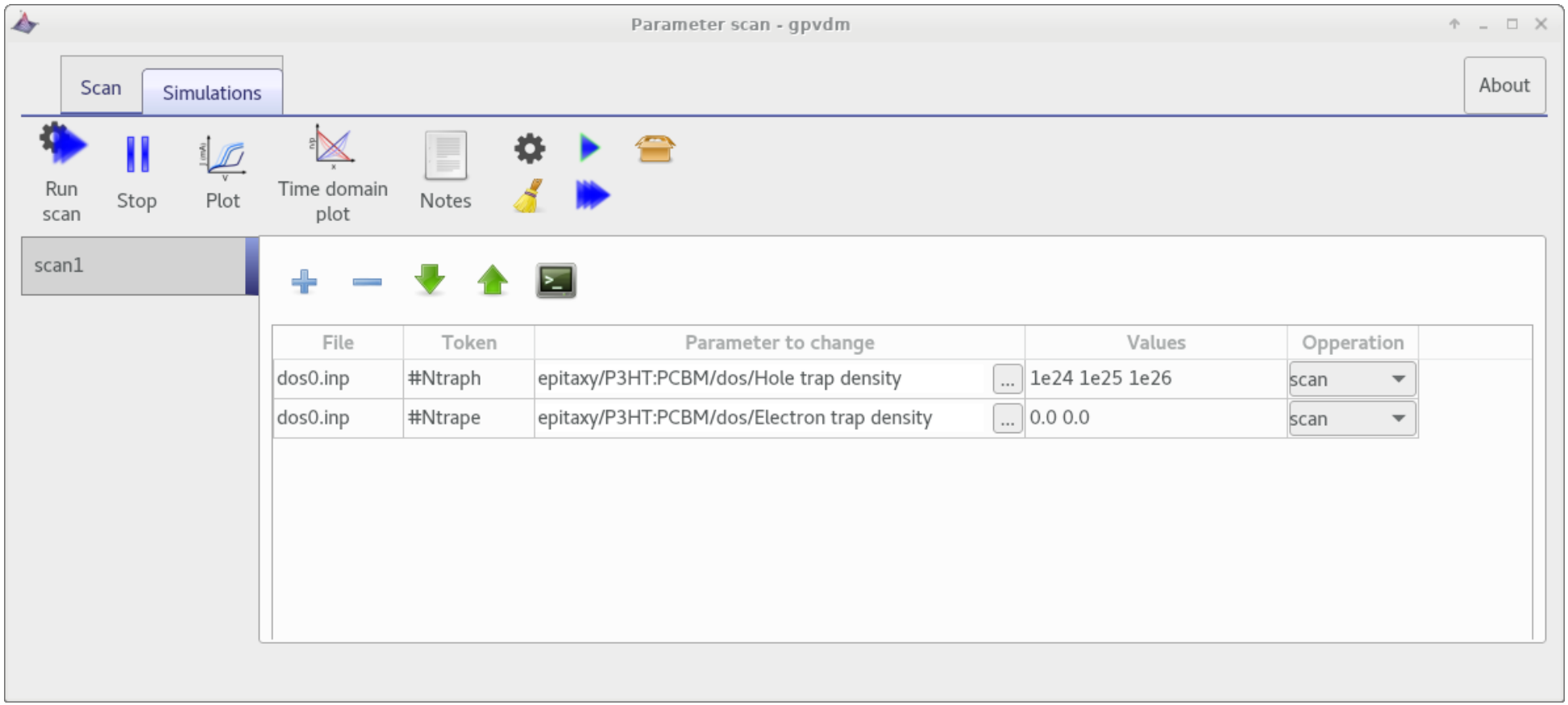


This shows the file/section of the file which will be edited (generated automatically).

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})

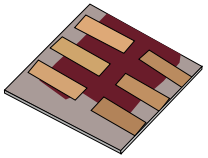
But we want to simulate a symmetric device (where Ntraph=Ntrape)...

