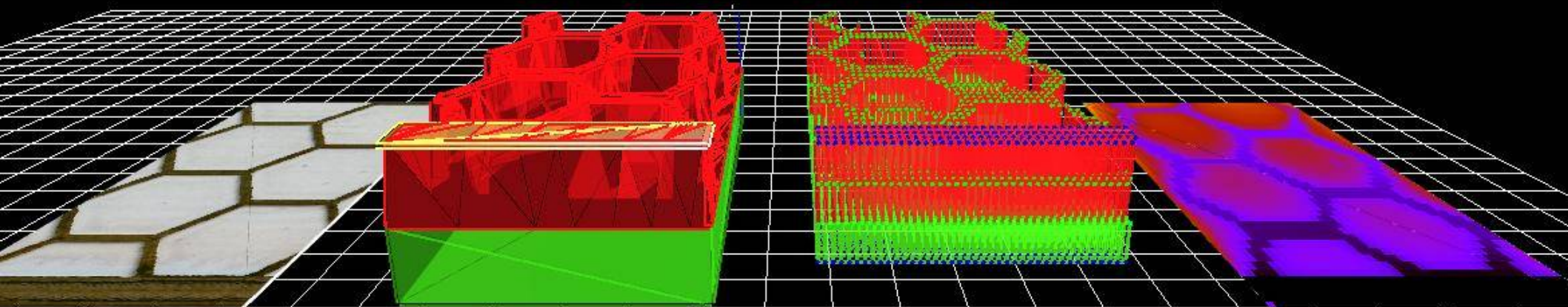
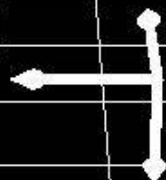


# Making a new simulation in *OghmaNano*



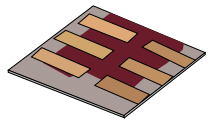
<https://www.oghma-nano.com>



Dr. Roderick MacKenzie  
roderick.mackenzie@durham.ac.uk

Autumn 2022

# Your first OghmaNano simulation



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

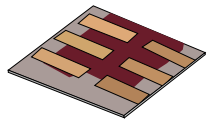
The screenshot shows the main application window titled "Organic and hybrid Material Nano Simulation tool" with a menu bar including File, Simulation type, Simulation Editors, Electrical, Optical, Thermal, Databases, and About. The "File" menu is open, and the "New simulation" option is highlighted with a red box. A dialog box titled "New simulation" is open, asking "Which type of device would you like to simulate?". The "New simulation" button in the dialog is also highlighted with a red box. The dialog contains a grid of device options, each with a small icon and a label:

- P3HT:PCBM solar cell (PCE=4%)
- 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
- papers

At the bottom of the dialog, there is a checkbox for "Show hidden" 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](mailto: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

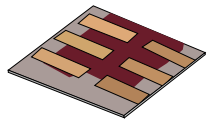
Layer editor Contacts Electrical parameters Emission parameters Substrate xz-size XY YZ XZ

