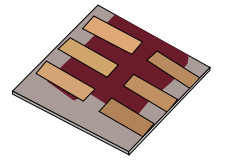
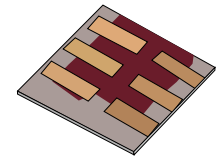


# Overview



- What is gpvdm/theoretical overview?
- Installing gpvdm
- Running simple simulations
  - Your first gpvdm simulation
  - Changing electrical parameters
- Optical simulations and the materials database
- Perovskite solar cells and time domain simulations
- OFET simulations and finite difference meshing.**
- Editing the device structure using the layer editor
- Meshing and dumping

# Make a new OFET simulation



The screenshot shows the 'General-purpose Photovoltaic Device Model' (gpvdm) software interface. The main window has a menu bar with 'File', 'Home', 'Simulations', 'Configure', 'Databases', and 'Information'. The 'File' menu is open, showing 'New simulation', 'Open simulation', and 'Export data'. The 'New simulation' button is highlighted with a red box. Below the menu bar, there is an 'Information' tab with the following text:

**General-purpose photovoltaic device model**  
~~~~~  
<https://www.gpvdms.com>

To make a new simulation click *New Simulation* in the menu, to open an existing simulation select *Open simulation*.

There is more help on the [man pages](#).

Please report bugs to: [roderick.mackenzie@nottingham.ac.uk](mailto:roderick.mackenzie@nottingham.ac.uk)

Follow the gpvdm project:  
[Youtube](#) [Twitter](#)

The status bar at the bottom left shows the path: `/home/rod/t/gpvdms5.0/gui`

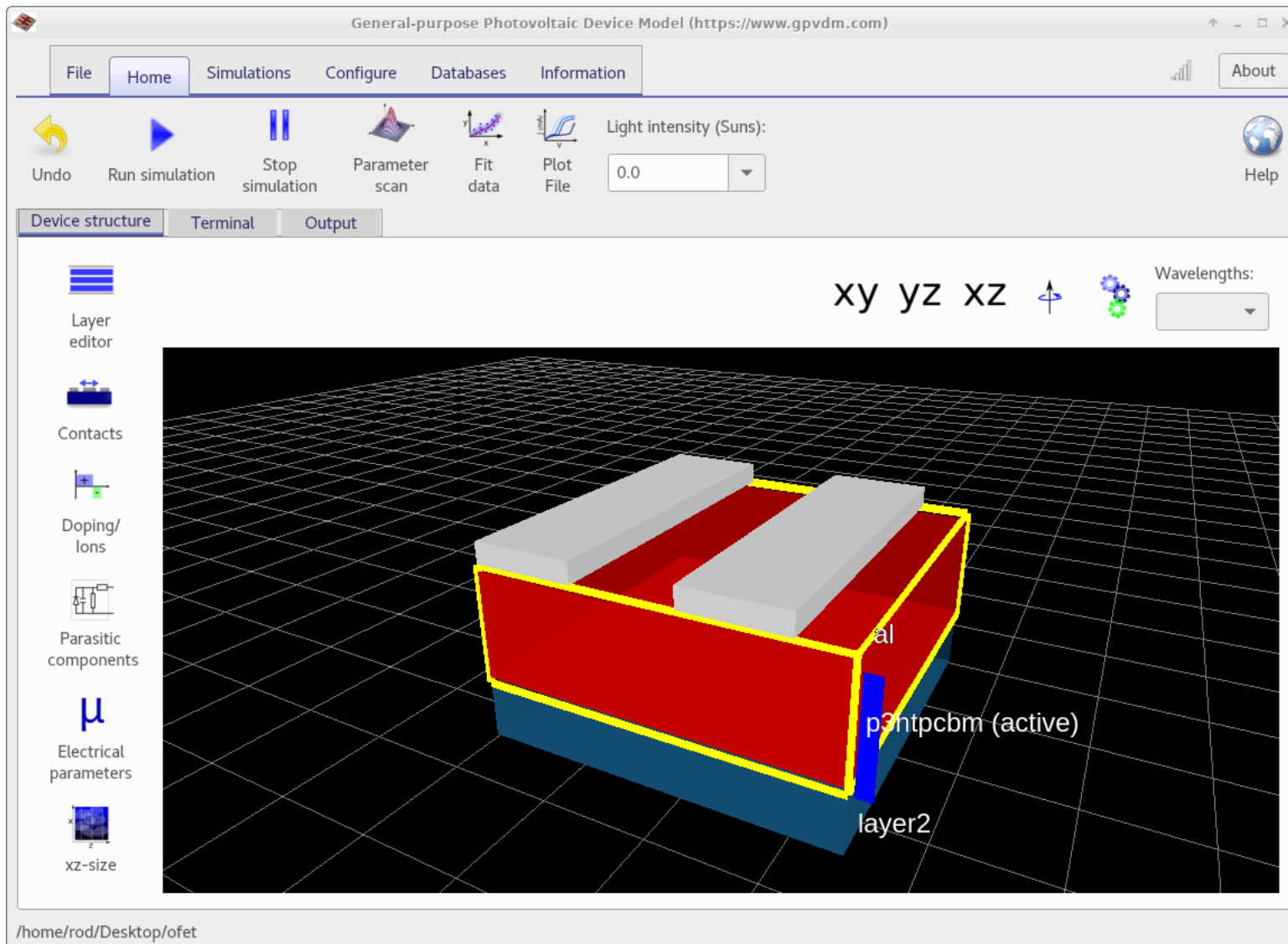
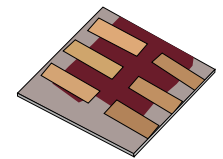
The 'New simulation' dialog box is open, titled 'New simulation (https://www.gpvdms.com)'. It asks 'Which type of device would you like to simulate?'. The options are:

- Organic solar cell (p3htpcbm.gpvdms)
- Perovskite solar cell (perovskite.gpvdms)
- a-Si solar cell (a-silicon.gpvdms)
- Organic bi-layer device (bilayer.gpvdms)
- OFET (ofet.gpvdms)** (highlighted with a red box)
- cigs