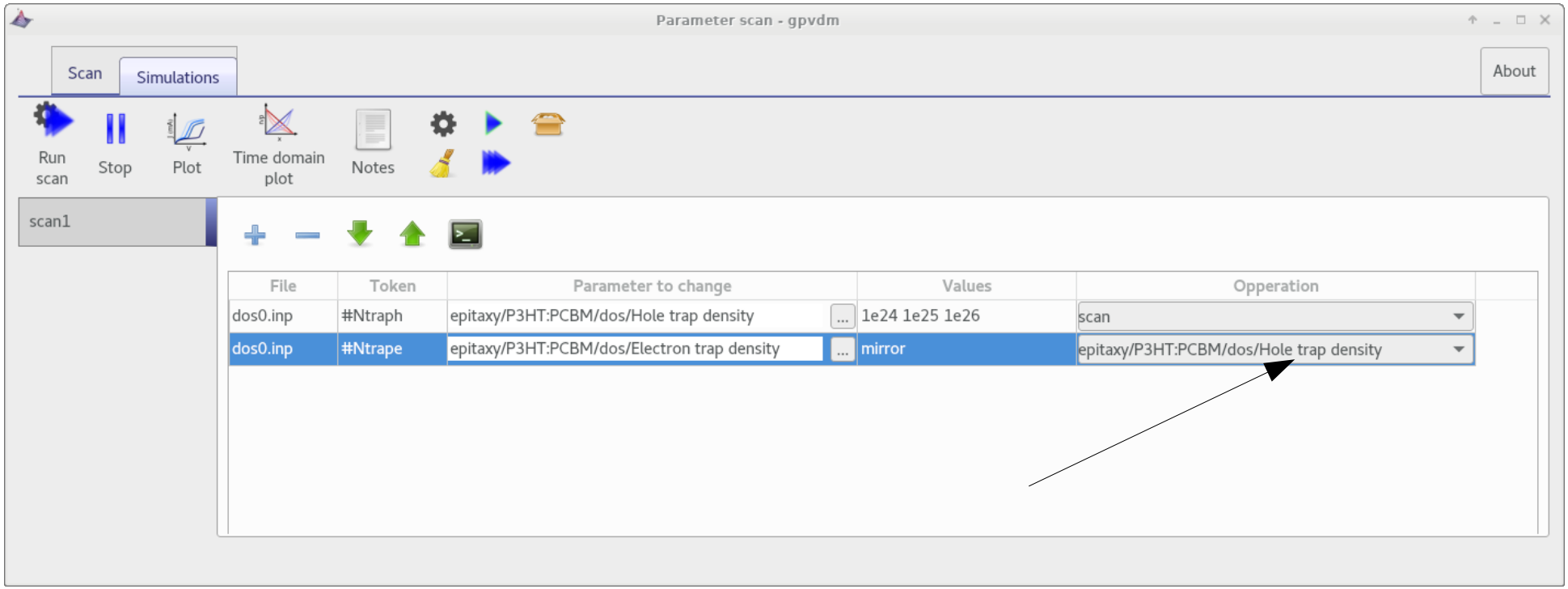




So using the '+' button add another row and then using the '...' buttons make it look like the above..

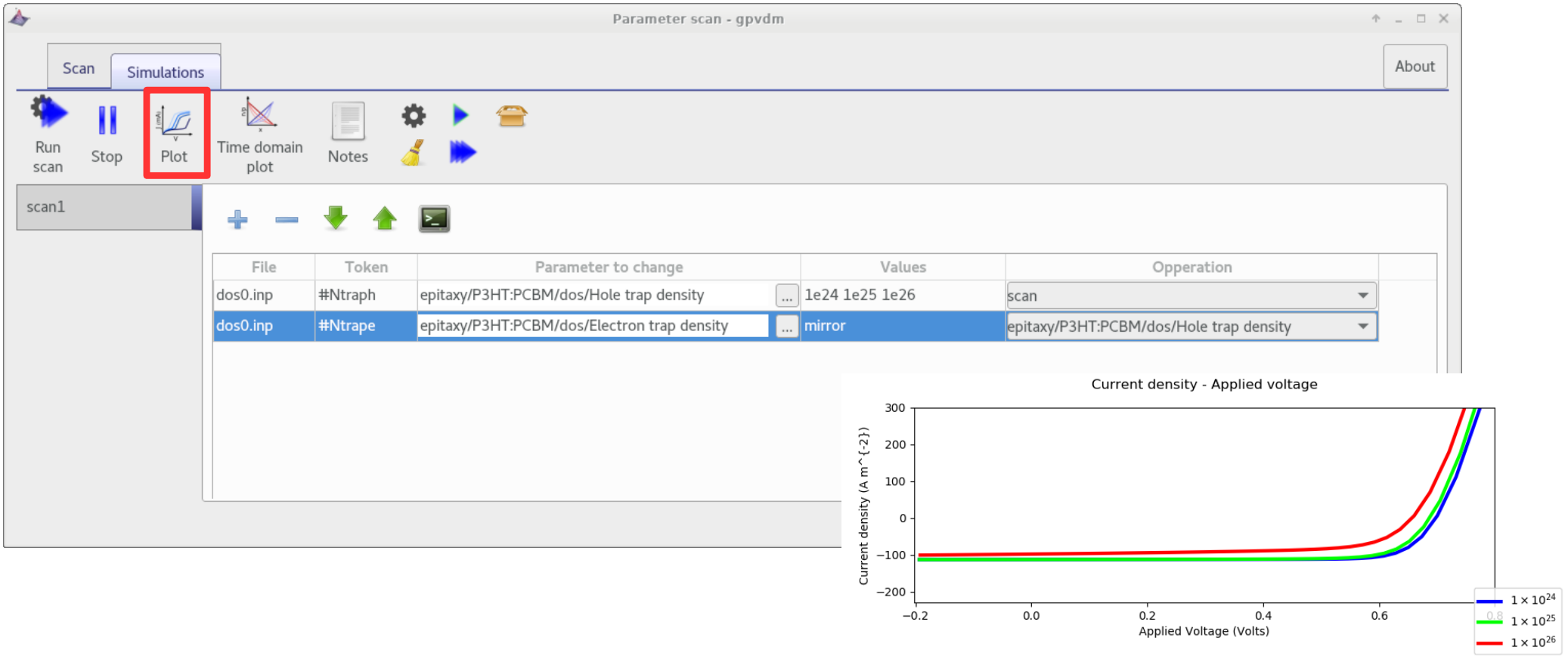
But we want to simulate a symmetric device (where Ntraph=Ntrape)...





