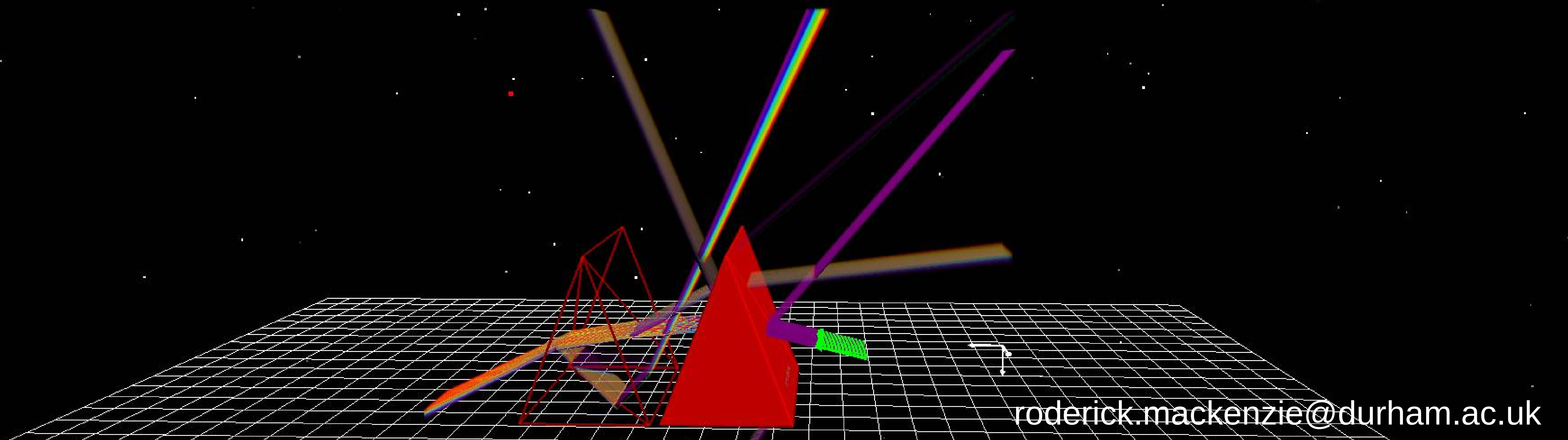
Simulating light in opto-electronic devices, solar cells, sensors, and bio-sensors using OghmaNano



roderick.mackenzie@durham.ac.uk

Download the software:

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

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

Outline of the talk

- In this talk we will cover:
  - **What are optical simulations?**
  - Why perform optical simulations?
  - What you need for accurate optical simulations
    - » Optical spectra
    - » Refractive index data (n)
    - » Optical absorption data (k)
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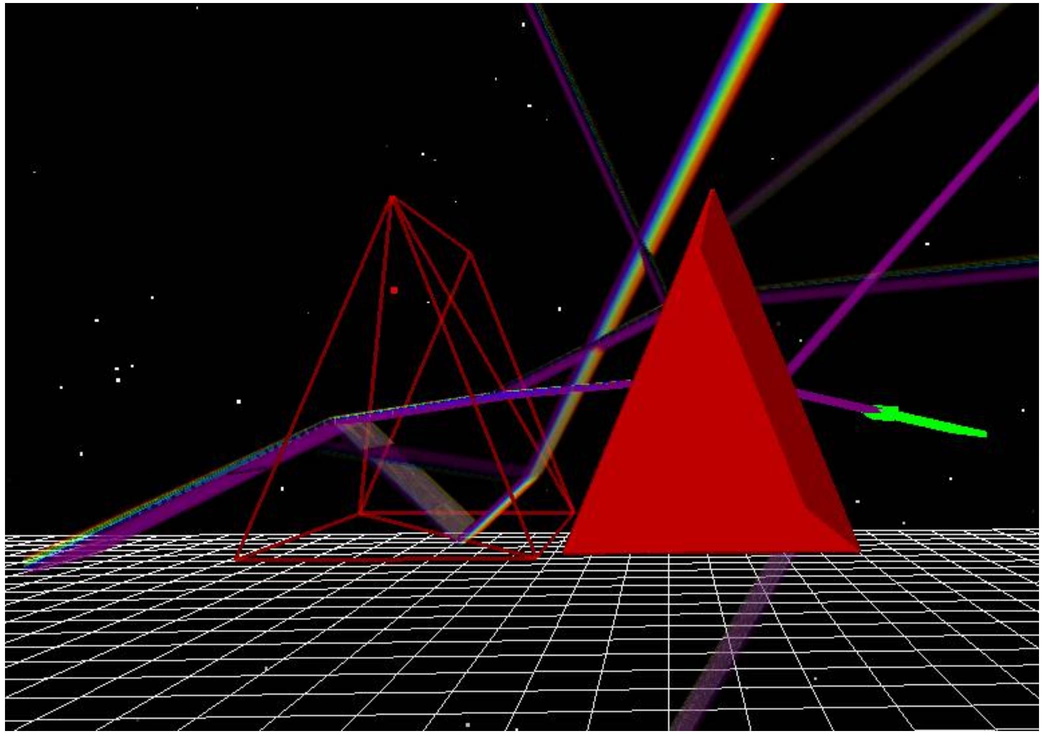
  - Setting up device structures
  - Running optical simulations using gpvdm.
  - Light sources
  - Output

What are optical simulations?

•Optical simulations enable you to understand how light interacts with your device.

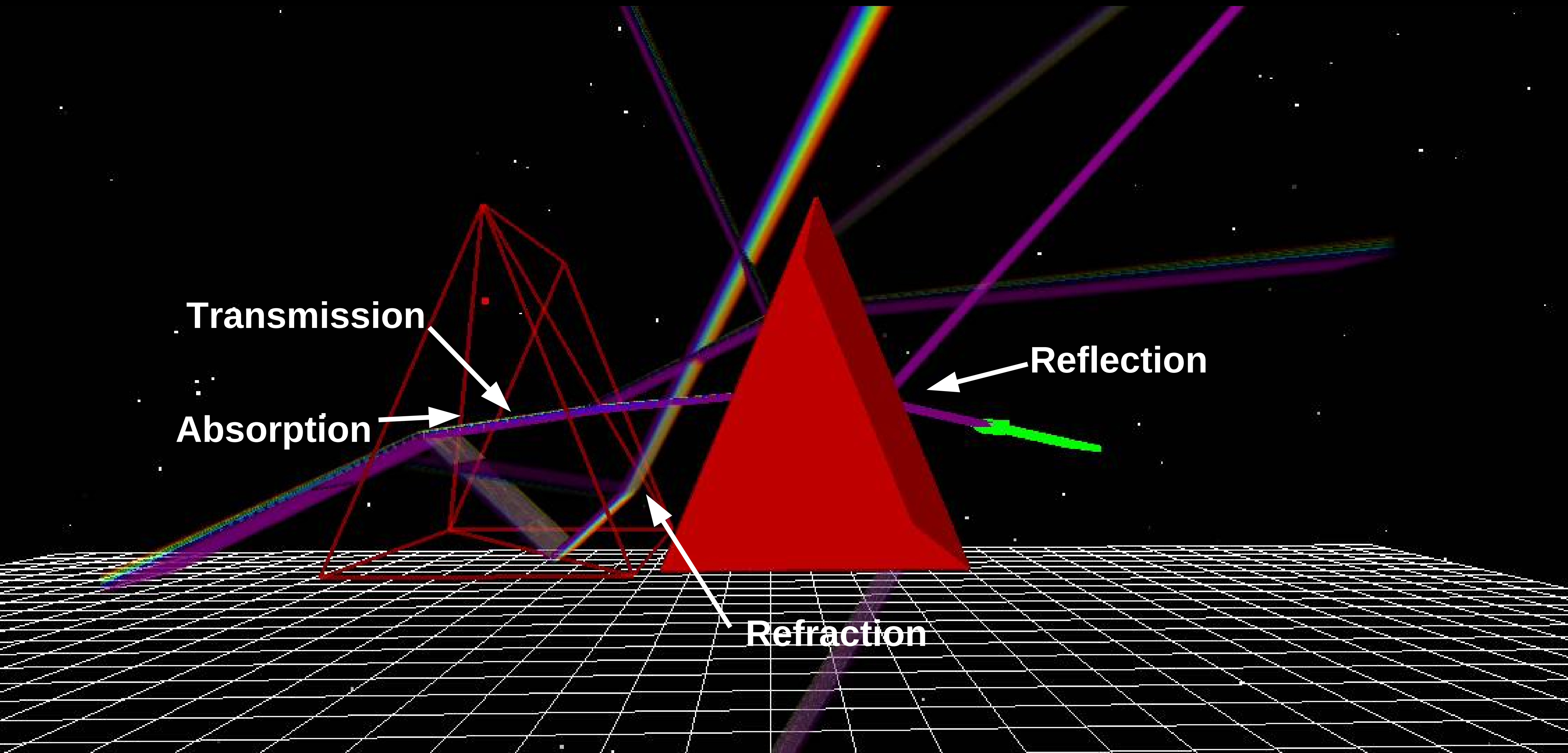
•The front cover of this slide deck was an example of a simple optical simulation it showed light interacting with two prisms



•You are able to predict
- **Reflections**
- **Transmission**
- **Absorption**
- **Refraction**

•And understand what this means for your device performance
- What ever type of device it is.

Let’s look at this picture in a bit more detail



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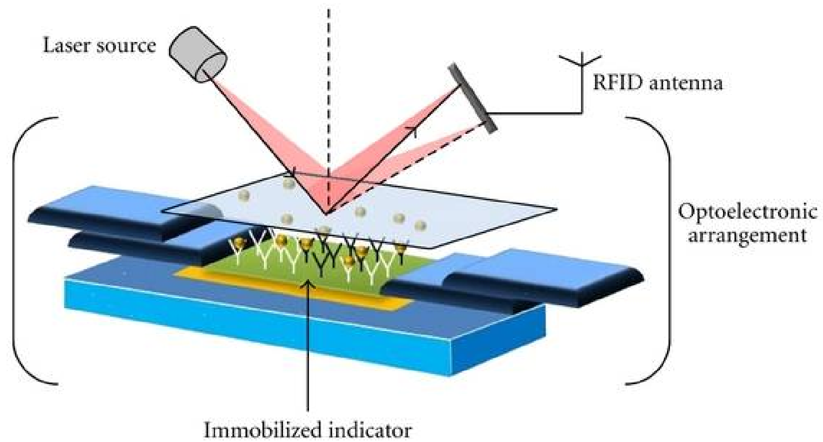
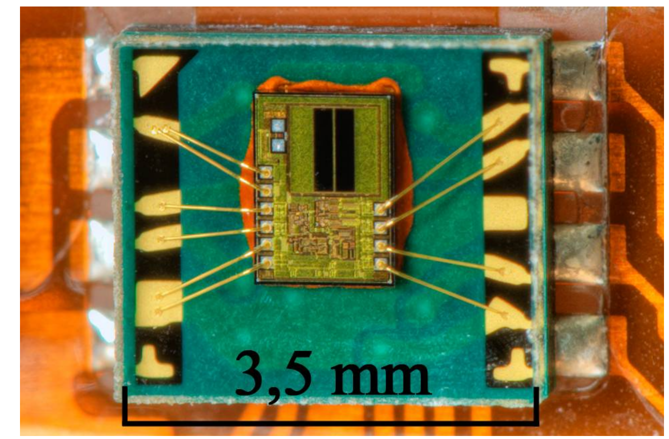
Why perform optical simulations?

•Understanding how light interacts with devices is important for designing many classes of device including:

Solar cells



Bio-sensors



Optical sensors, DVD or telecommunications

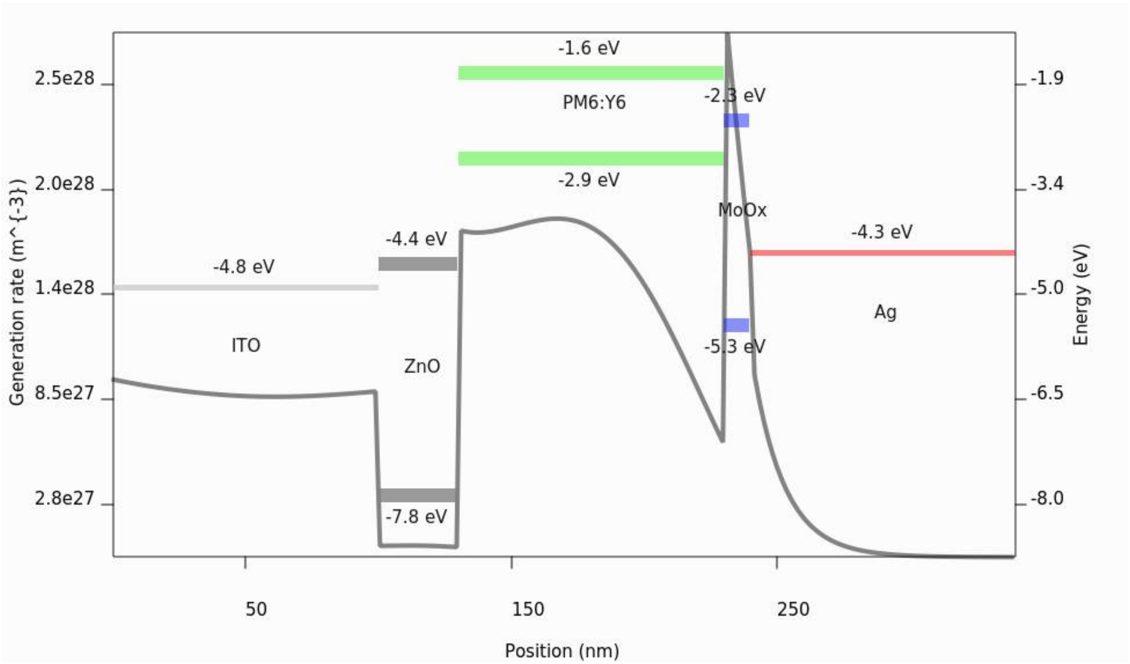
•If you have photons in your device you will want to perform optical simulations at some point.

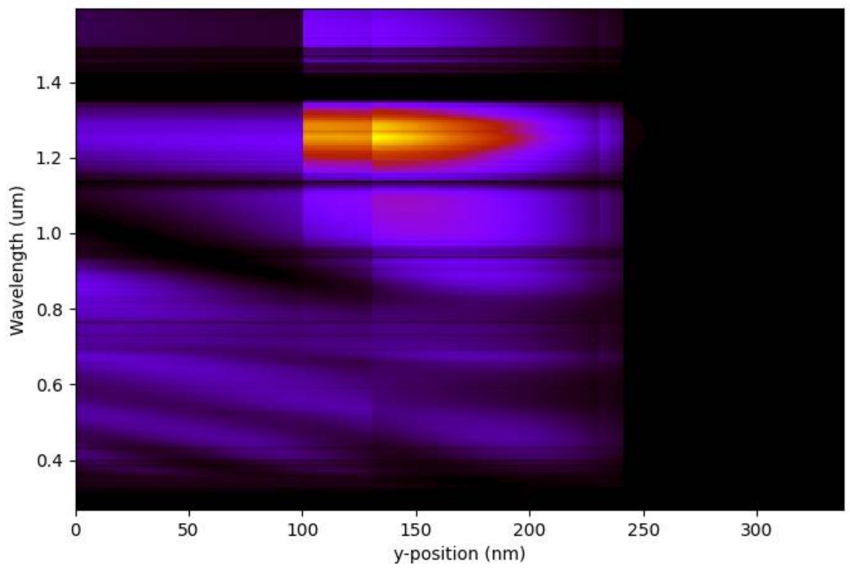
https://doi.org/10.1155/2011/348218

https://commons.wikimedia.org/wiki/File:Photodetector_(dvd_drive).jpg

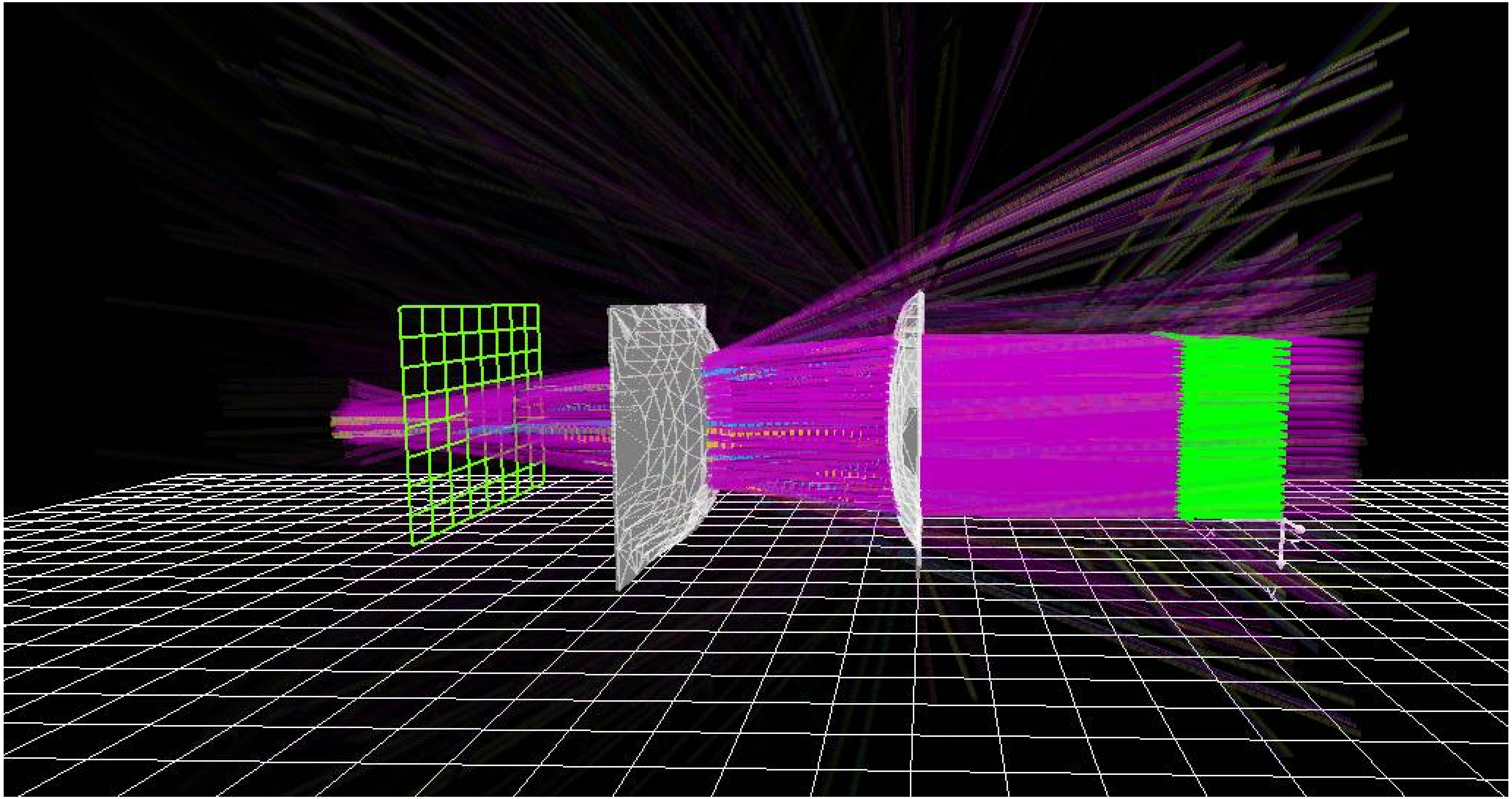
Why perform optical simulations?
Solar cell example:

- Optical simulations can tell you:
  - Where photons are being absorbed
  - At what wavelength
  - If your device is as efficient as it could be.