At the bottom of the dialog box, there is a 'Show hidden' checkbox, a 'Cancel' button, and a 'Next' button (highlighted with a red box).

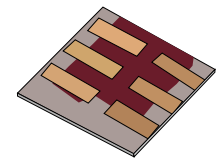
- This will use a 2D solver instead of the 1D solver.

# This will create a new 2D simulation



- Notice the contacts which are 2D structures.

# Adding another electrically active layer



General-purpose Photovoltaic Device Model (<https://www.gpvd.com>)

File Home Simulations Configure Databases Information

New simulation Open simulation Export data

Device structure Terminal Output

Layer editor

Contacts

Doping/ions

Parasitic components

Electrical parameters

xz-size

xy yz xz

Wavelengths:

Layer editor <https://www.gpvd.com>

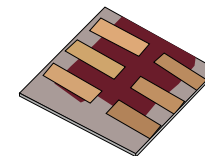
| Layer name | Thicknes | Optical material    | Layer type  |
|------------|----------|---------------------|-------------|
| al         | 4e-08    | metal/al            | contact     |
| p3htp3cm   | 2e-07    | blends/p3htp3cm     | active layr |
| C60        | 1e-07    | small_molecules/c60 | active layr |
| layer2     | 1e-07    | metal/au            | contact     |

/home/rod/Desktop/ofet

- Click on the layer editor and then the +.

- Use the up and down arrows to move the layer to the correct place.

# Take a look at the electrical mesh to make sure it adds up to the width/height.



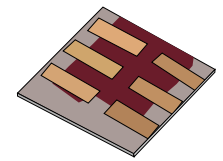
The screenshot shows the 'Electrical Mesh Editor' window with the following data:

| Direction | Thickness | Mesh points | Step multiply | Left/Right |
|-----------|-----------|-------------|---------------|------------|
| x         | 0.0034641 | 10.0        | 1.0           | Left       |
| y         | 3e-07     | 10.0        | 1.0           | Left       |

The x-axis scale is labeled 'Thickness (mm)' with values from 0.5 to 3.0. The y-axis scale is labeled 'Thickness (nm)' with values from 50 to 250. An arrow points from the y-axis scale to the '3e-07' value in the table.