ITO  
PEDOT:PSS  
P3HT:PCBM (active)  
Al

/home/rod/oghma/oghma8.0

## Click the play button

# The core solver will be run on CPU 0

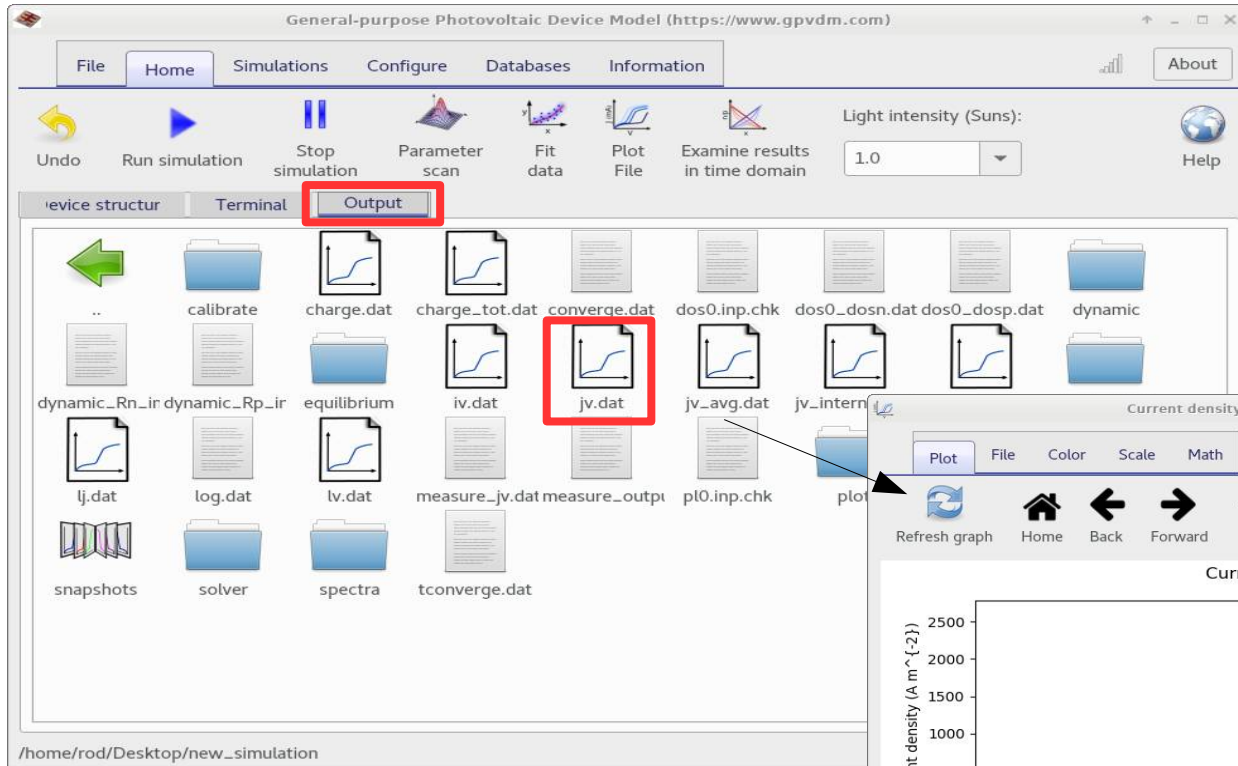
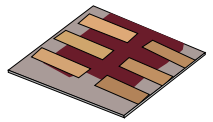


```
Organic and hybrid Material Nano Simulation tool (https://www.oghma-nano.com)
File Simulation type Simulation Editors Electrical Optical Thermal Databases Information
Questions? Contact: roderick.mackenzie@durham.ac.uk About
New simulation Open simulation Export Zip Run simulation Parameter scan Fit to experimental data Optical Simulation Machine Learning Edit Probes
Script Editor

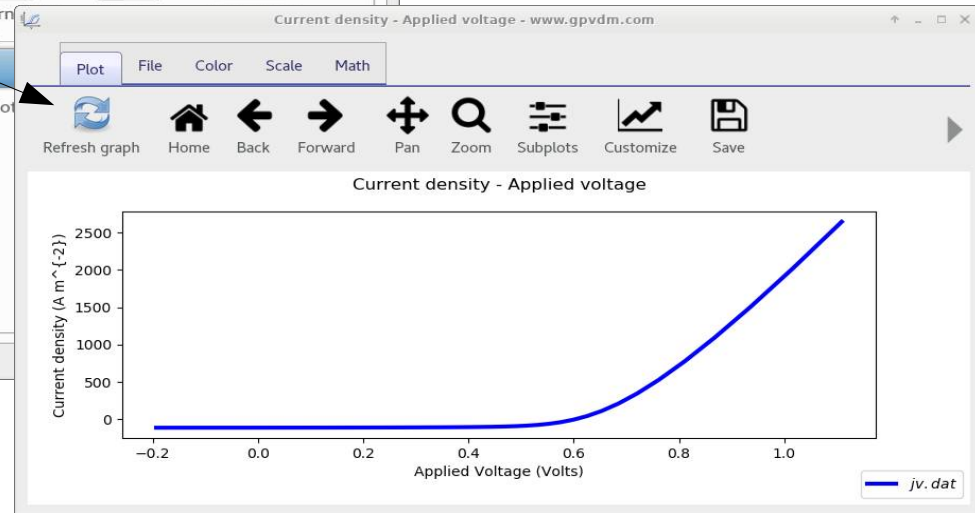
device structure Terminal Output Tutorials/Documentation
CPU 0 top= 0.36 V, -1.09e+02 A/m^2, btm= 0.00 V, -1.09e+02 A/m^2 f()=9.225806e-09 2.784912 ms
CPU 0 top= 0.38 V, -1.08e+02 A/m^2, btm= 0.00 V, -1.08e+02 A/m^2 f()=8.960899e-09 2.794922 ms
CPU 1 top= 0.40 V, -1.07e+02 A/m^2, btm= 0.00 V, -1.08e+02 A/m^2 f()=8.765618e-09 2.794189 ms
CPU 1 top= 0.42 V, -1.06e+02 A/m^2, btm= 0.00 V, -1.06e+02 A/m^2 f()=8.414331e-09 2.988770 ms
CPU 2 top= 0.44 V, -1.05e+02 A/m^2, btm= 0.00 V, -1.05e+02 A/m^2 f()=7.583864e-09 2.793945 ms
CPU 2 top= 0.46 V, -1.02e+02 A/m^2, btm= 0.00 V, -1.02e+02 A/m^2 f()=5.804115e-09 2.836914 ms
CPU 2 top= 0.48 V, -9.92e+01 A/m^2, btm= 0.00 V, -9.92e+01 A/m^2 f()=3.795407e-09 2.800049 ms
CPU 3 top= 0.50 V, -9.48e+01 A/m^2, btm= 0.00 V, -9.48e+01 A/m^2 f()=2.125123e-09 3.133057 ms
CPU 3 top= 0.52 V, -8.83e+01 A/m^2, btm= 0.00 V, -8.83e+01 A/m^2 f()=1.022912e-09 2.913086 ms