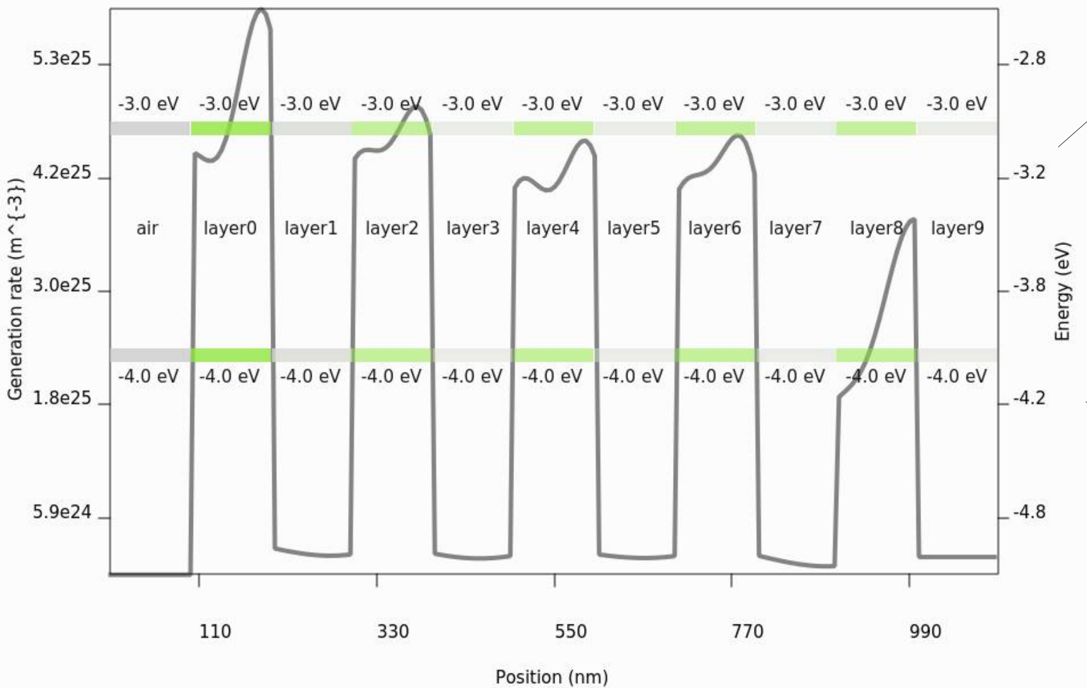


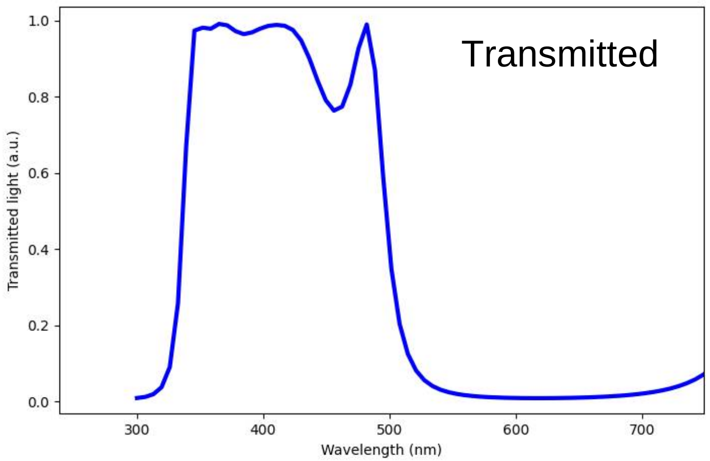
Why perform optical simulations?
Designing optical systems

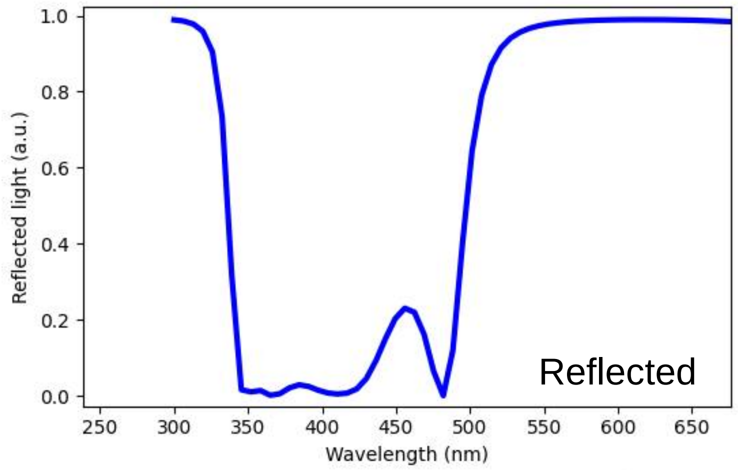


Why perform optical simulations? Optical filter example:

- Optical simulations allow you to:
  - Play with the layer thickness before fabrication
  - Play with the material properties before fabrication.







Why perform optical simulations?
They are easy to run and produce very reliable results

- All you need is the:
  - ***Optical spectra*** of the incident light
  - The ***refractive index*** of the material as a function of wavelength
  - The ***absorption of the material*** as a function of wavelength
  - And your ***device structure***

If you have this information your simulations will be 100% accurate.

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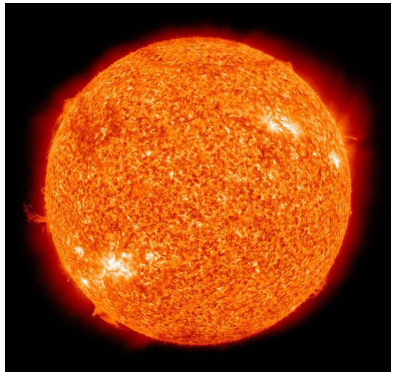
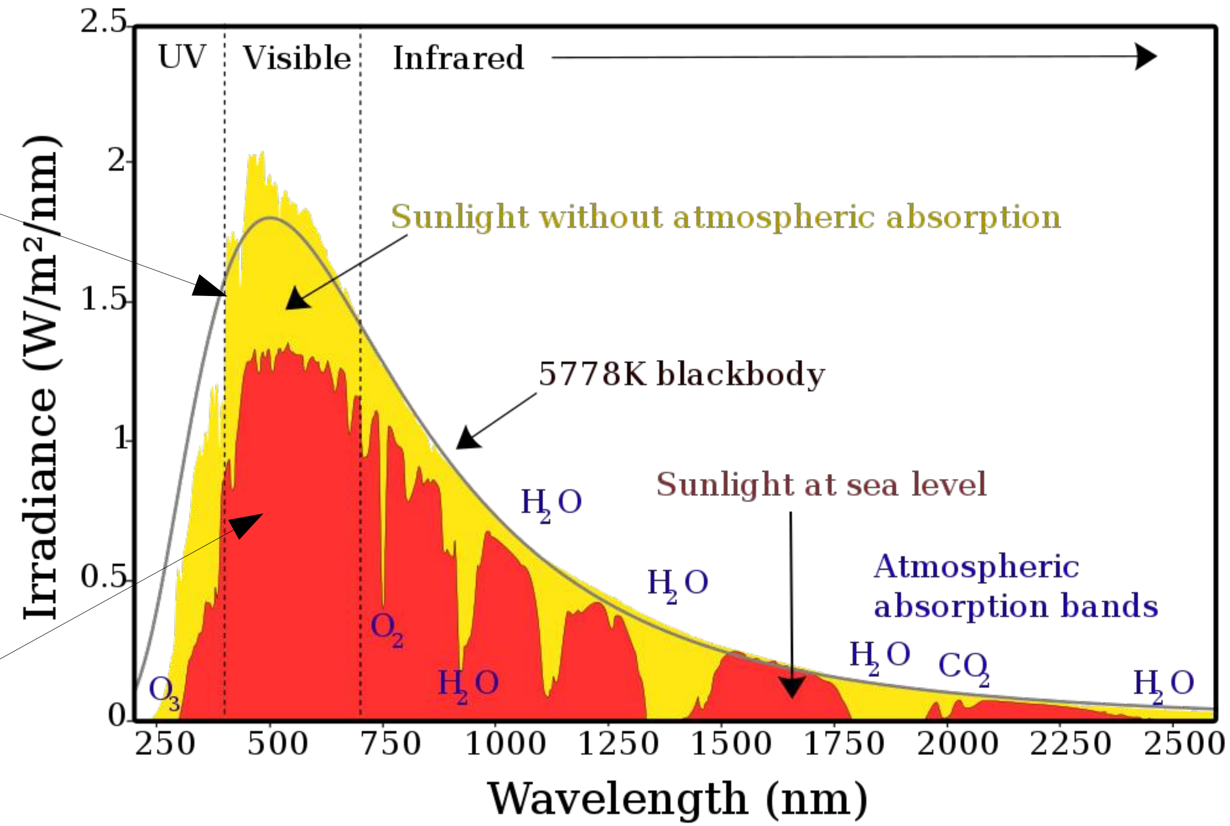
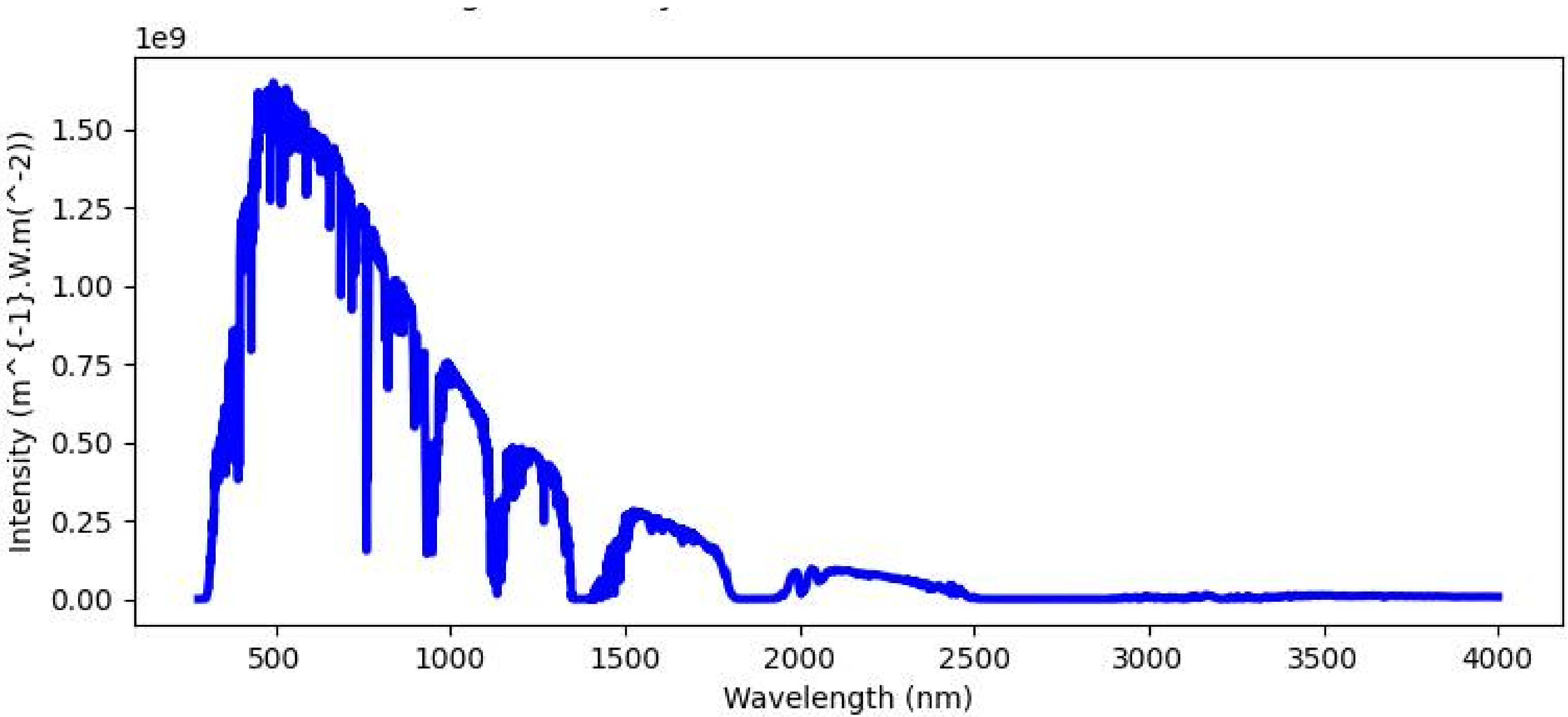
The optical spectra of the Sun AM0, AM1.5G





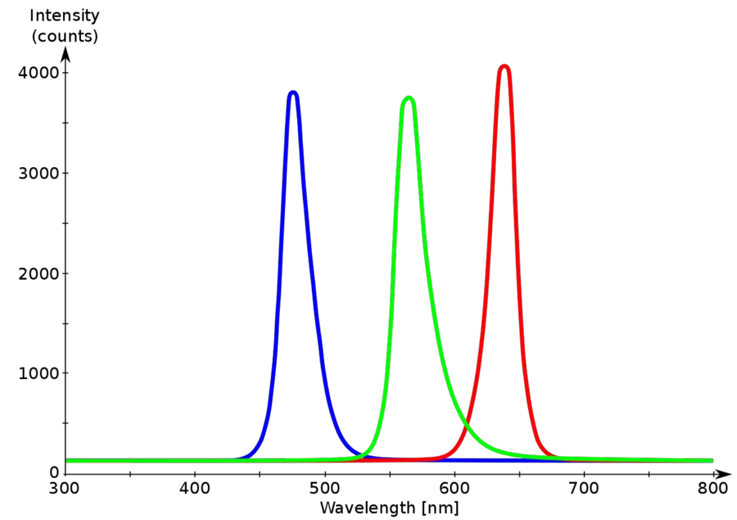
These spectra are known quantities.

AM1.5G in more detail

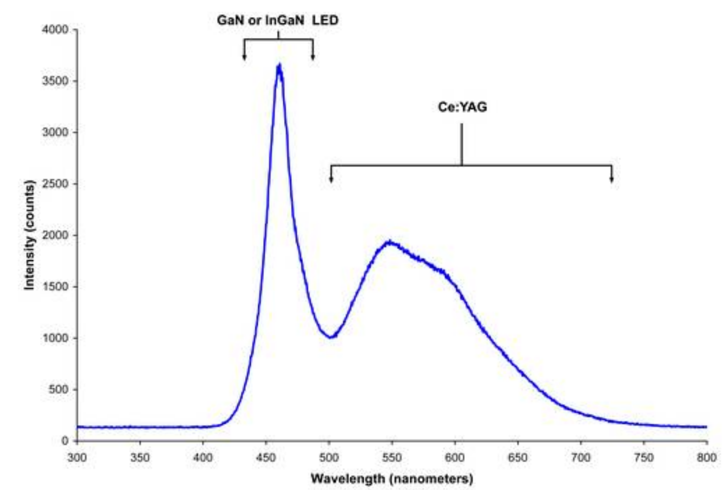


Other examples of spectra commonly used in science/Engineering:

- Blue, Green and Red LEDs.