- This values should have updated so that the mesh matches the width of the active layers. 65

# Let's now look at the contacts



General-purpose Photovoltaic Device Model (<https://www.gpvdm.com>)

File Home Simulations Configure Databases Information

Undo Run simulation Stop simulation Parameter scan Fit data Plot File Light intensity (Suns): 0.0 Help

Device structure Terminal Output

Layer editor

**Contacts**

Doping/Ions

Parasitic components

Electrical parameters

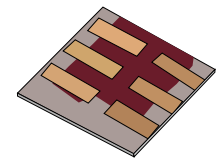
xy yz xz Wavelengths:

Edit contacts ([www.gpvdm.com](https://www.gpvdm.com))

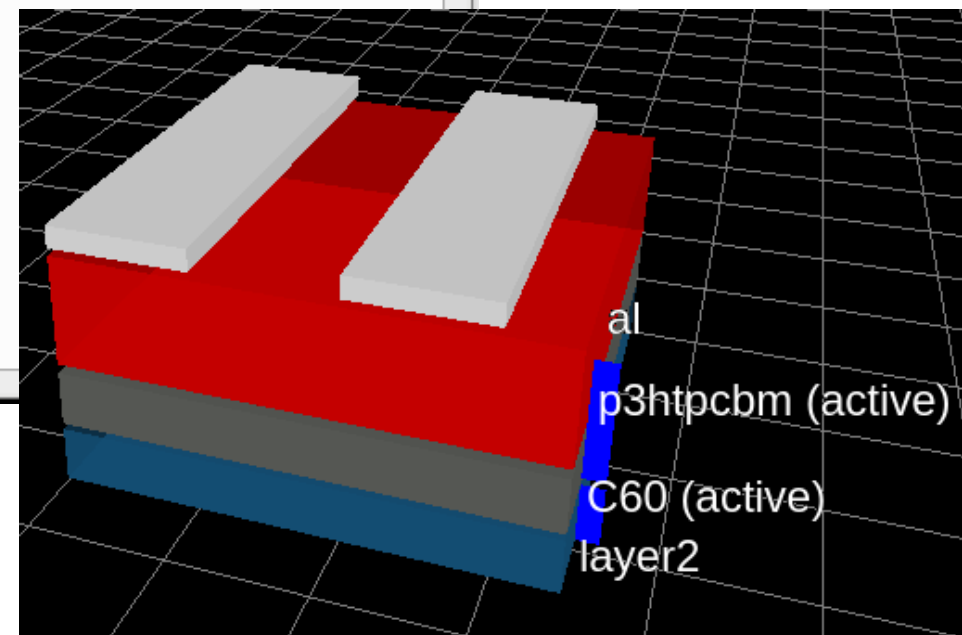
| Name   | Top/Bottom | Active contact | Start | Width     | Depth | Voltage |
|--------|------------|----------------|-------|-----------|-------|---------|
| top    | top        | false          | 0.0   | 0.001     | 0.0   | -1.0    |
| top2   | top        | false          | 0.002 | 0.001     | 0.0   | 0.0     |
| bottom | bottom     | true           | 0.0   | 0.0034641 | 5e-08 | 0.0     |

/home/rod/Desktop/ofet

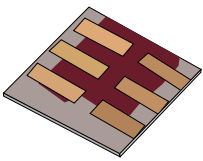
# The human readable name of the contact, you can call them what you want.



| Name   | Top/Bottom | Active contact | Start | Width     | Depth | Voltage |
|--------|------------|----------------|-------|-----------|-------|---------|
| top    | top        | false          | 0.0   | 0.001     | 0.0   | -1.0    |
| top2   | top        | false          | 0.002 | 0.001     | 0.0   | 0.0     |
| bottom | bottom     | true           | 0.0   | 0.0034641 | 5e-08 | 0.0     |

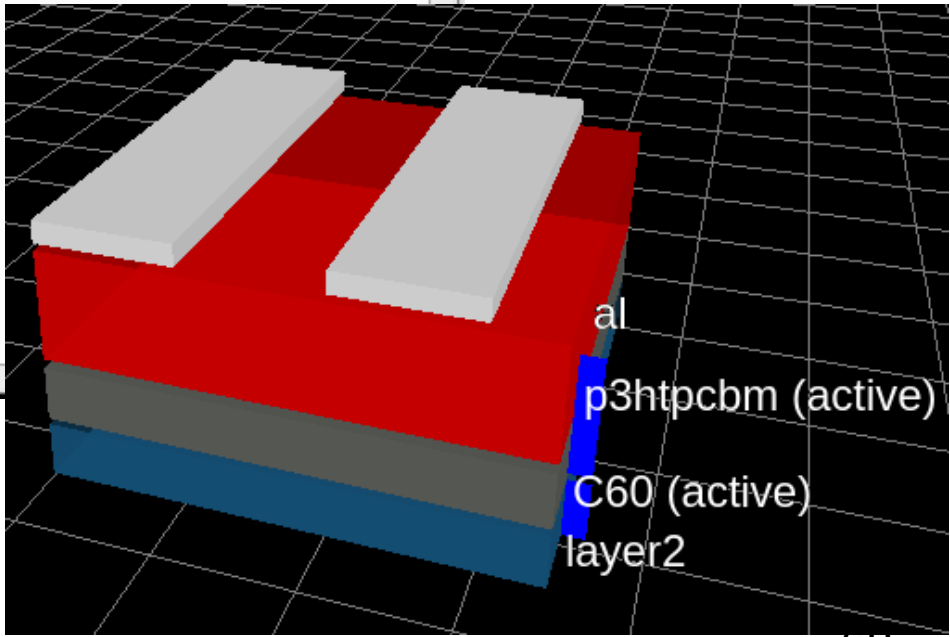