CPU 4 top= 0.54 V, -7.87e+01 A/m^2, btm= 0.00 V, -7.88e+01 A/m^2 f()=4.628513e-10 2.777832 ms
CPU 4 top= 0.56 V, -6.44e+01 A/m^2, btm= 0.00 V, -6.44e+01 A/m^2 f()=1.973159e-10 2.863037 ms
CPU 5 top= 0.58 V, -4.28e+01 A/m^2, btm= 0.00 V, -4.28e+01 A/m^2 f()=9.135184e-11 2.669922 ms
CPU 5 top= 0.60 V, -1.04e+01 A/m^2, btm= 0.00 V, -1.04e+01 A/m^2 f()=1.206325e-09 3.277832 ms
CPU 6 top= 0.62 V, 3.79e+01 A/m^2, btm= 0.00 V, 3.79e+01 A/m^2 f()=3.016961e-11 3.008057 ms
CPU 6 top= 0.64 V, 1.09e+02 A/m^2, btm= 0.00 V, 1.09e+02 A/m^2 f()=2.265345e-11 3.102051 ms
CPU 7 top= 0.66 V, 2.13e+02 A/m^2, btm= 0.00 V, 2.13e+02 A/m^2 f()=2.189347e-11 4.281982 ms
CPU 7 top= 0.68 V, 3.60e+02 A/m^2, btm= 0.00 V, 3.60e+02 A/m^2 f()=-2.367089e-11 3.309814 ms
CPU 7 top= 0.70 V, 5.65e+02 A/m^2, btm= 0.00 V, 5.65e+02 A/m^2 f()=3.047228e-11 2.974854 ms
CPU 7 top= 0.72 V, 8.44e+02 A/m^2, btm= 0.00 V, 8.45e+02 A/m^2 f()=4.172688e-11 2.854004 ms
Cluster top= 0.74 V, 1.22e+03 A/m^2, btm= 0.00 V, 1.22e+03 A/m^2 f()=6.145060e-11 3.283936 ms
Cluster top= 0.76 V, 1.70e+03 A/m^2, btm= 0.00 V, 1.70e+03 A/m^2 f()=-1.444342e-10 2.790039 ms
Cluster top= 0.78 V, 2.33e+03 A/m^2, btm= 0.00 V, 2.33e+03 A/m^2 f()=-2.338285e-10 2.807129 ms
Cluster top= 0.80 V, 3.11e+03 A/m^2, btm= 0.00 V, 3.11e+03 A/m^2 f()=-2.006914e-10 2.877930 ms
Stopping because of Vexternal 1.163852e+00>1.100000e+00
Solved 9245 Equations
unload DLLs
Bytes, written 905798 , read 406934
Files, read 23 written 601
```