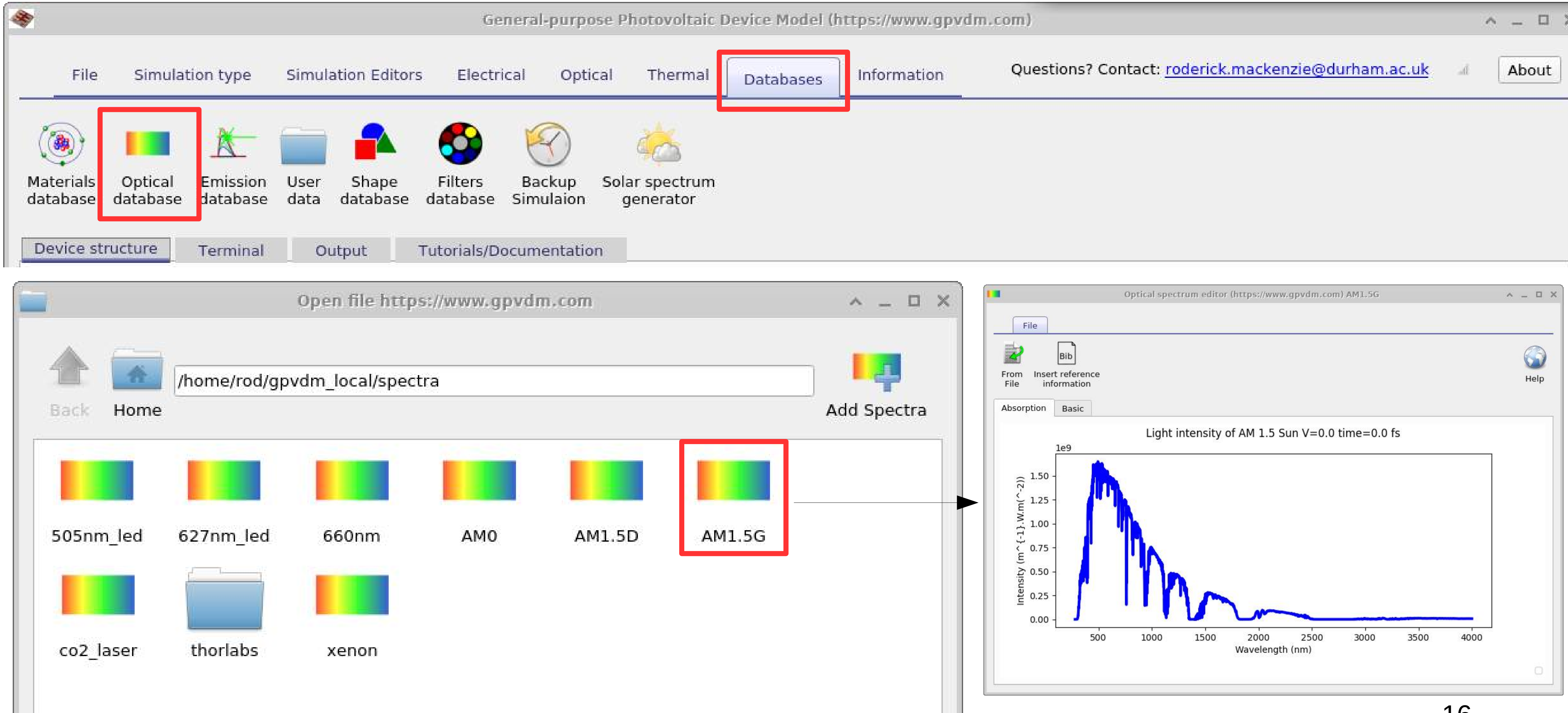


- White LEDs

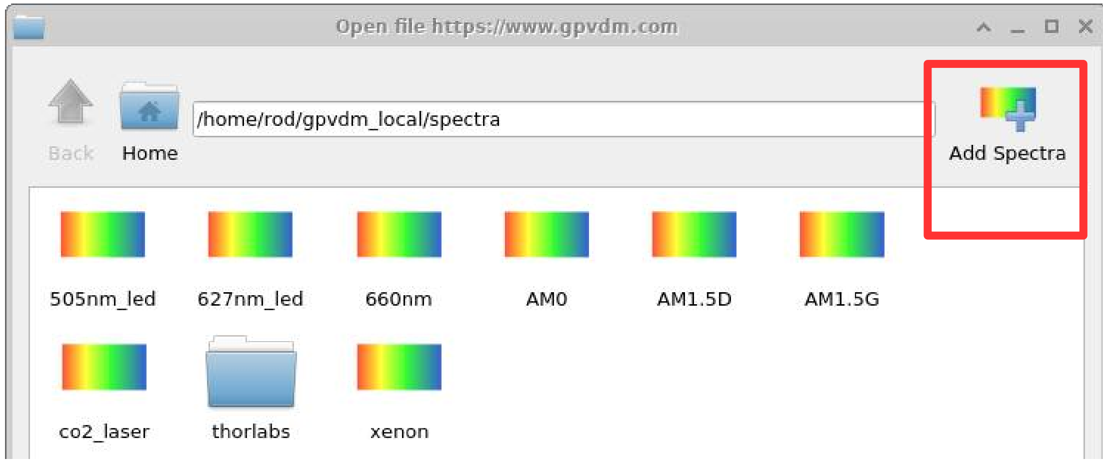


https://commons.wikimedia.org/wiki/File:Red-YellowGreen-Blue_LED_spectra.png

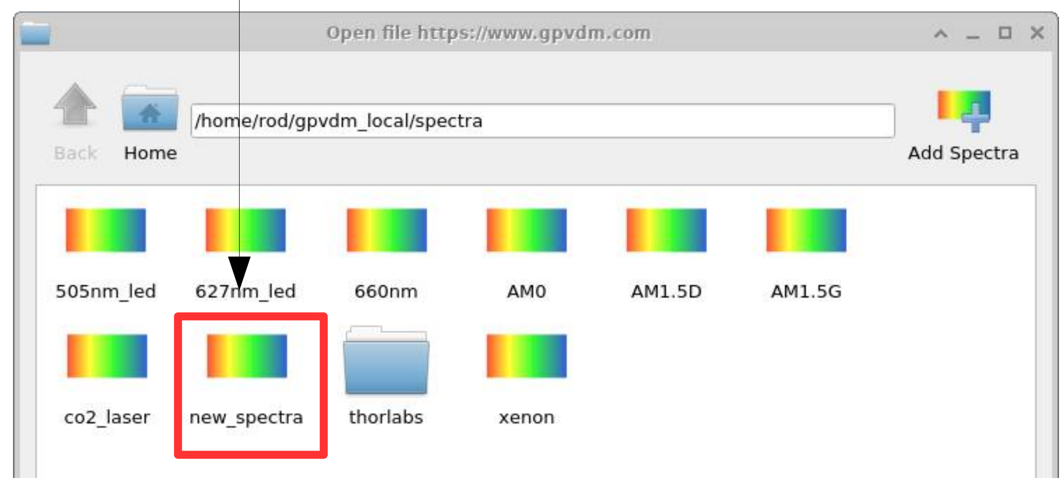
You can access the spectra in from the database tab:



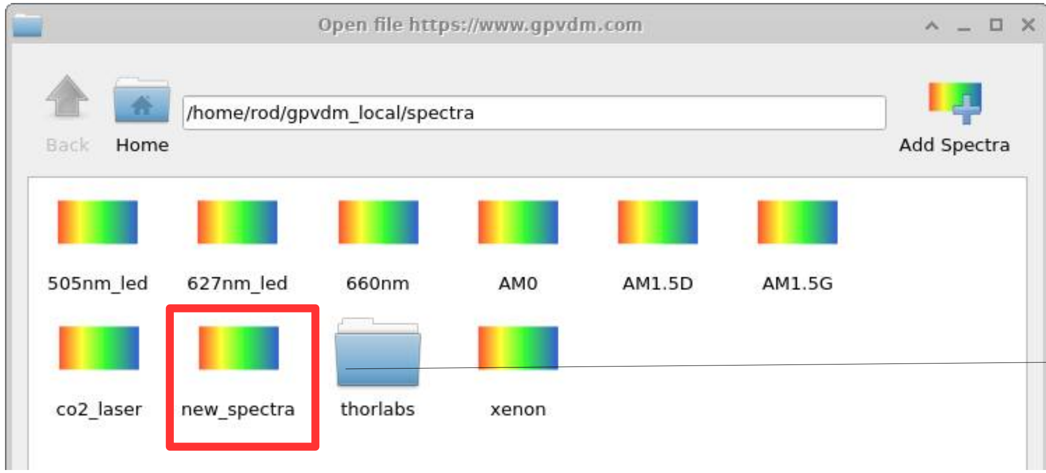
Sometimes you will want to import your own spectra say from a lamp or other source in your lab:

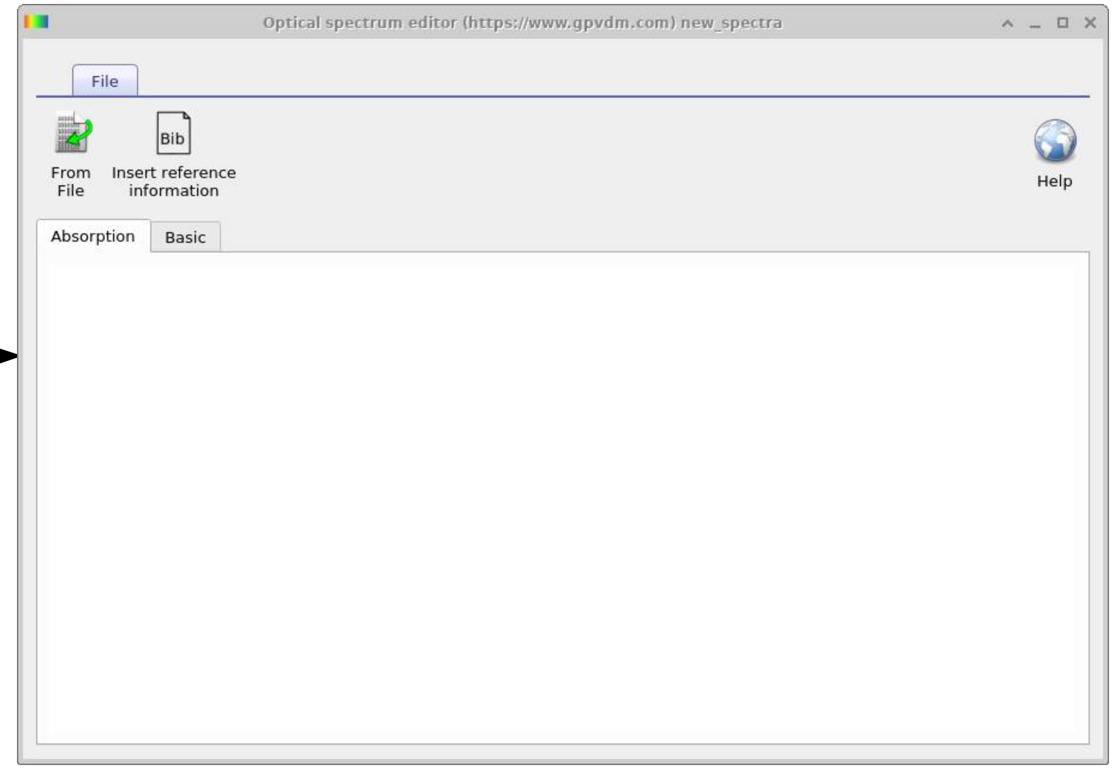


- Click on the “Add spectra” button
- Type a new name
- Open the new spectra by double clicking.



Opening your new spectrum window

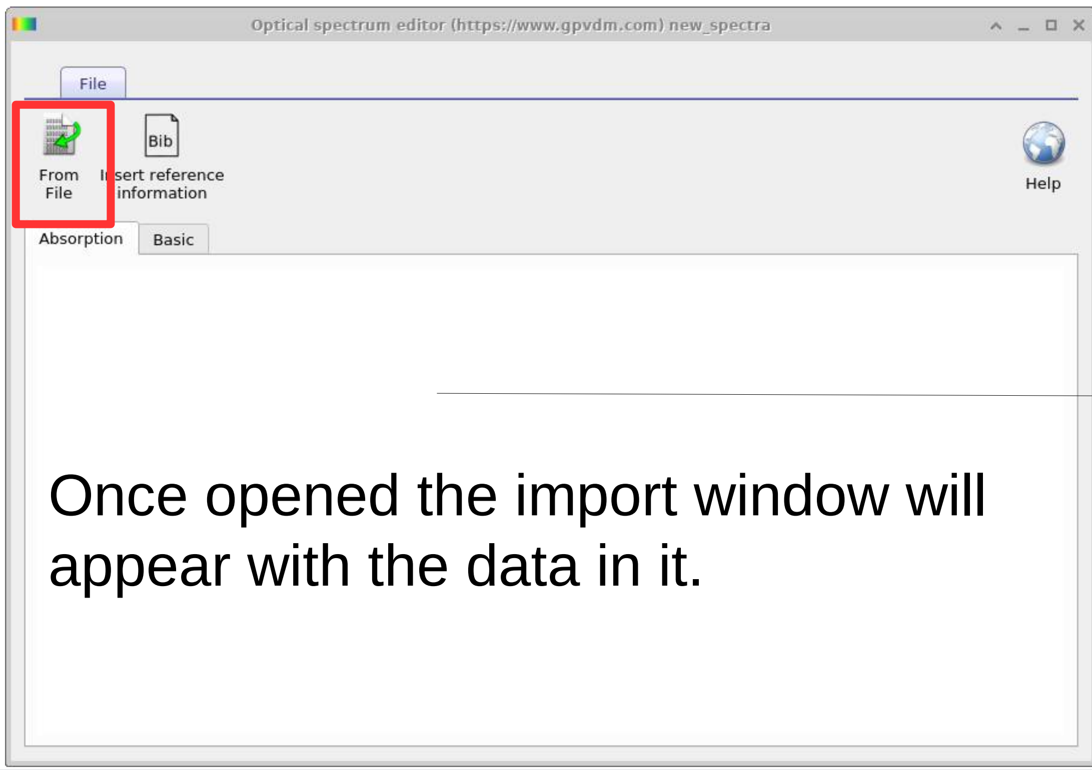




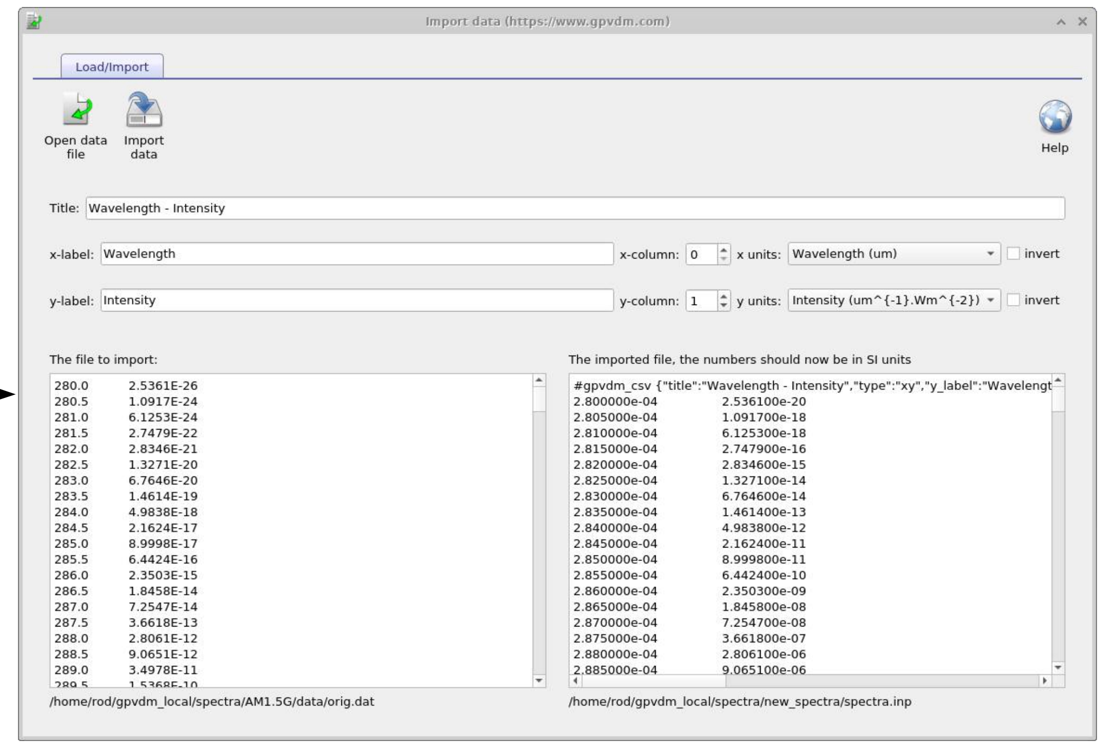
- This will open and empty spectrum window.
- We now need some data to fill it.

Importing a spectra

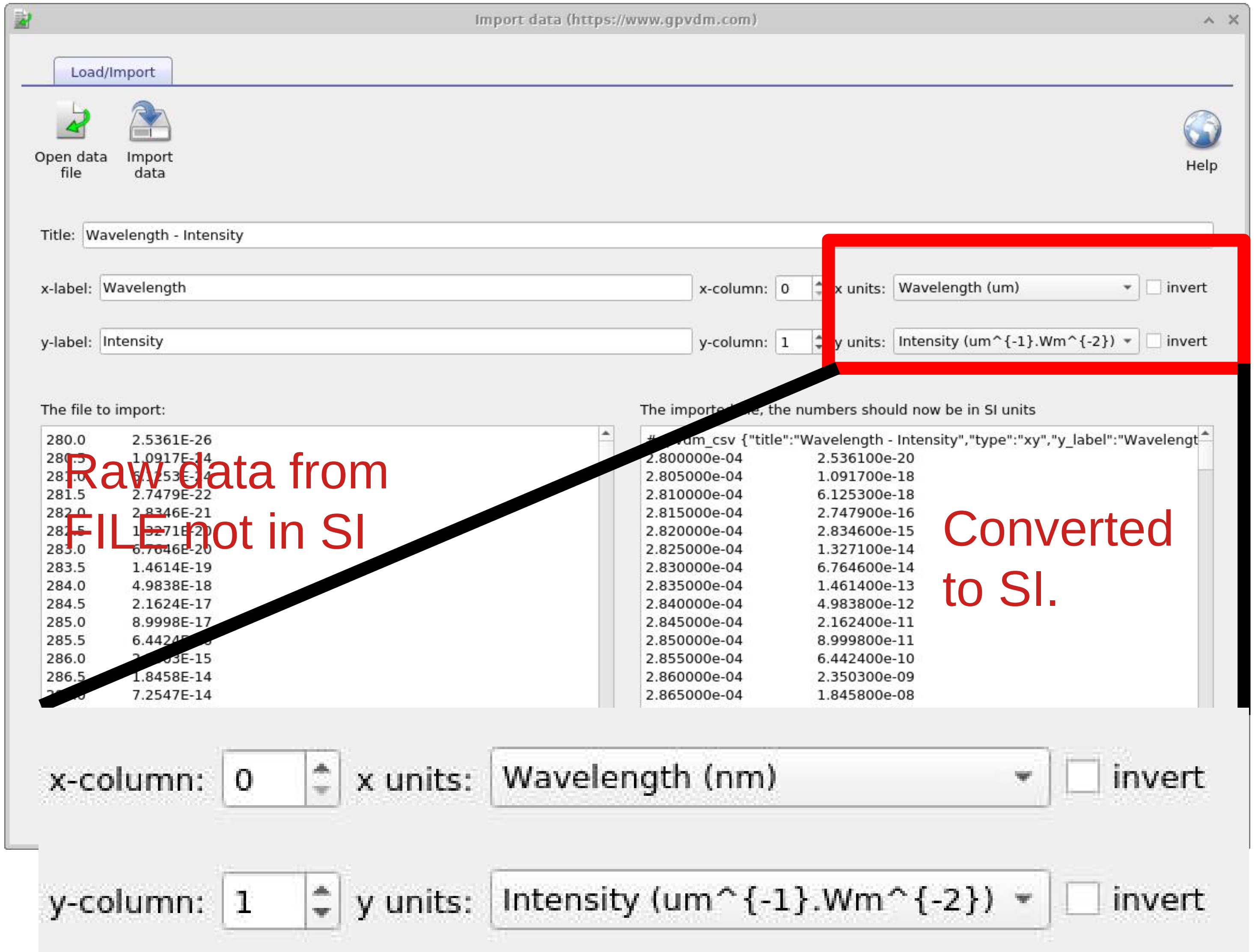
- Download the solar spectra of the sun from:
- https://www.gpvdm.com/demo/solar_spectra_demo.txt
- And save it to your home directory.
- Then open it using “File Import” (red box below)



Once opened the import window will appear with the data in it.