# Is the contact at the top or bottom of the device.



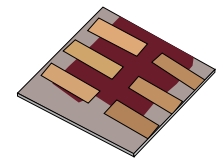
Edit contacts (www.gpvd.com)

| Name   | Top/Bottom | Active contact | Start | Width     | Depth | Voltage |
|--------|------------|----------------|-------|-----------|-------|---------|
| top    | top        | false          | 0.0   | 0.001     | 0.0   | -1.0    |
| top2   | top        | false          | 0.002 | 0.001     | 0.0   | 0.0     |
| bottom | bottom     | true           | 0.0   | 0.0034641 | 5e-08 | 0.0     |



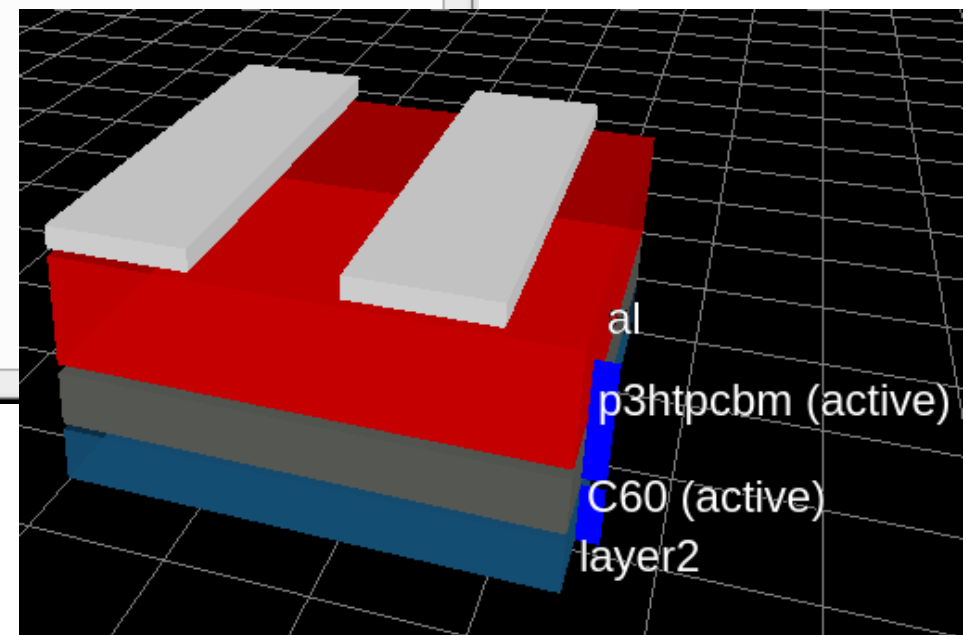