- Blue is CPU usage, red is disk usage, if you simulation is running slowly, writing to the hard disk is **always** the bottleneck, SSDs highly recommended.
- Don't run your simulation in Dropbox/OneDrive or any type of network drive, network communication is far too slow to run simulations.

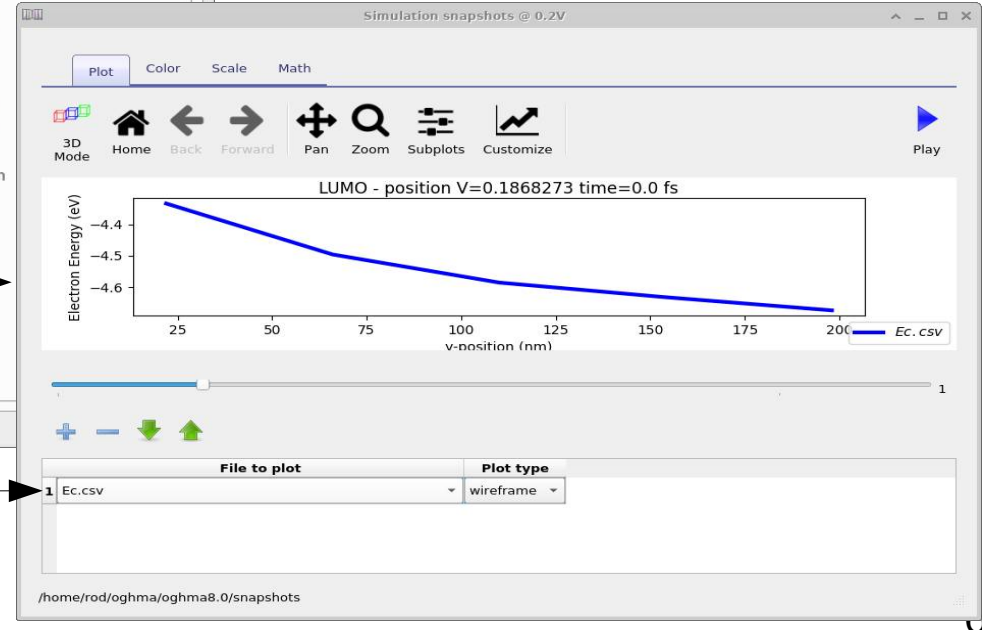
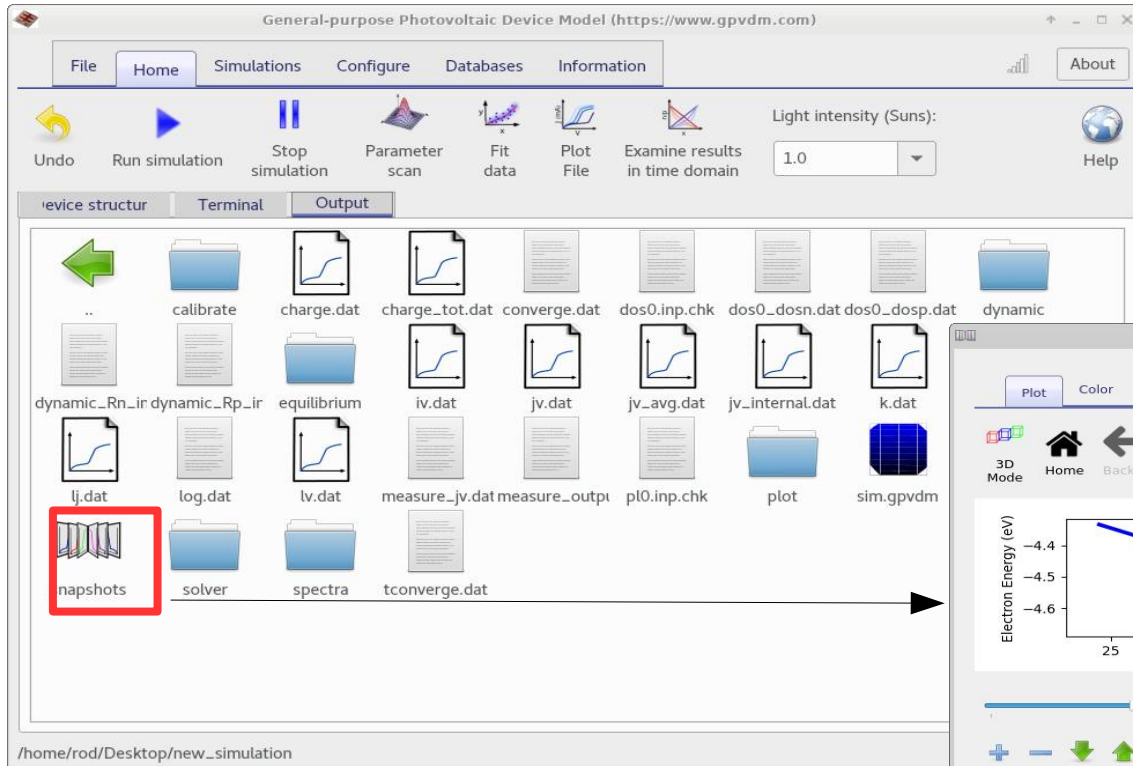
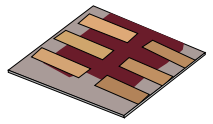
# Examining the results.