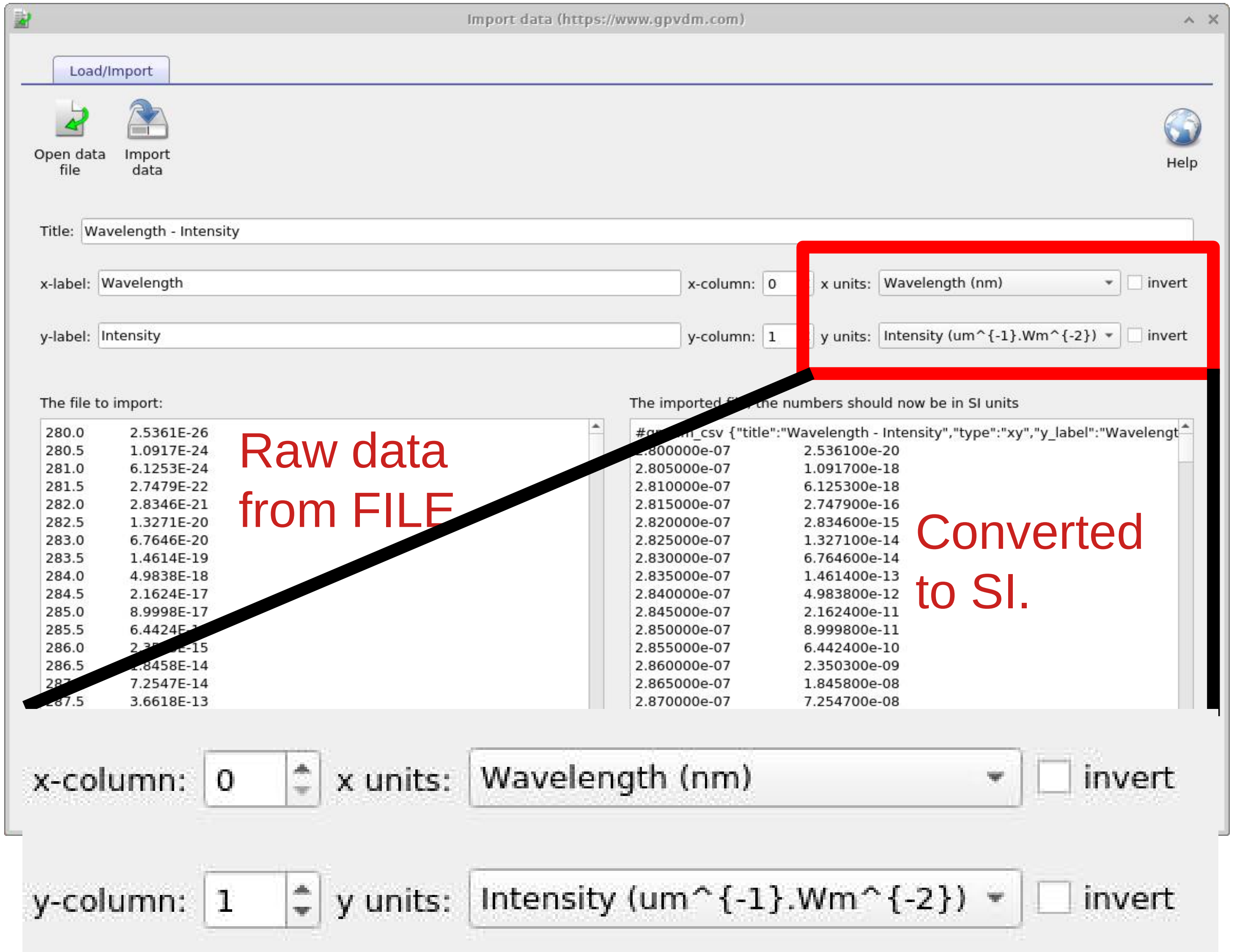


Closer look at the data importer tool



- The model needs all data to be in SI units.
- The data you downloaded had units of Wavelength (nm) v.s. Intensity (um^{-1}Wm^{-2}). Intensity is already SI, wavelength in nm is not.
- To convert the data to SI, select from the drop down boxes what units the INPUT DATA is in.
- The converted data will be displayed in the right hand text box.

Closer look at the data importer tool



- You should see on the right hand side of the window nm has been converted into units of meters.
- Always perform a sanity check on the imported data by looking at the numbers in each column – do they make sense?
- They should always be in SI units. There should be no InF values, and no NaN values if anything

Try at home demo

- You can download the data used in this example from:

  https://www.gpvdm.com/demo/solar_spectra_demo.txt

- Have a go at importing the data your self.

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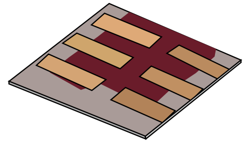
Refractive index:
Snells law and the speed of light

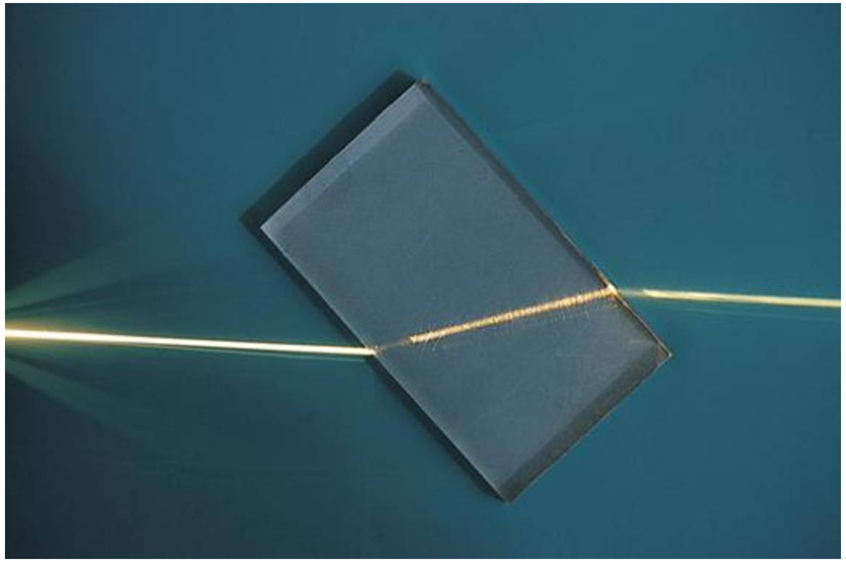


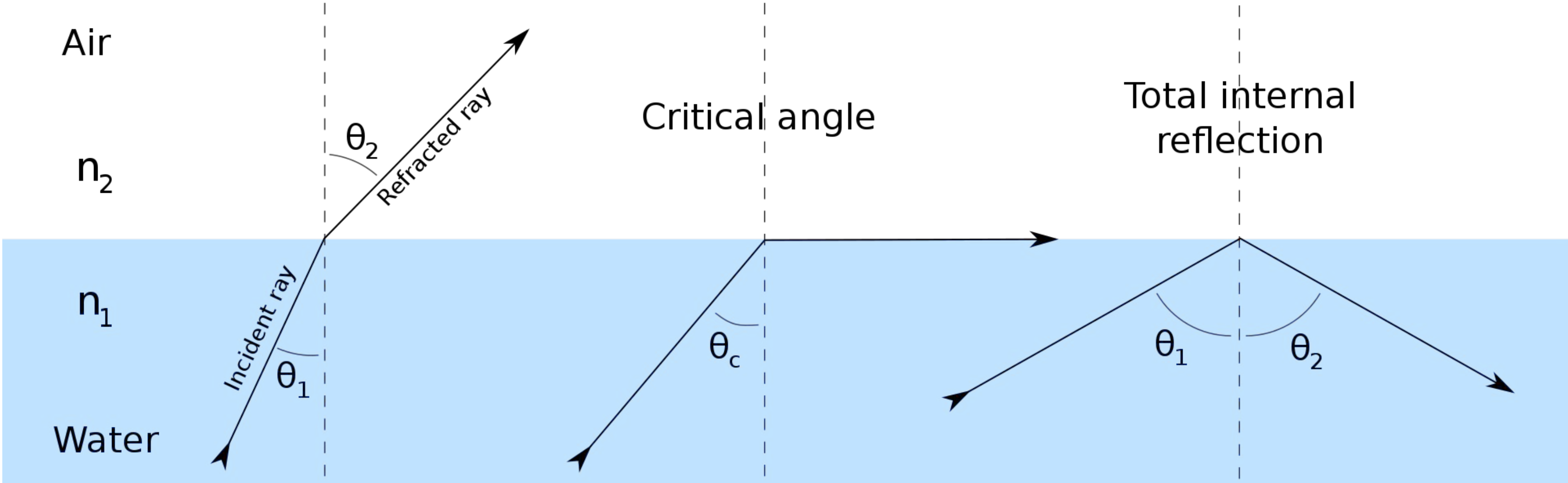
•Refractive index governs by how might light is bent when entering or leaving an object.

• Snells law describes this bending of light:

$$n_1 \sin \theta_1 = n_2 \sin \theta_2$$

•Refractive index also governs the speed of light in an object.



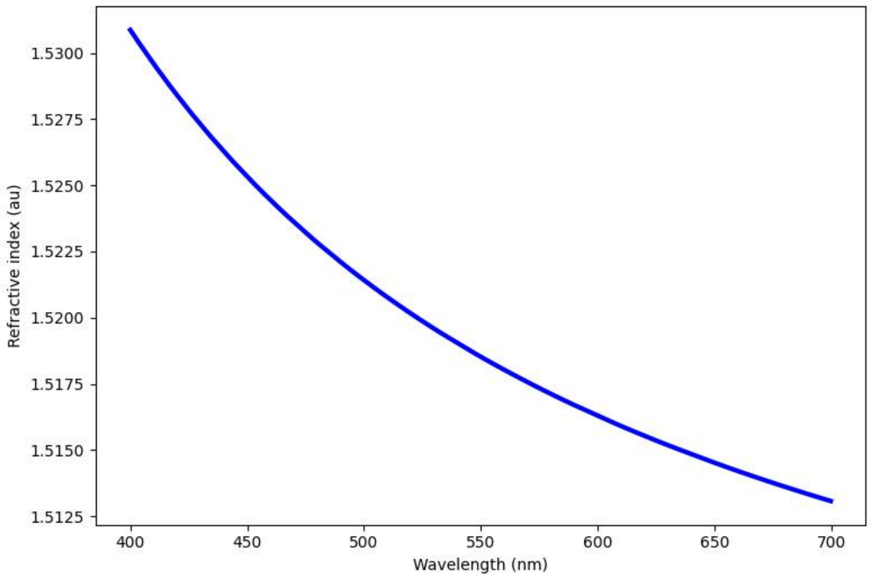


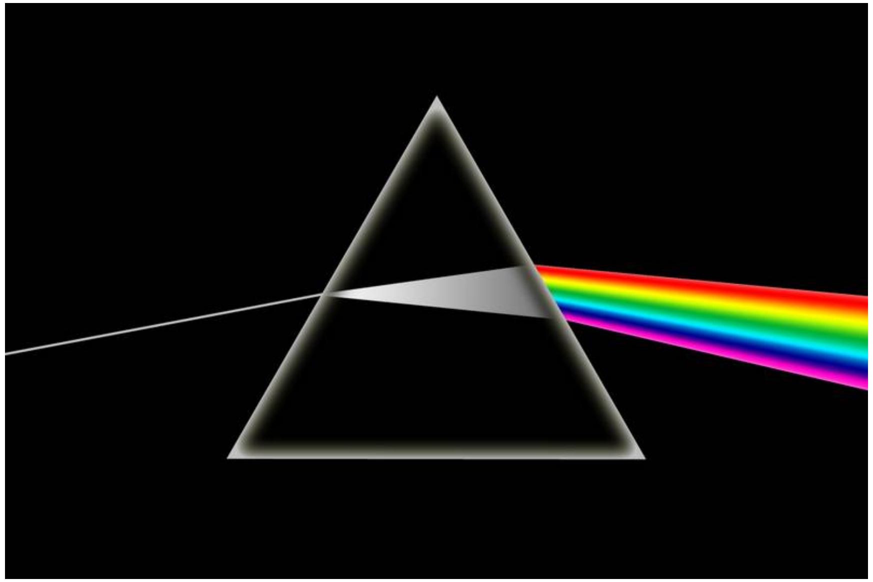
Refractive index: Variation as a function of wavelength

•The reason you see light being split in a prism is due to a combination of Snells law and materials having different refractive index values at different wavelengths.

$$n_1 \sin \theta_1 = n_2 \sin \theta_2$$

•Below is a plot of the refractive index of glass as a function of wavelength.



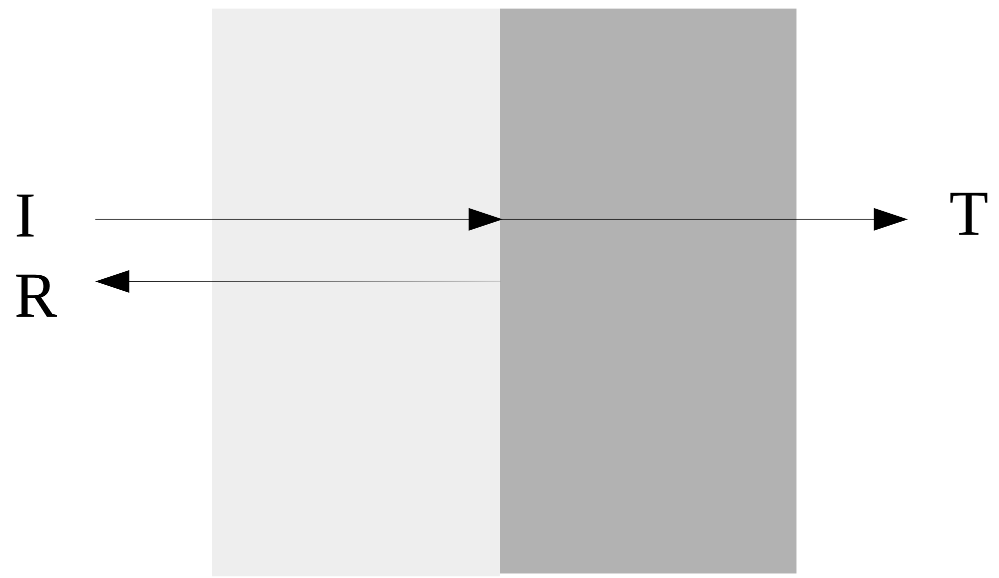


Refractive index (n): Reflection

- Refractive index also governs how much light is reflected/transmitted at an interface:

$$R=\left|\frac{n_1-n_2}{n_1+n_2}\right|^2$$

$$T=1-R$$



- For this talk I'm not going to go further into Snell's law or these relations, I just want you to appreciate the how refractive index influences optical simulations.