# The contact to which the voltage ramp/transient/frequency pulse is applied.

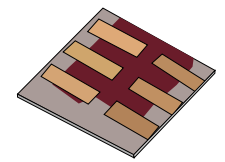


Edit contacts (www.gpvd.com)

| Name   | Top/Bottom | Active contact | Start | Width     | Depth | Voltage |
|--------|------------|----------------|-------|-----------|-------|---------|
| top    | top        | false          | 0.0   | 0.001     | 0.0   | -1.0    |
| top2   | top        | false          | 0.002 | 0.001     | 0.0   | 0.0     |
| bottom | bottom     | true           | 0.0   | 0.0034641 | 5e-08 | 0.0     |

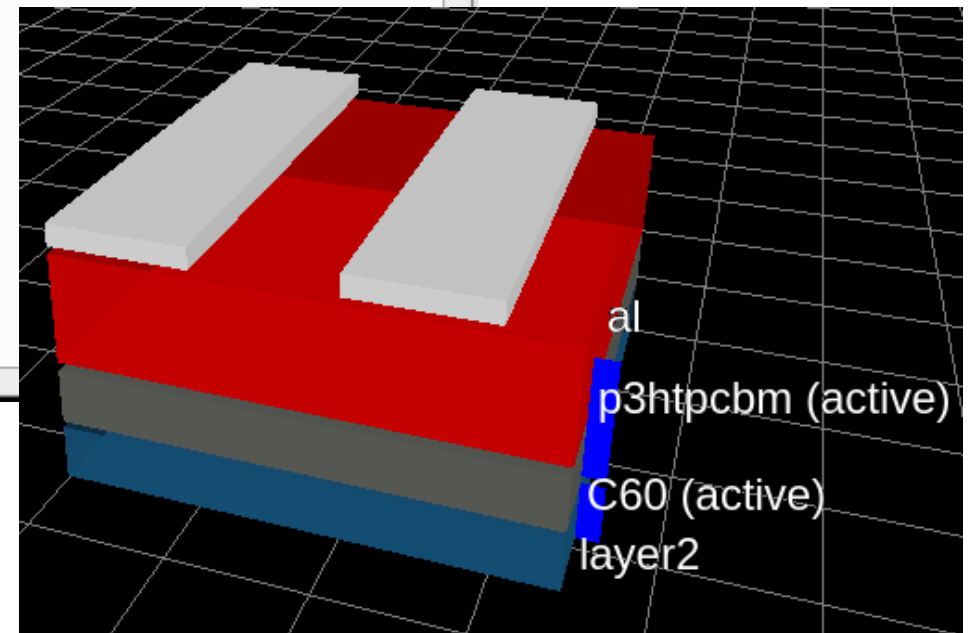


# Start of the contact from the left of the device in meters.

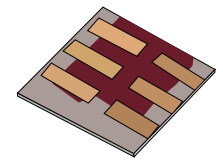


Edit contacts (www.gpvd.com)

| Name   | Top/Bottom | Active contact | Start | Width     | Depth | Voltage |