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

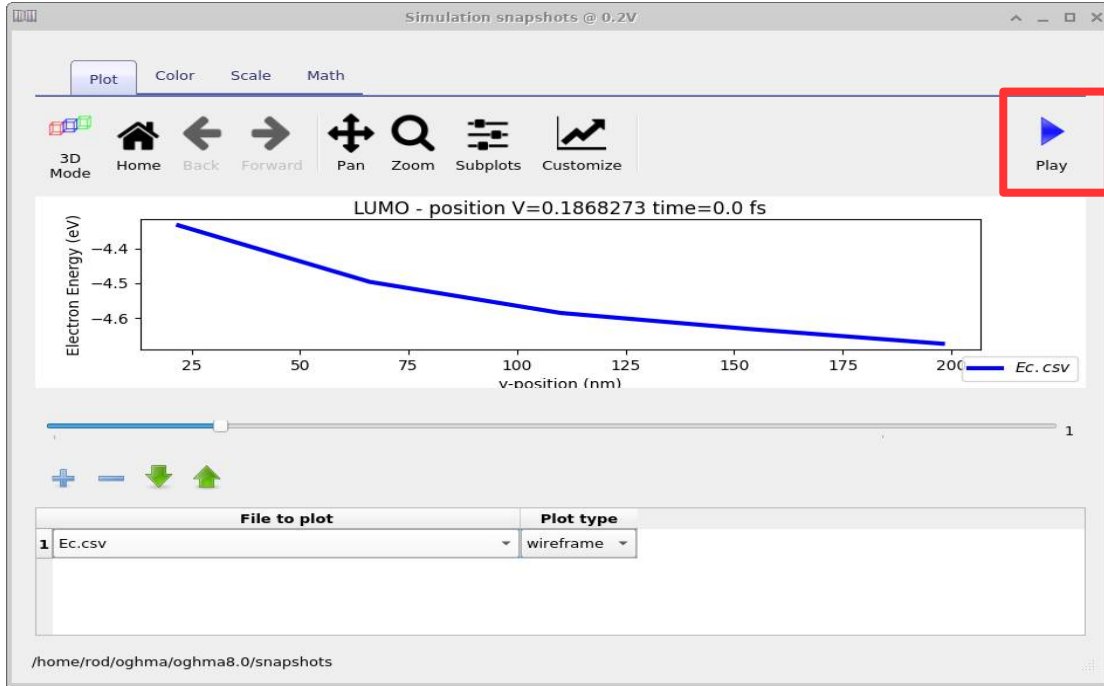
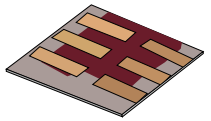


The snapshots window, this is used to show changes in the device as a function of voltage and time.