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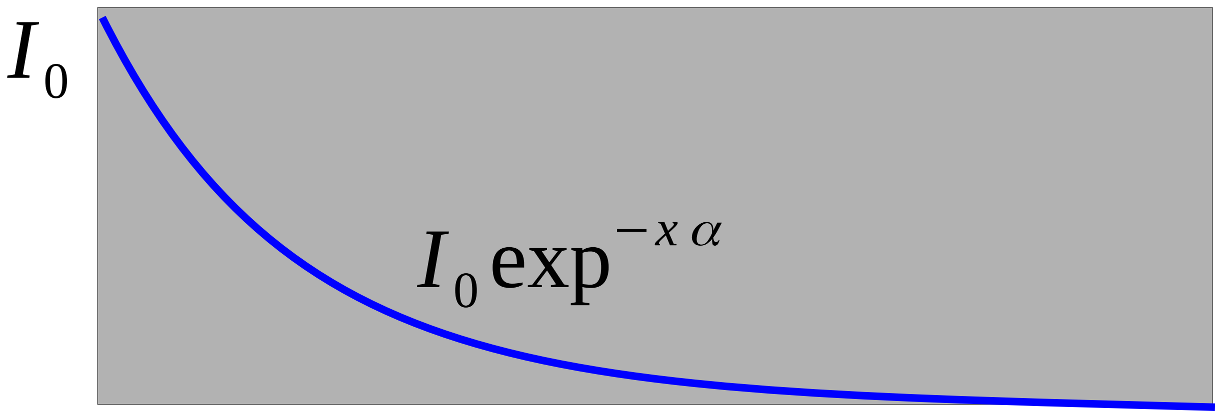
Optical absorption

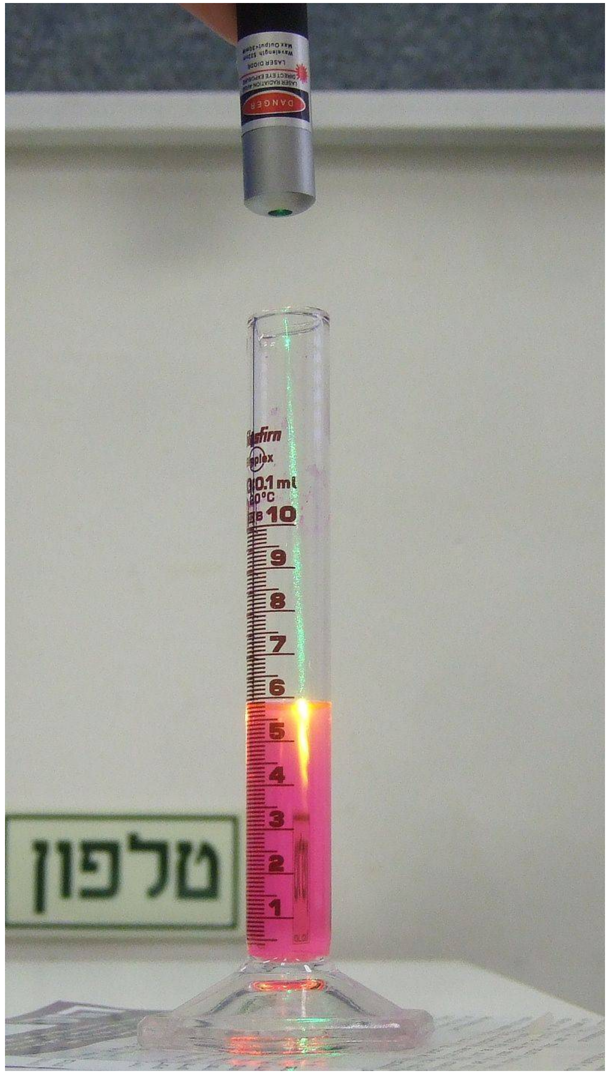
•Optical absorption is the process where by light is absorbed as it passes through a material.

•If follows the equation

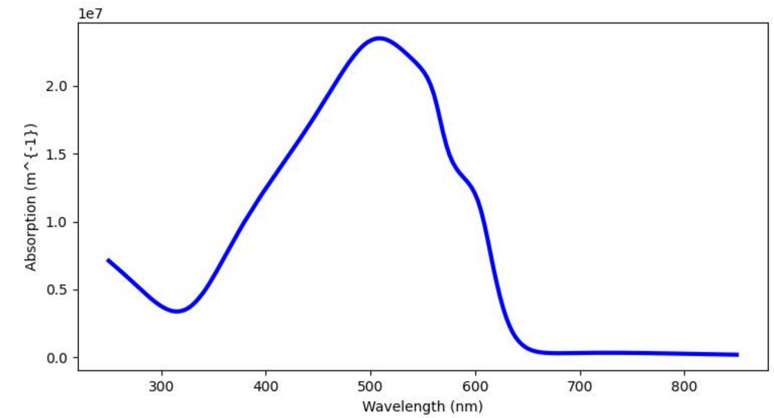
$$I(x) = I_0 \exp^{-x\alpha}$$

• Where I_0 is the initial photon flux, I(x) is the photon flux at position x in the medium and alpha is the absorption coefficient.





Optical absorption: Absorption coefficient (alpha)



- The alpha in this equation also changes as a function of wavelength, an example is given to the left for PTB7 a commonly used polymer in organic electronics.

- So the equation

$$I(x) = I_0 \exp^{-x\alpha}$$

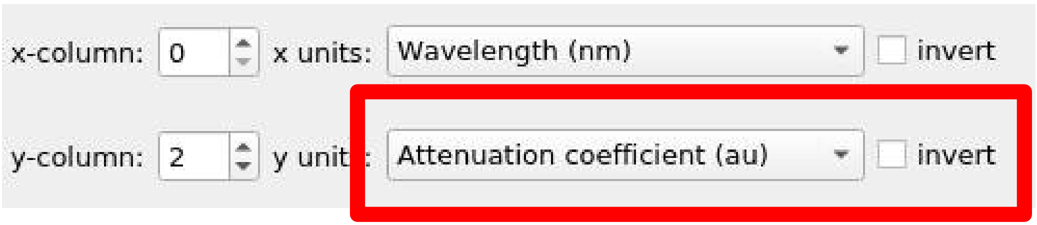
- Should really be written as a function of wavelength:

$$I(x,\lambda) = I_0 \exp^{-x\alpha(\lambda)}$$

- Alpha has units of length^{-1}, in this case as the model works only in SI, m^{-1}.

Optical absorption: Attenuation coefficient (k)

- As a final note you often hear about **n/k** data
- This is a complex number representing both the n term and the alpha term:
- This is written as $\bar{n} = n + j\kappa = n + j\dfrac{\lambda\alpha}{4\pi}$
- The relationship between alpha and k is given as $\alpha = \dfrac{4\pi\kappa}{\lambda}$
- The model takes **alpha** (m^{-1}) as an input, so using the above formula you can convert values of k found in the literature for use in the model.
- The model also has an option to convert k to alpha in the import window:



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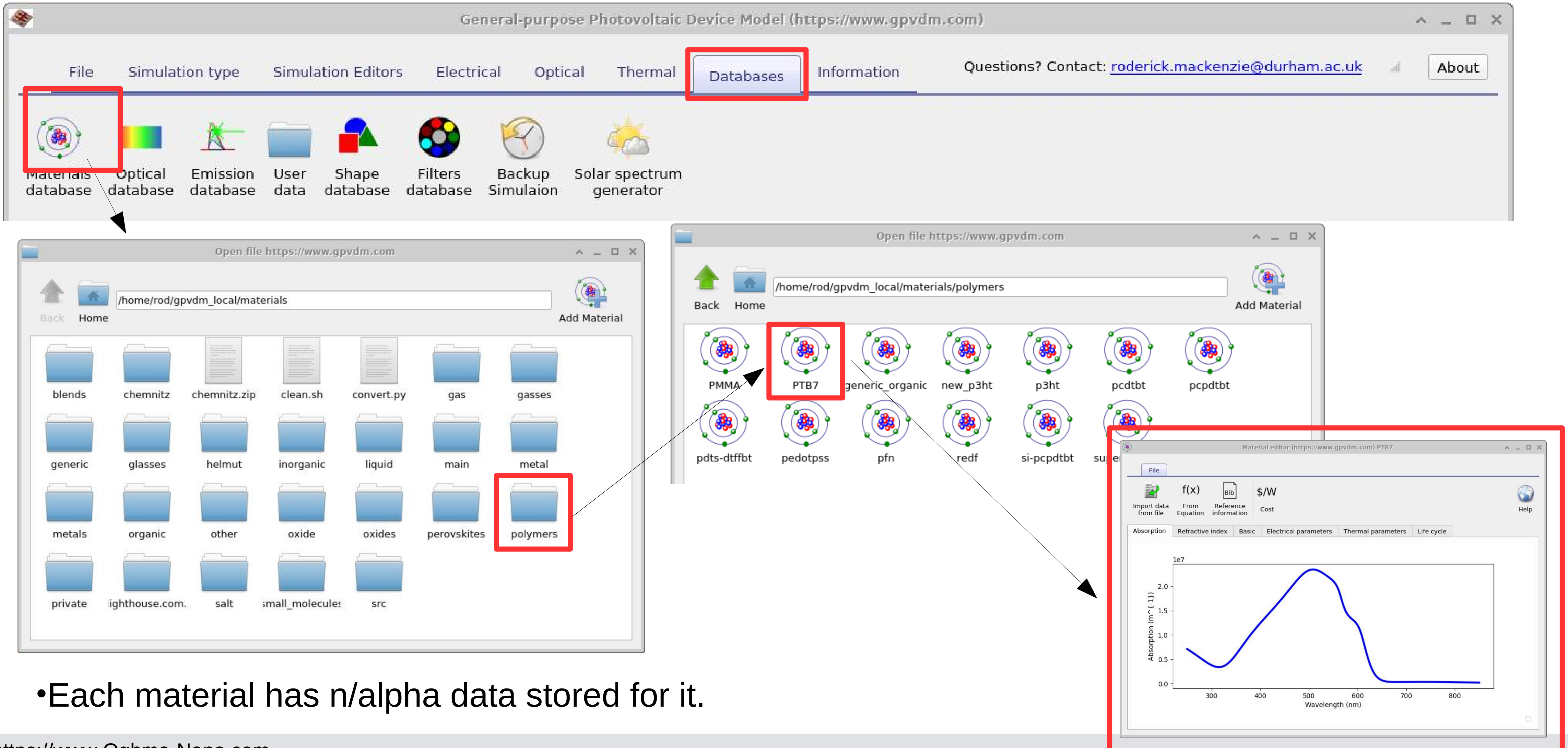
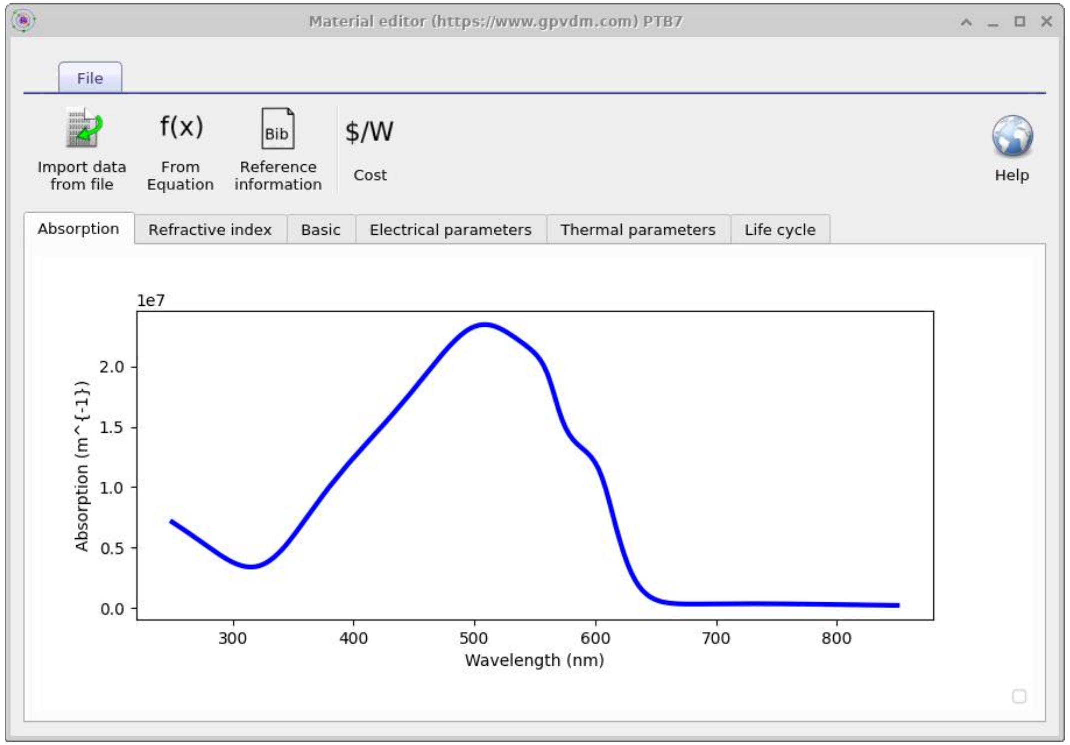
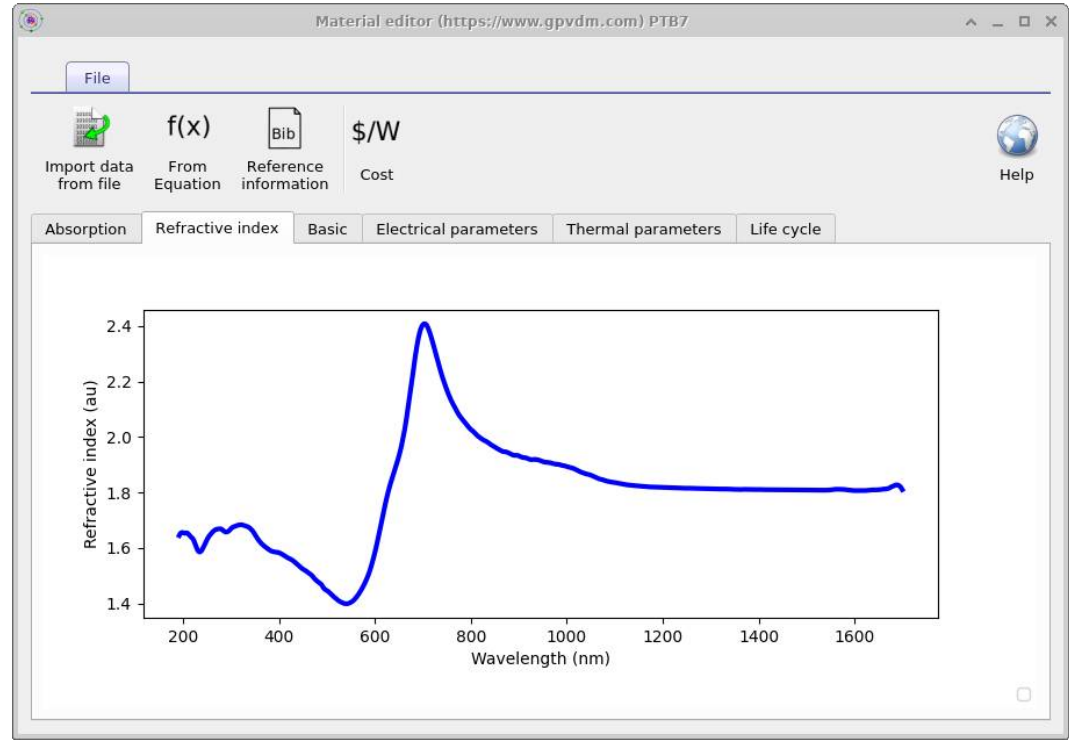
The materials database:
This has lots of materials in it that you can explore



- Each material has n/alpha data stored for it.

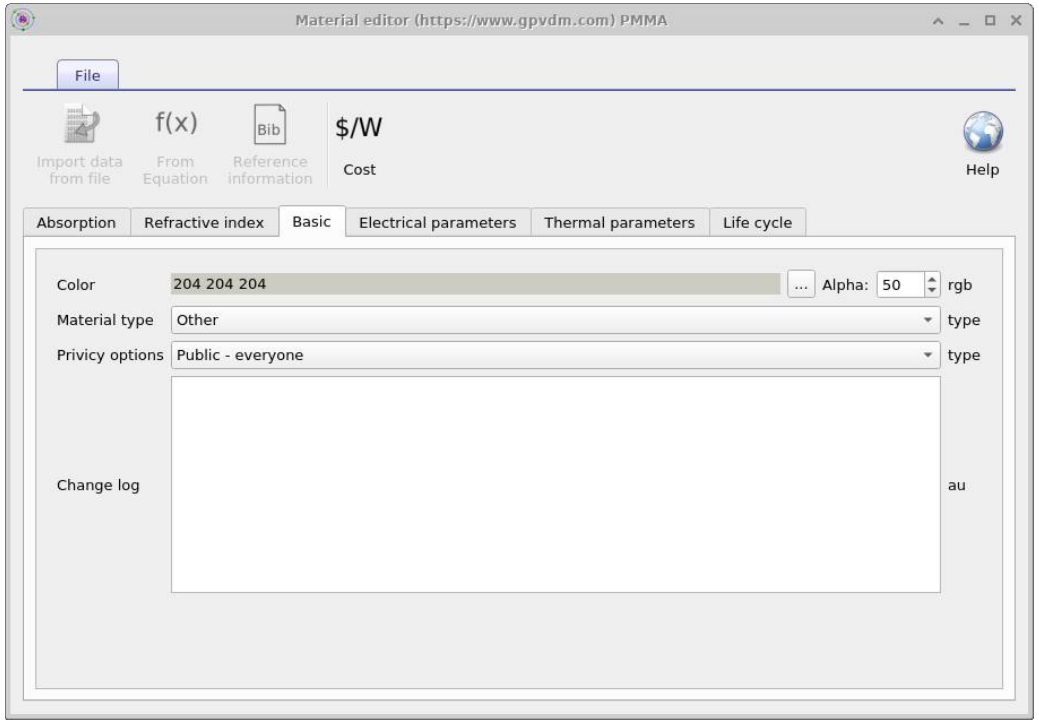
The materials database: n/alpha

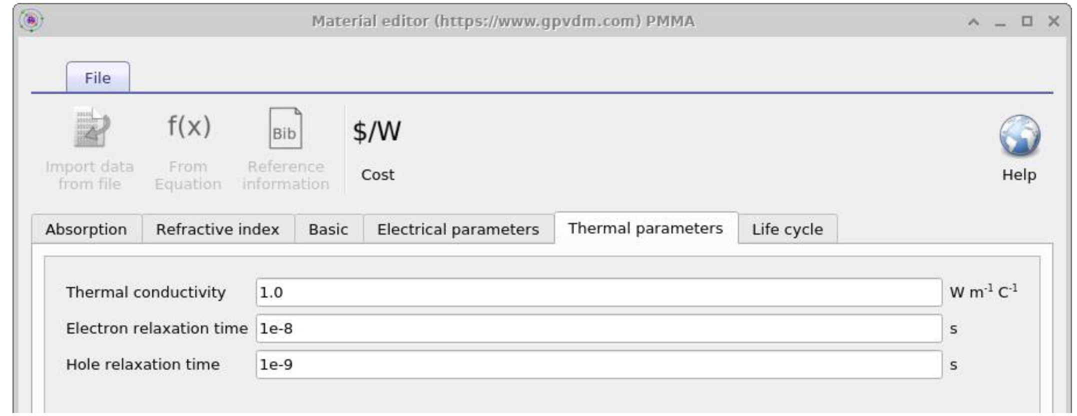


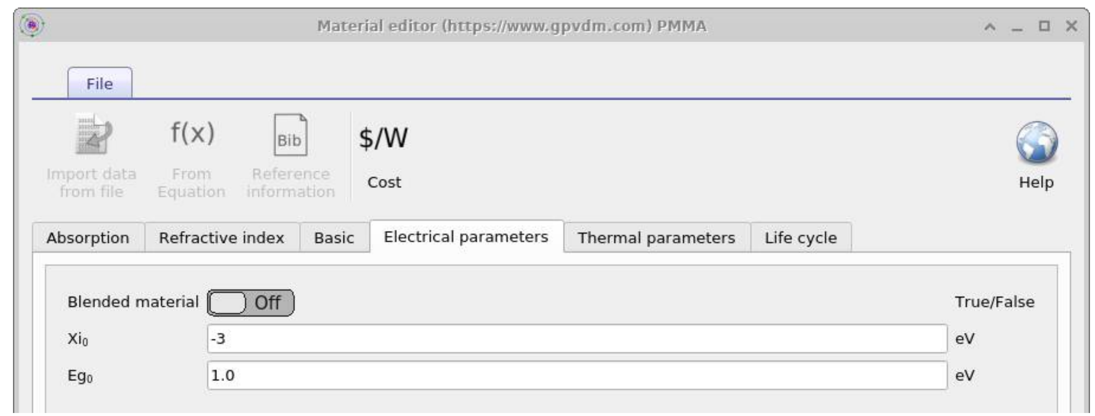


- Each material has both refractive index and absorption data associated with it.