|--------|------------|----------------|-------|-----------|-------|---------|
| top    | top        | false          | 0.0   | 0.001     | 0.0   | -1.0    |
| top2   | top        | false          | 0.002 | 0.001     | 0.0   | 0.0     |
| bottom | bottom     | true           | 0.0   | 0.0034641 | 5e-08 | 0.0     |

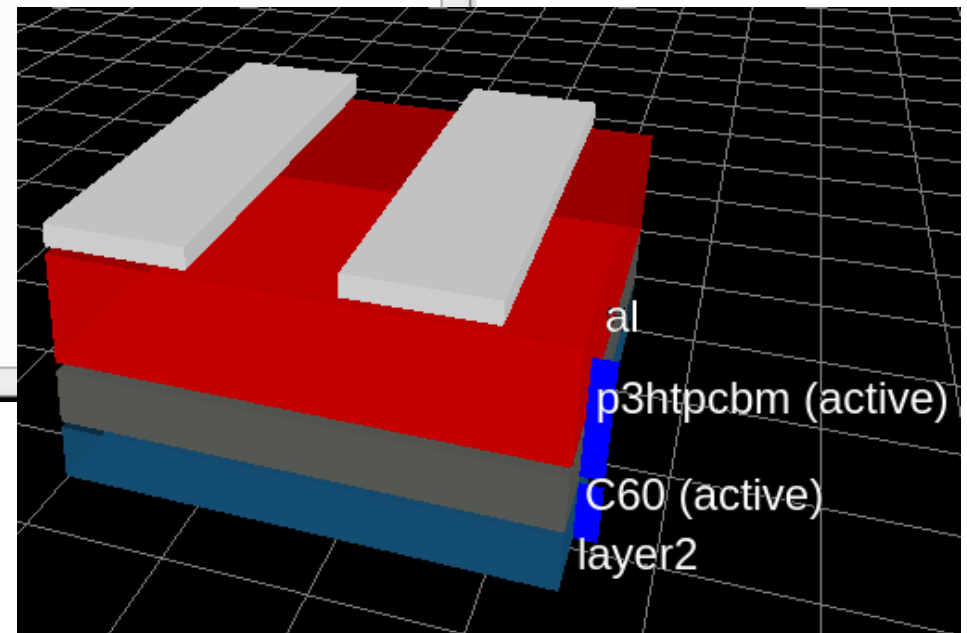


# Width of the contact in meters

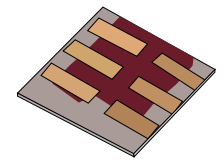


Edit contacts (www.gpvd.com)

| Name   | Top/Bottom | Active contact | Start | Width     | Depth | Voltage |
|--------|------------|----------------|-------|-----------|-------|---------|
| top    | top        | false          | 0.0   | 0.001     | 0.0   | -1.0    |
| top2   | top        | false          | 0.002 | 0.001     | 0.0   | 0.0     |
| bottom | bottom     | true           | 0.0   | 0.0034641 | 5e-08 | 0.0     |