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

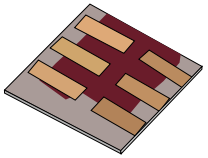
Plotting the results.

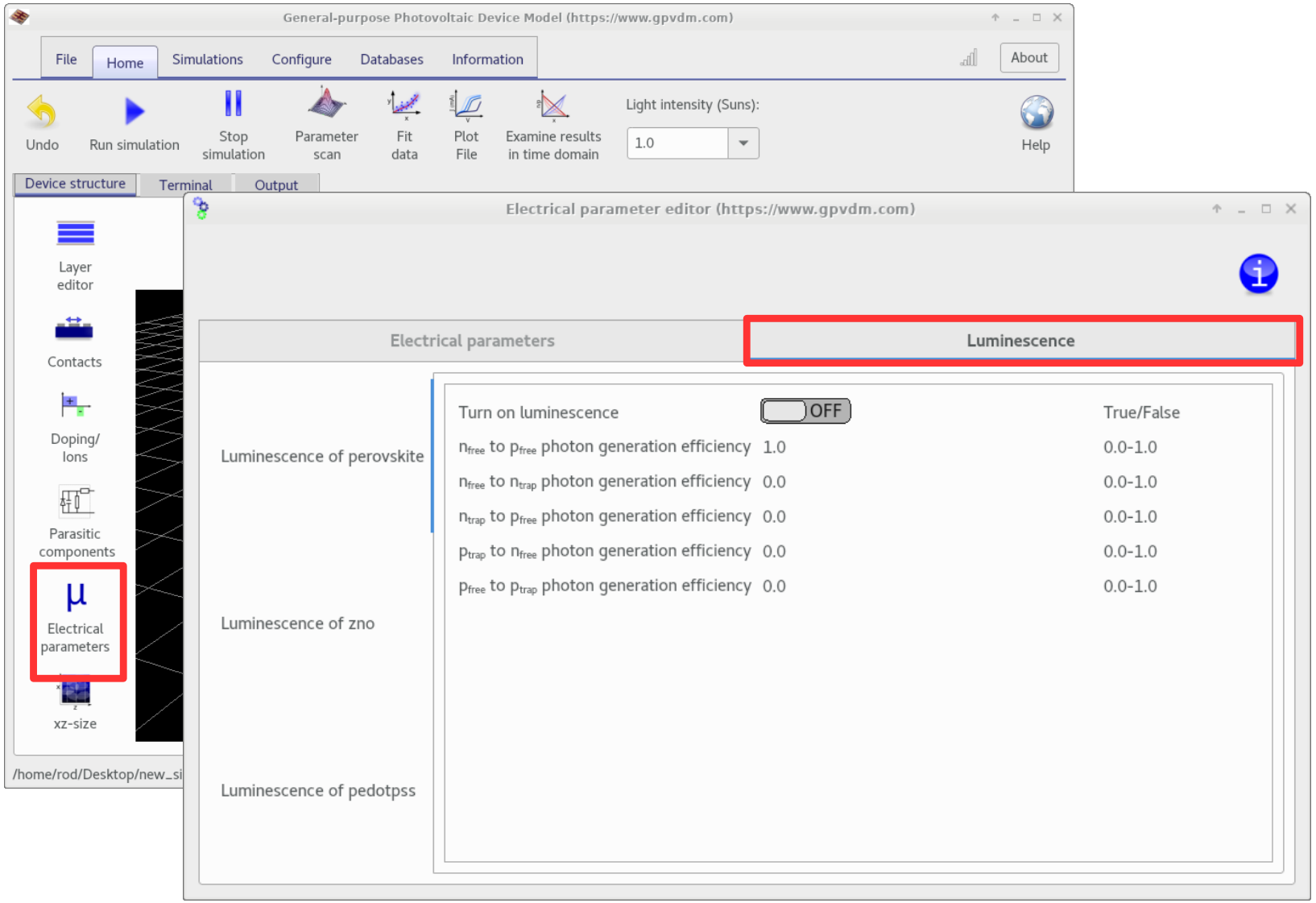


- Click plot, and plot the file scan1/1e24/jv.dat.

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

A final note on the electrical parameter window...





- We can assign a photon generation efficiency to each recombination process, so we an get a predicted PL/EL spectrum…

- We can only do this because we know where the carriers are in energy space across the device.