The materials database: Other parameters







- Other tabs show other basic material parameters

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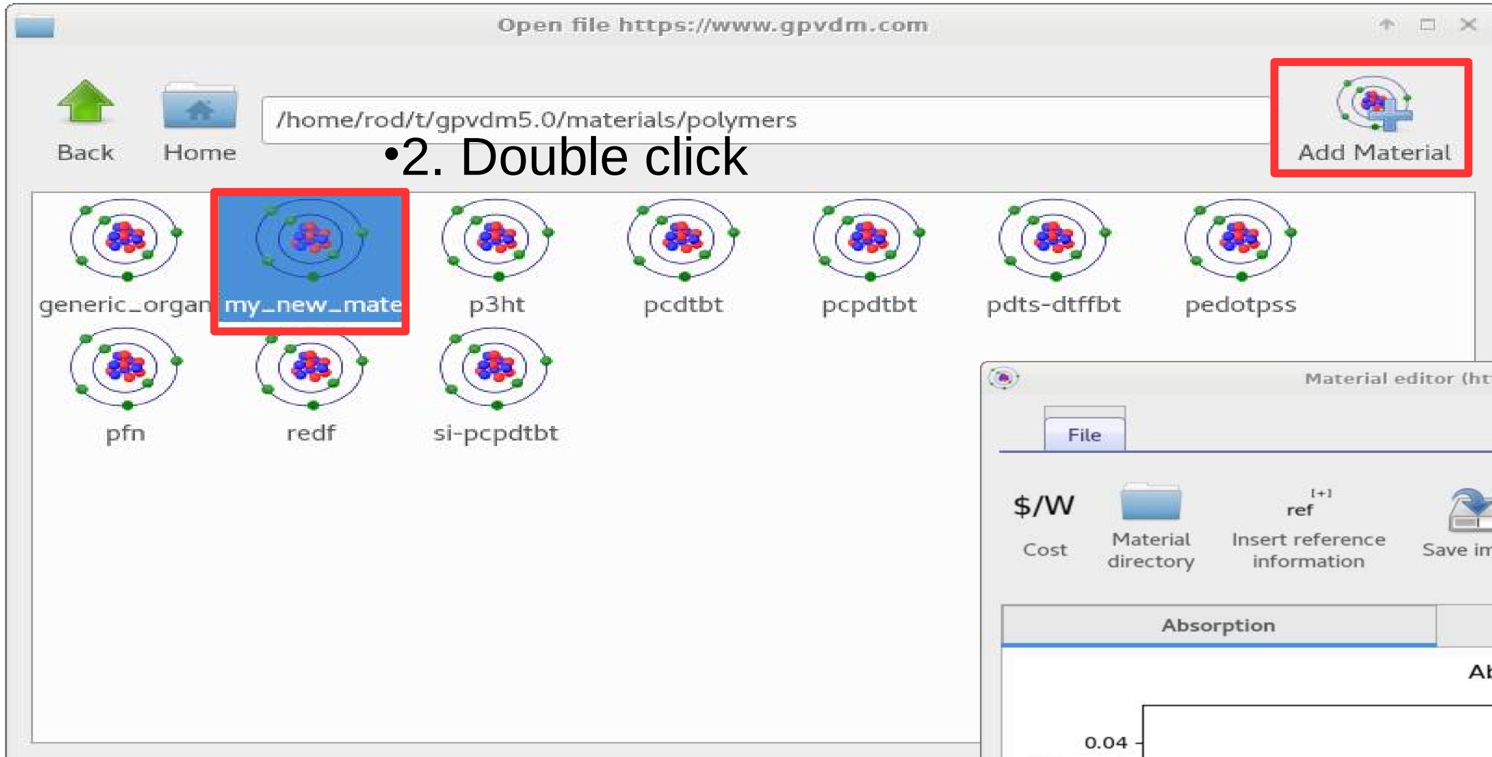
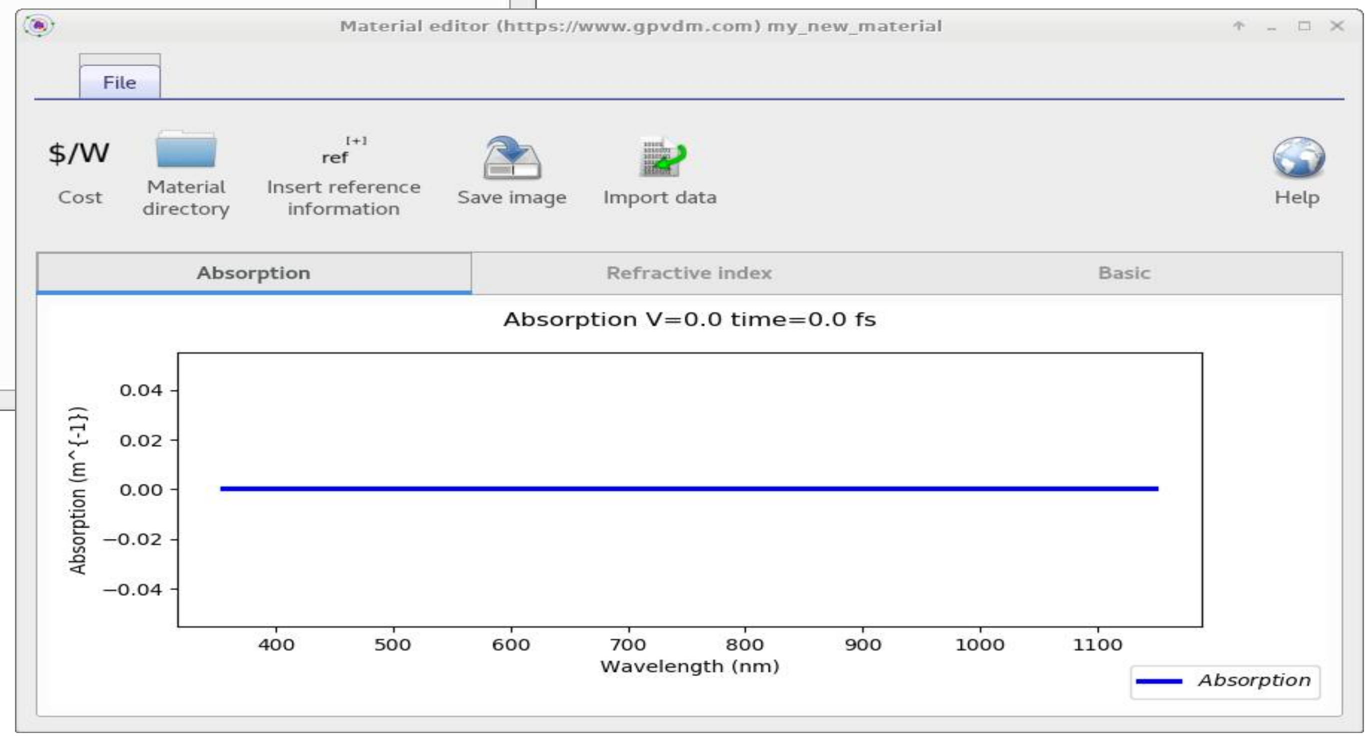
Making a new material



•1. Click

•2. Double click

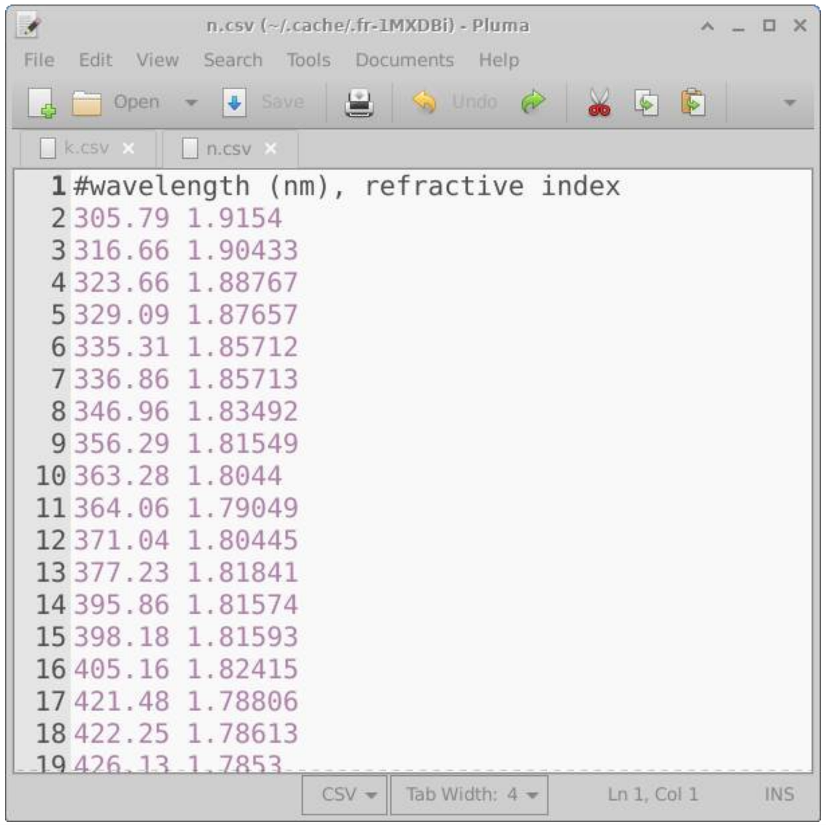


•The material file has no data….

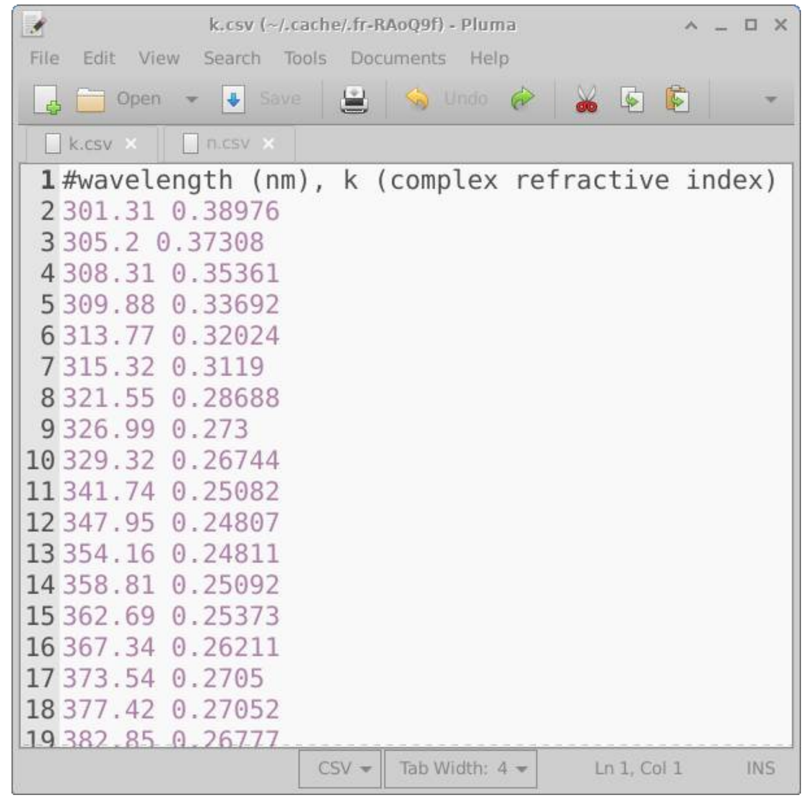
Let’s get hold of some data to import… usually you would get this from experiment or a publication.

- Download this zip archive https://www.gpvdm.com/demo/ptb7pc70bm_demo.zip and UNZIP it.

- You should have two files….

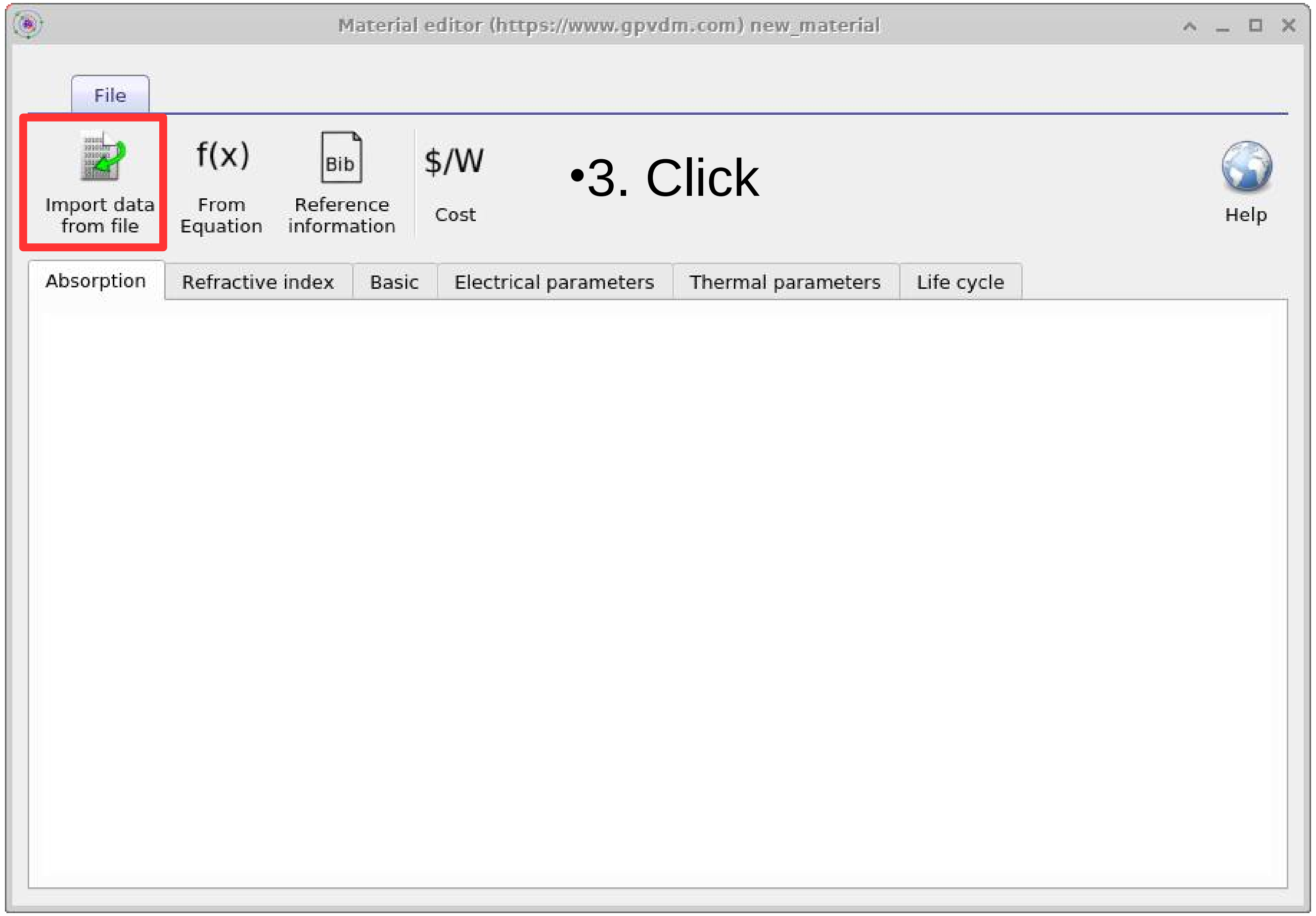



```
1 #wavelength (nm), refractive index
2 305.79 1.9154
3 316.66 1.90433
4 323.66 1.88767
5 329.09 1.87657
6 335.31 1.85712
7 336.86 1.85713
8 346.96 1.83492
9 356.29 1.81549
10 363.28 1.8044
11 364.06 1.79049
12 371.04 1.80445
13 377.23 1.81841
14 395.86 1.81574
15 398.18 1.81593
16 405.16 1.82415
17 421.48 1.78806
18 422.25 1.78613
19 426.13 1.7853
```