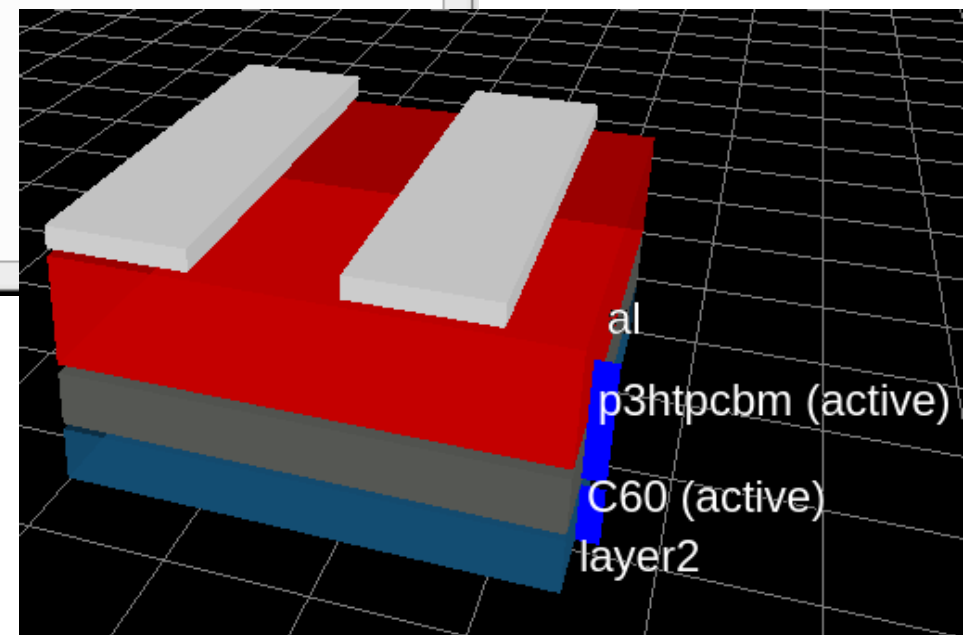
# The voltage applied to the contact.



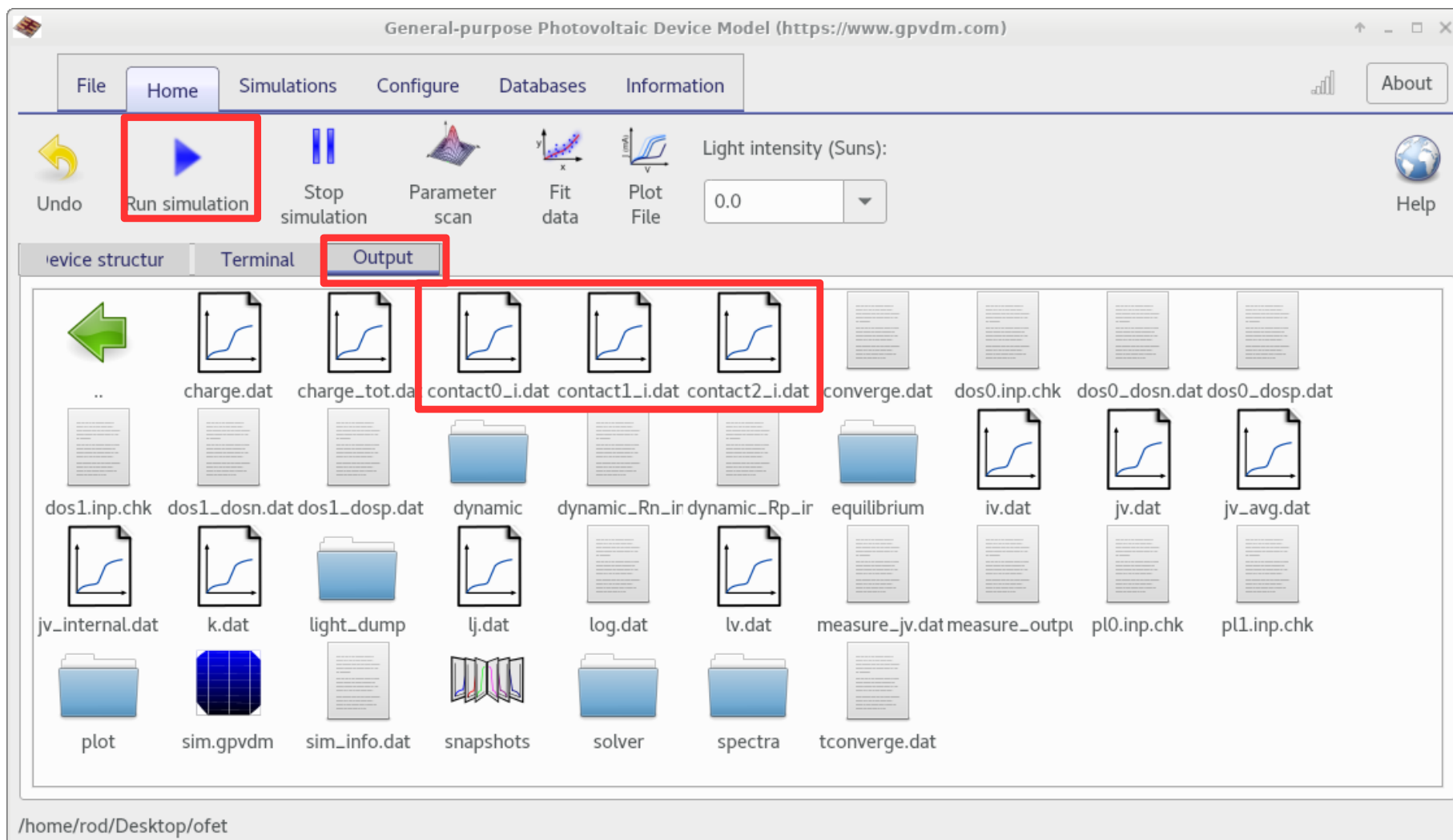
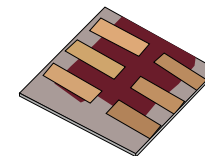
Edit contacts (www.gpvdm.com)

| Name   | Top/Bottom | Active contact | Start | Width     | Depth | Voltage |
|--------|------------|----------------|-------|-----------|-------|---------|
| top    | top        | false          | 0.0   | 0.001     | 0.0   | -1.0    |
| top2   | top        | false          | 0.002 | 0.001     | 0.0   | 0.0     |
| bottom | bottom     | true           | 0.0   | 0.0034641 | 5e-08 | 0.0     |

- So in this case we are applying -1V to **top**, 0V to **top2** and applying a voltage ramp to **bottom** – as we are in *JV simulation mode*.

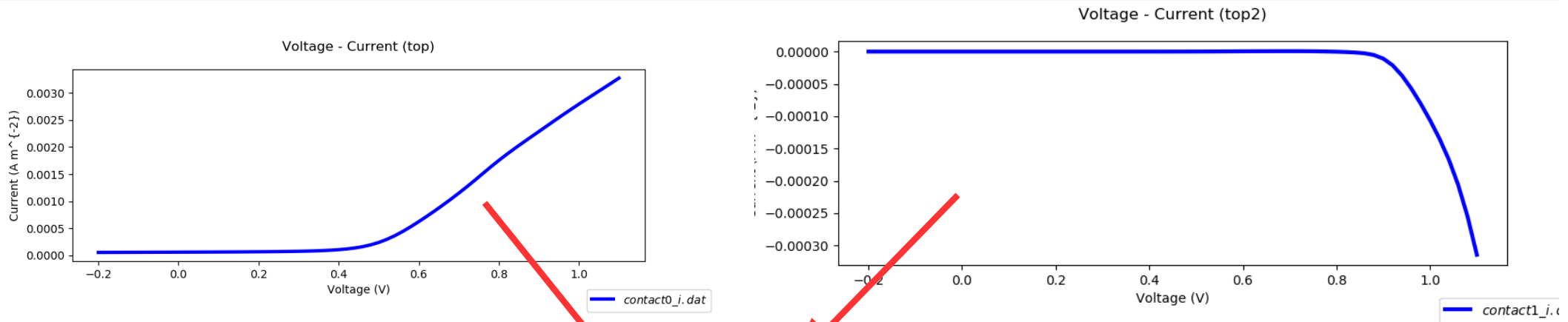
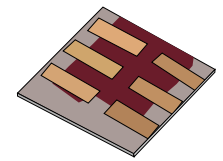