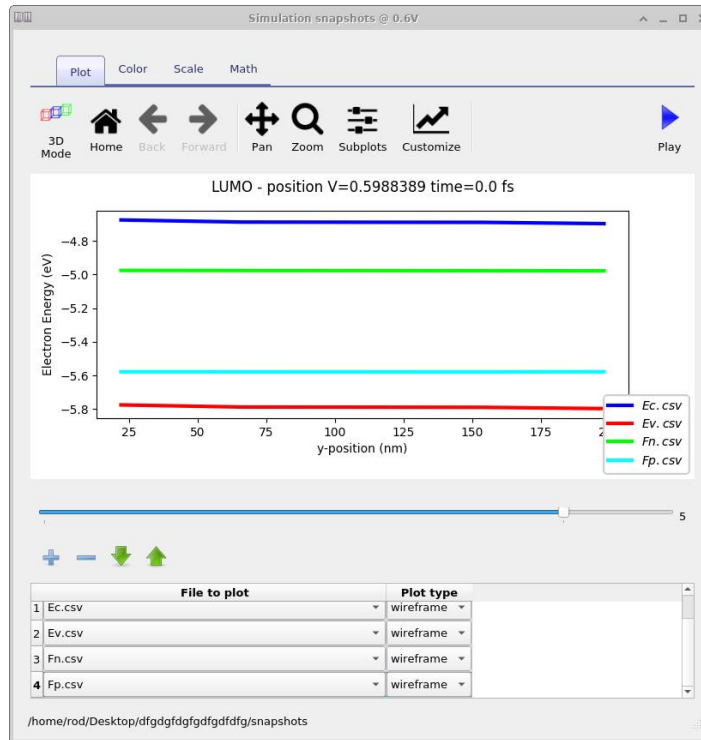
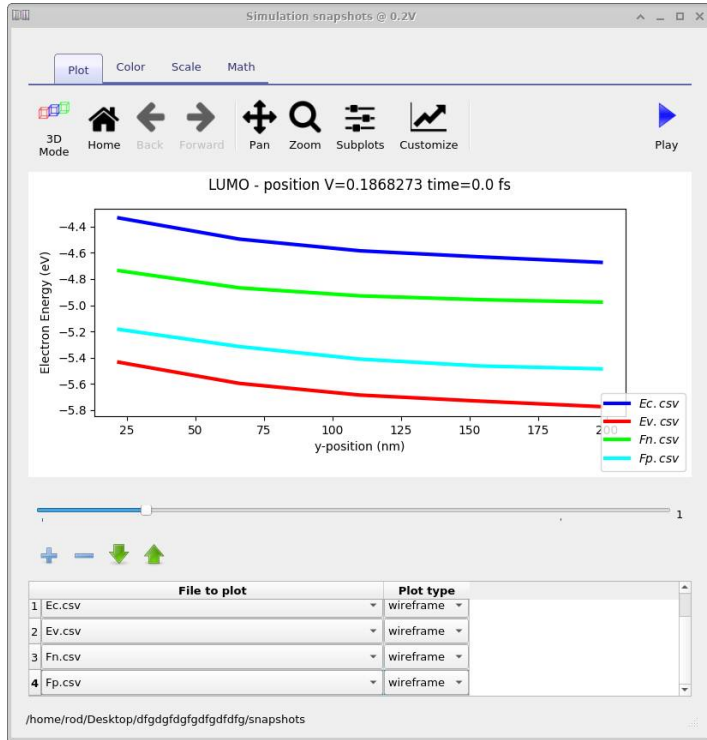
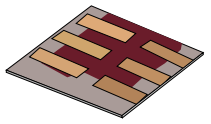
Set this to Ec.csv (The Conduction band/LUMO)

# Using the snapshots window



- Click play and the simulation will iterate through each voltage step. If you were doing a time domain simulation it would do the same.

# More complex snapshot plots



- You can also add multiple outputs to the snapshots window.
- In this example we are plotting  $E_c$  (conduction band),  $E_v$  (valance band),  $F_n$ ,  $F_p$  at the same time.