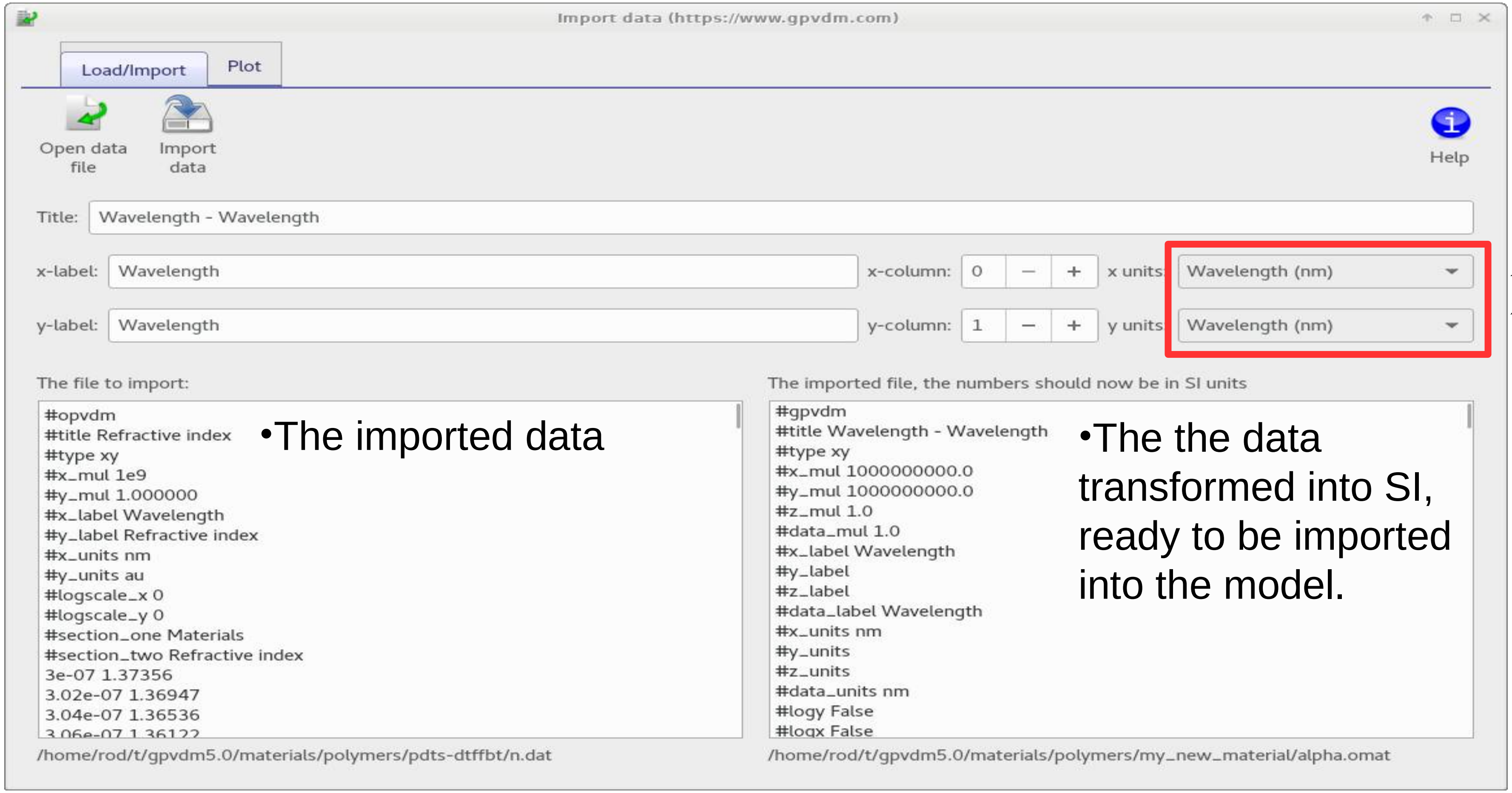

```
1 #wavelength (nm), k (complex refractive index)
2 301.31 0.38976
3 305.2 0.37308
4 308.31 0.35361
5 309.88 0.33692
6 313.77 0.32024
7 315.32 0.3119
8 321.55 0.28688
9 326.99 0.273
10 329.32 0.26744
11 341.74 0.25082
12 347.95 0.24807
13 354.16 0.24811
14 358.81 0.25092
15 362.69 0.25373
16 367.34 0.26211
17 373.54 0.2705
18 377.42 0.27052
19 382.85 0.26777
```

Let's import k.csv



- Select "Import the data from file" button.
- Select k.csv to import… from where ever you extracted n/k.csv
- Again the import window will pop up.

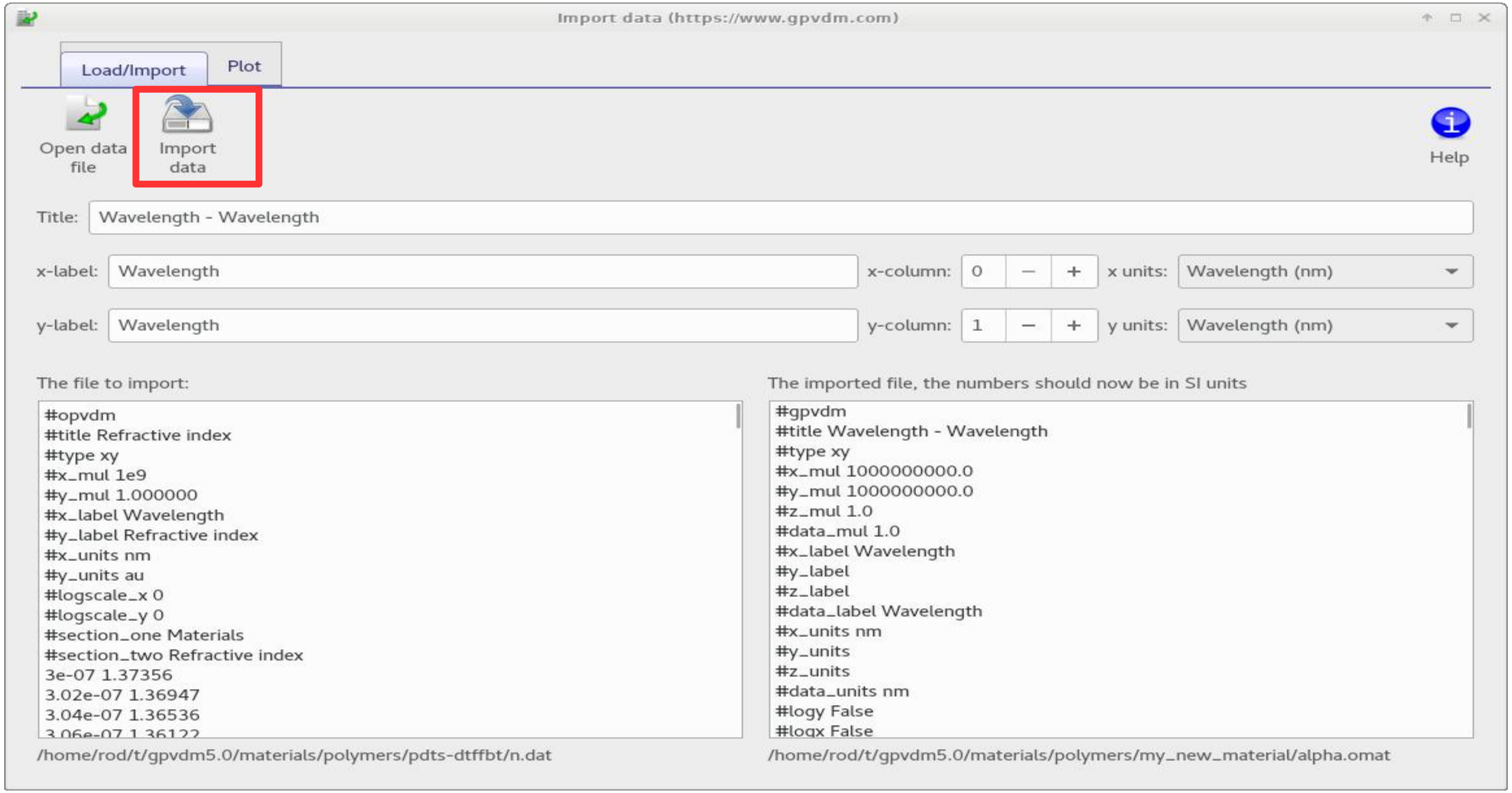
The raw data will be on the LHS of the import window The RHS will display the data converted to SI units.



•Set these to the units used in the RAW data file you imported.

•Set the values to **Wavelength (nm)**, and **Attenuation coefficient (au)**, the RHS will then be in SI, scroll down to inspect the file. Make sure it has been imported correctly

Then click import data and the data will be imported into the material..



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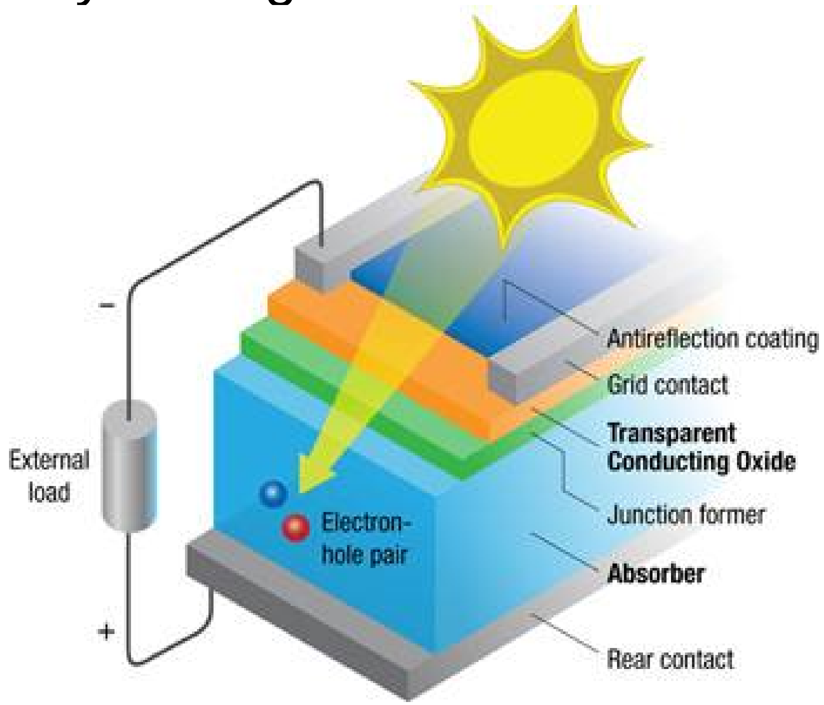
We are now going to do an example using a solar cell.

•There is currently a lot or research interest in these devices.

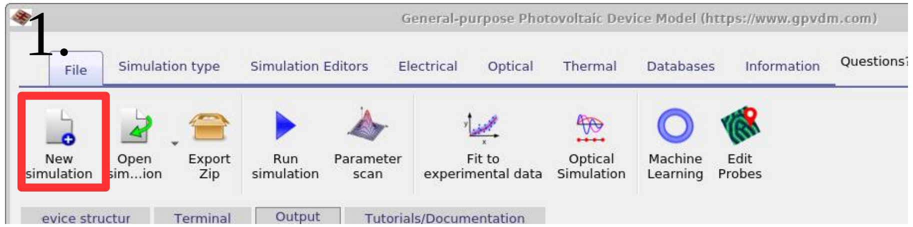
•For this we will use the transfer matrix method. This assumes light propagates in the device as a wave.

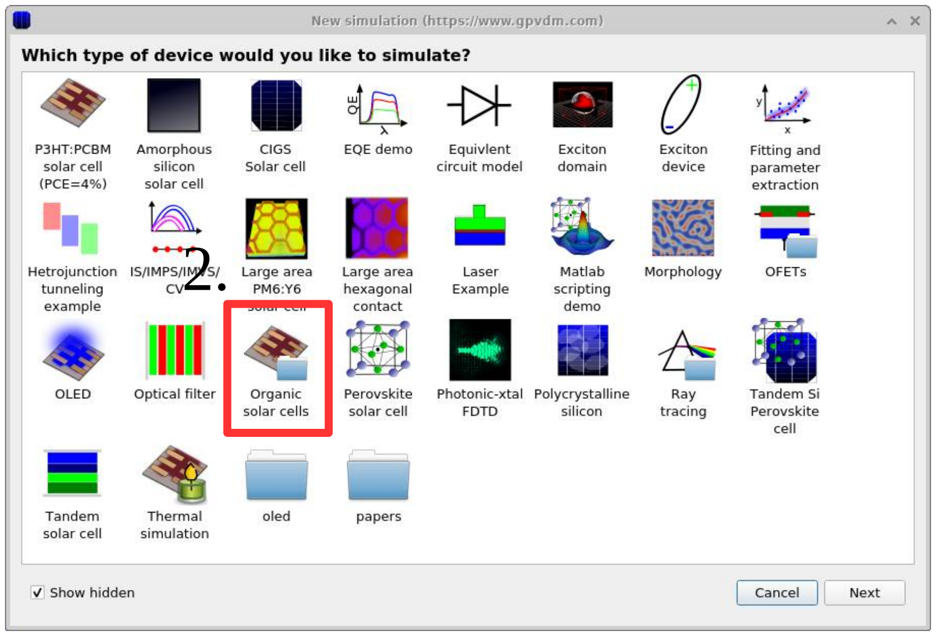
•Don't worry about this too much for now but it's different to ray tracing.