# Run the simulation..., by clicking on the play button.

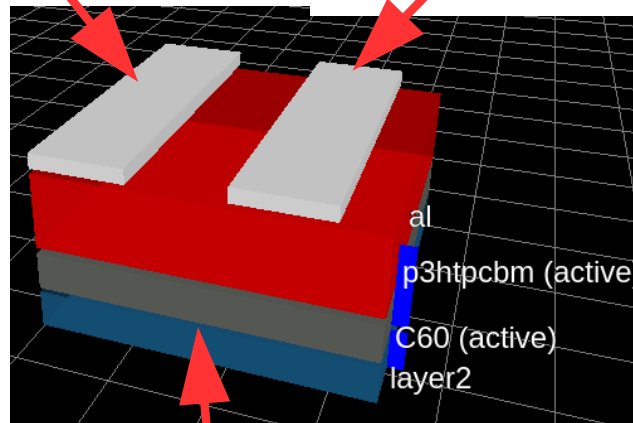


•Then let's look at the output.

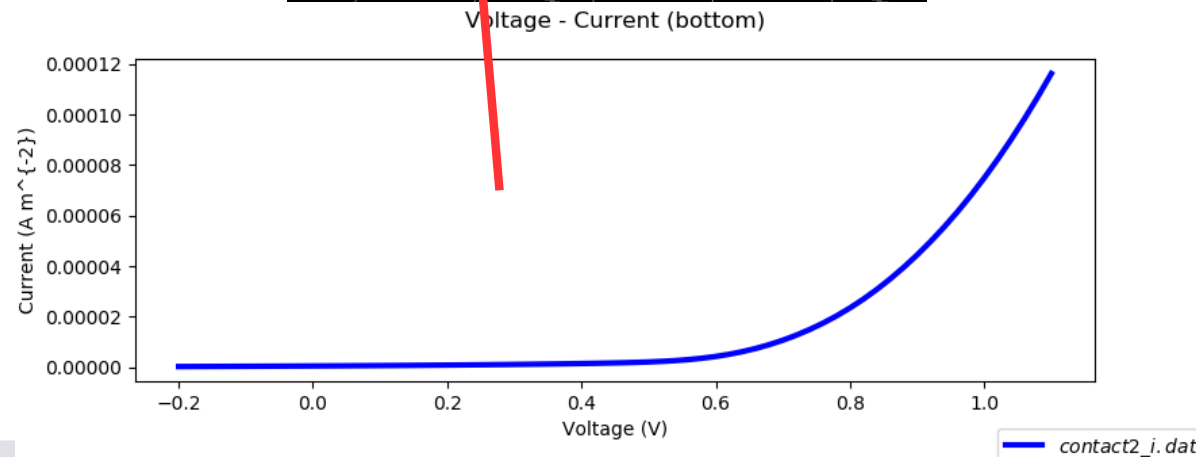
# Current in/out of the contacts and the gate current.



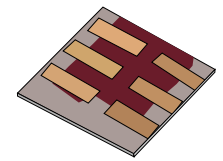
- Current going into left contact (+), current coming out of the right contact(-).



- Gate current much smaller than source/drain therefore amplification.



# Using the snapshot tool to view what is going on in 2D during the simulation.



- Click play in the snapshot window and select phi.dat, to view how the potential changes within the device.

The screenshot displays the General-purpose Photovoltaic Device Model (gpvdm) software interface. The main window shows a file explorer with various data files. A 'snapshots' folder is highlighted with a red box. An inset window titled 'Examine simulation results in time domain' is open, showing a 3D surface plot of potential V versus x and y position (nm). The plot shows a potential well structure. The 'Play' button in the inset window's toolbar is also highlighted with a red box. The main window's toolbar includes buttons for 'Run simulation', 'Stop simulation', 'Parameter scan', 'Fit data', and 'Plot File'. The inset window's toolbar includes 'Refresh graph', 'Home', 'Back', 'Forward', 'Pan', 'Zoom', 'Subplots', 'Customize', and 'Save'.