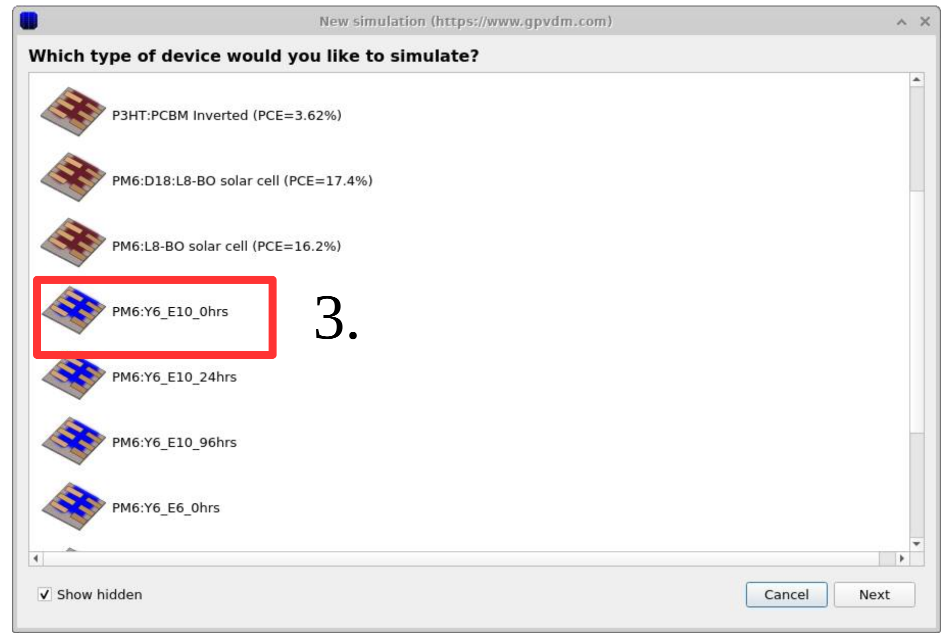


https://www.nrel.gov/pv/organic-photovoltaic-solar-cells.html

Make a new solar cell simulation

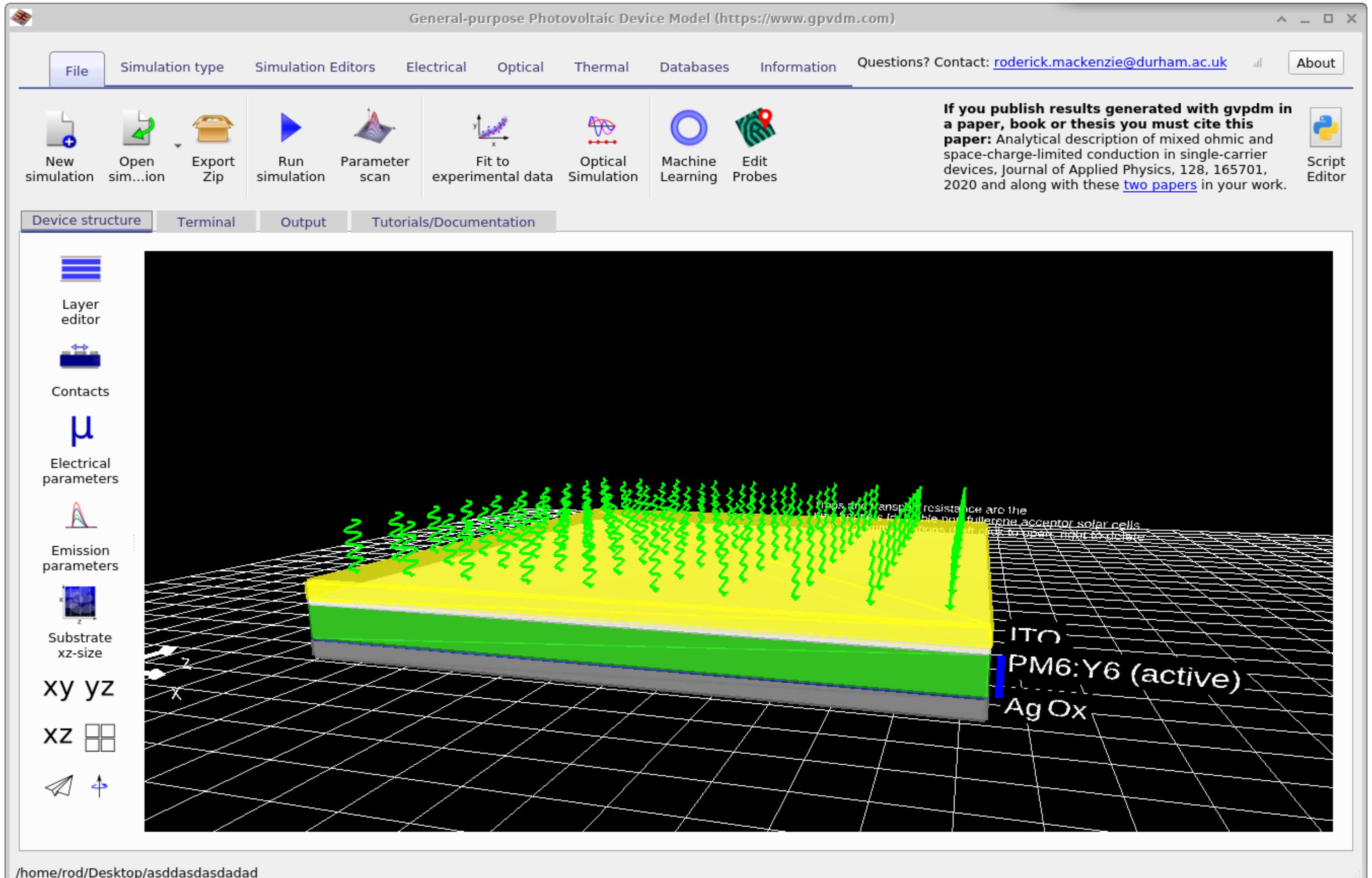






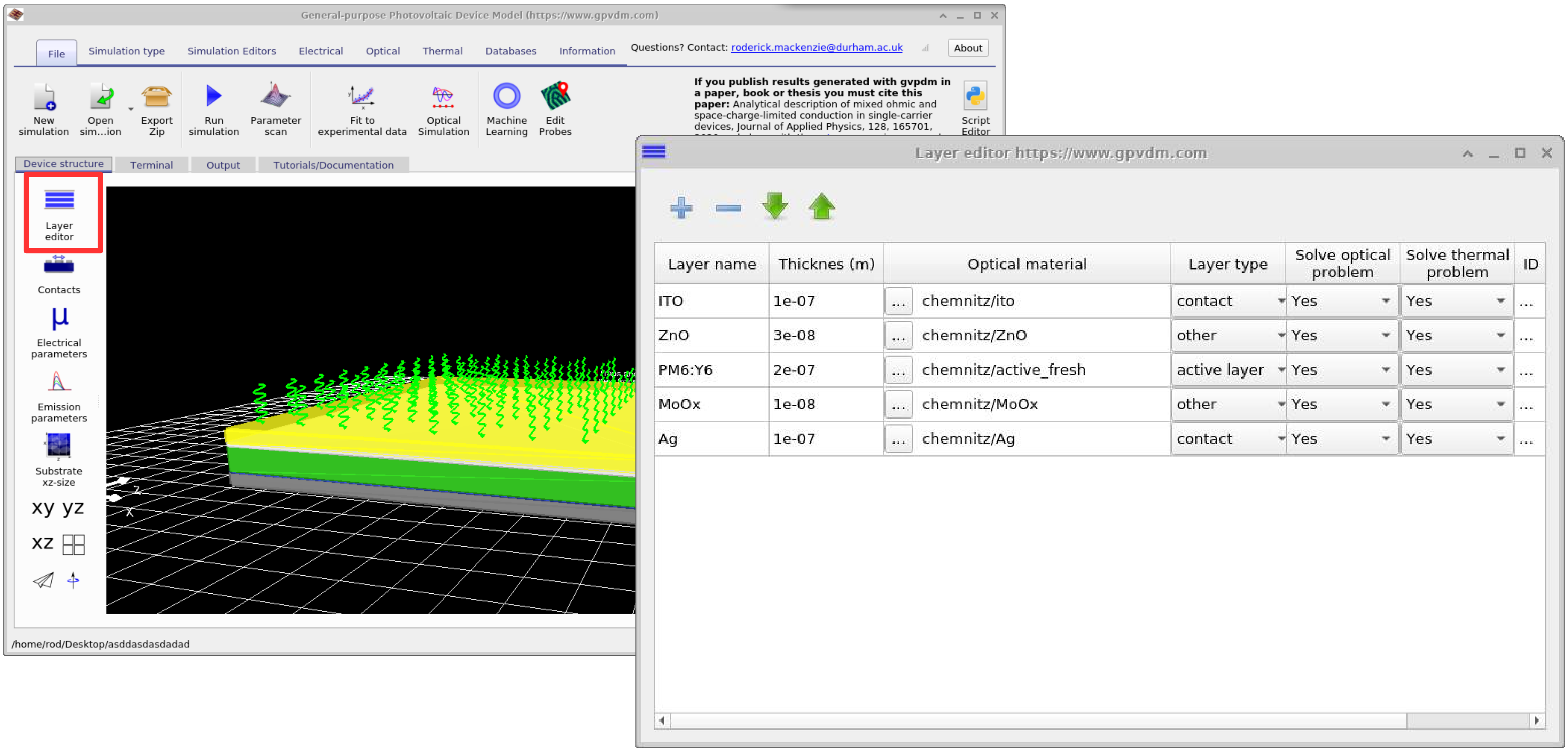
- We are going to select a PM6:Y6 Organic solar cell which is a modern type of organic solar cell.
- Save this example to your home directory.

You should get a window like this

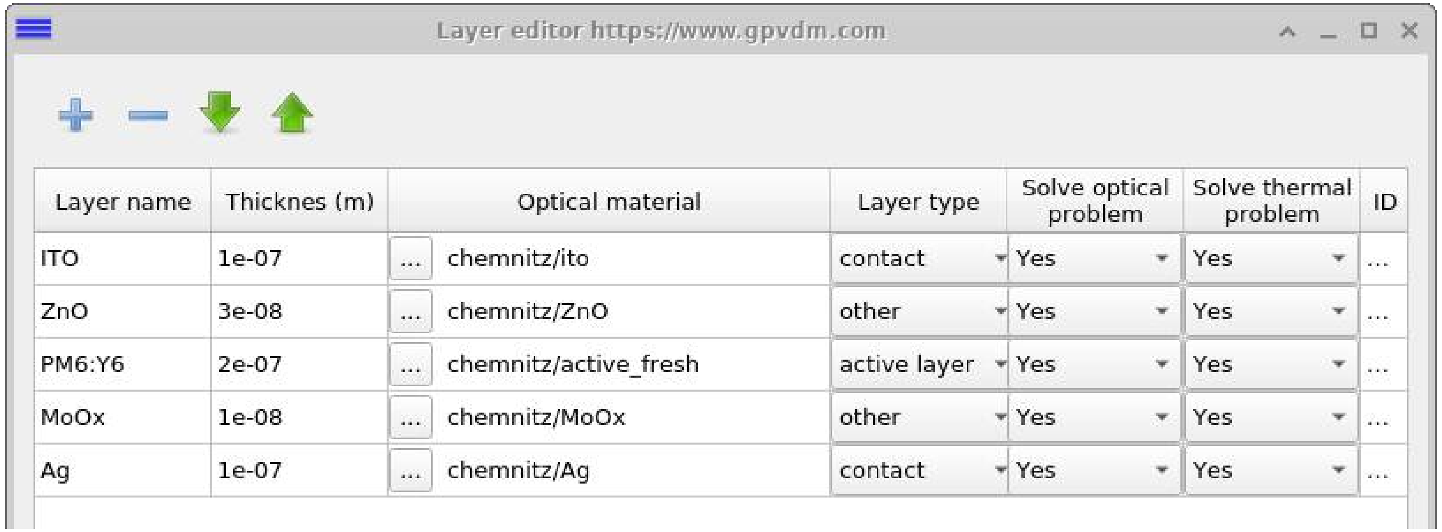


- You can see the solar cell is made up of around five layers.
- You can see light coming in from the top.
- If you click on the layer editor you can inspect the layers.

Opening the layer editor



The layer editor



Layer name	Thicknes (m)		Optical material	Layer type	Solve optical problem	Solve thermal problem	ID
ITO	1e-07	...	chemnitz/ito	contact	Yes	Yes	...
ZnO	3e-08	...	chemnitz/ZnO	other	Yes	Yes	...
PM6:Y6	2e-07	...	chemnitz/active_fresh	active layer	Yes	Yes	...
MoOx	1e-08	...	chemnitz/MoOx	other	Yes	Yes	...
Ag	1e-07	...	chemnitz/Ag	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.

•**Other columns:** Discuss elsewhere.

•You can use the + button to add layers, the – button to remove layers.

Homework task:

Layer editor https://www.gpvdm.com

Layer name	Thicknes (m)	Optical material	Layer type	Solve optical problem	Solve thermal problem	ID
ITO	1e-07	... chemnitz/ito	contact	Yes	Yes	...
ZnO	3e-08	... chemnitz/ZnO	other	Yes	Yes	...
PM6:Y6	2e-07	... chemnitz/active_fresh	active layer	Yes	Yes	...
MoOx	1e-08	... chemnitz/MoOx	other	Yes	Yes	...
Ag	1e-07	... chemnitz/Ag	contact	Yes	Yes	...

•Increase the thickness of the active layer to 300nm and change the material to chemnitz/active_aged.

•The materials are in the directory chemnitz, as the data was measured in the city of Chemnittz, Germany.

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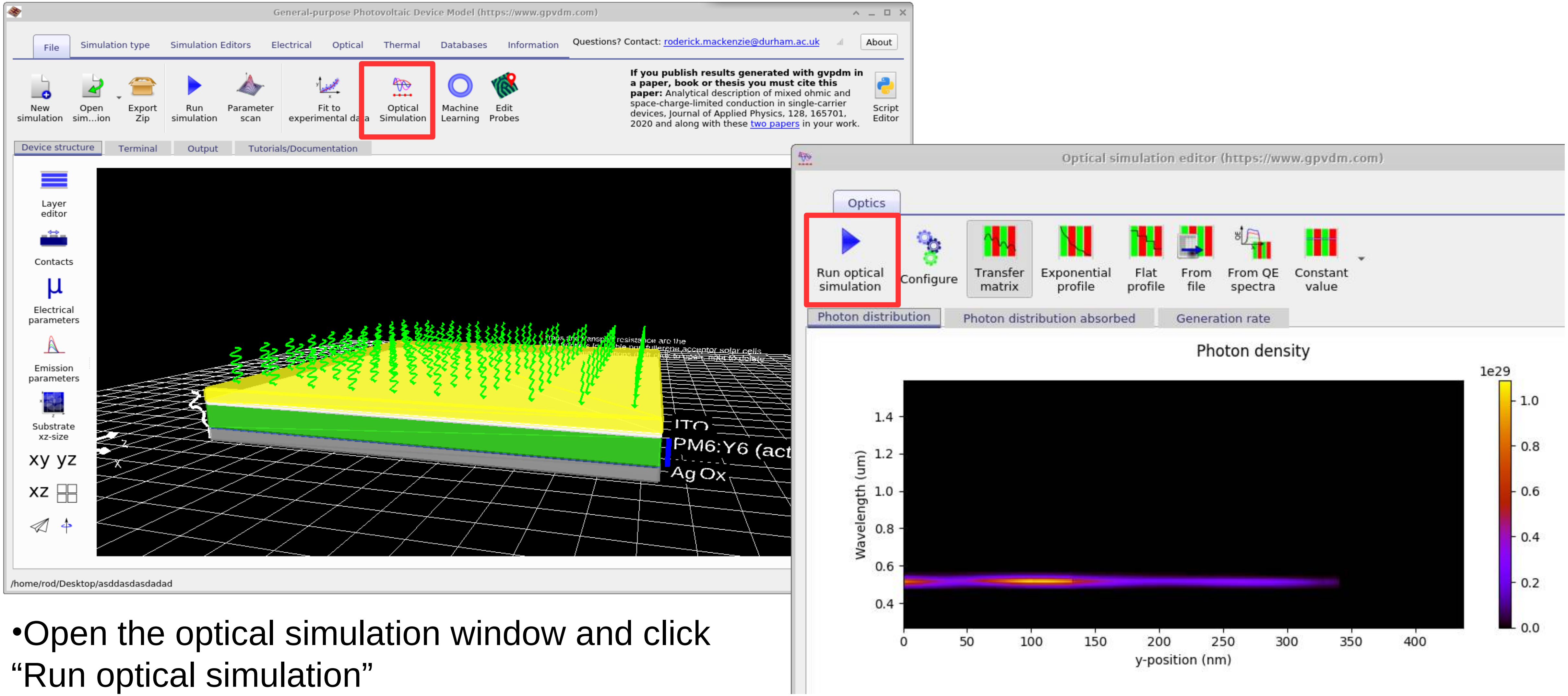
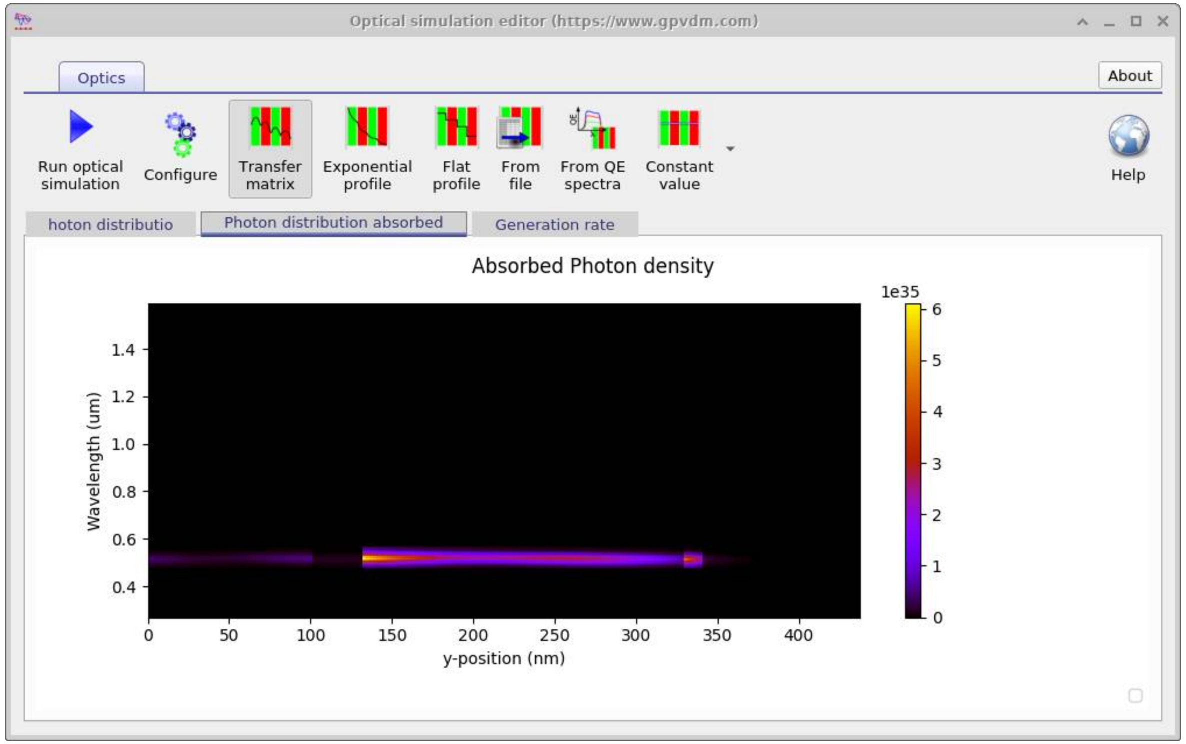
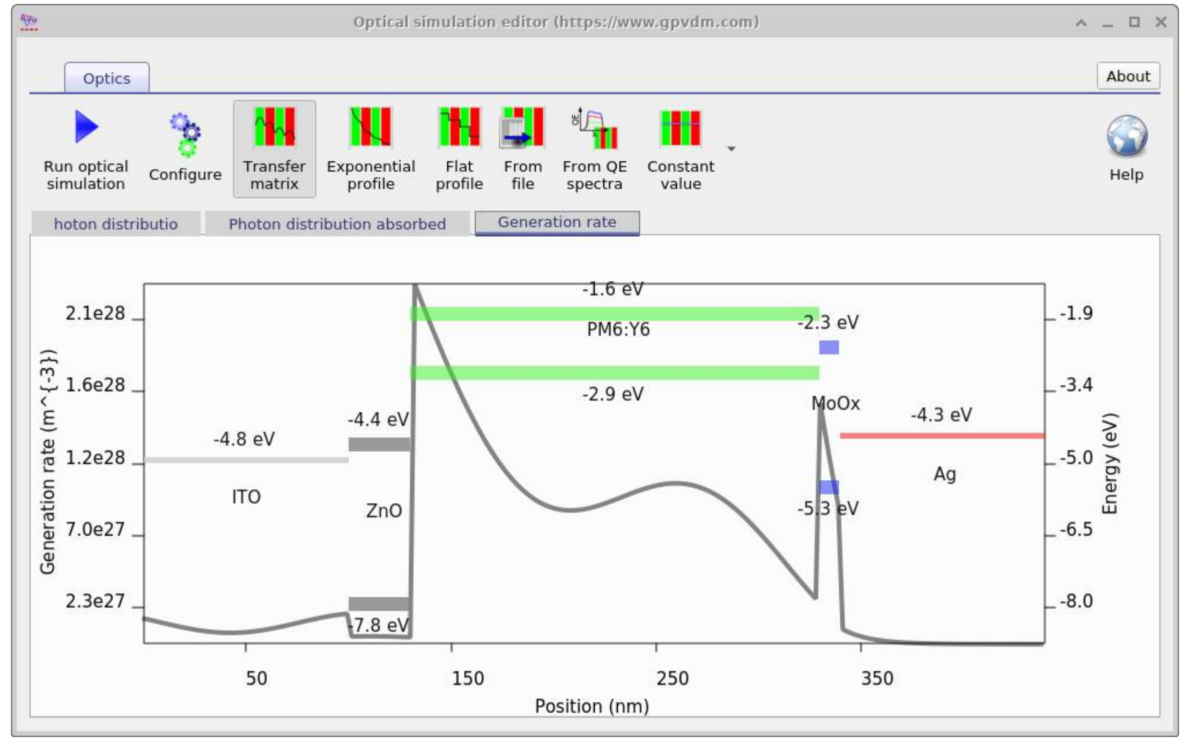
Running the full optical simulation...



- Open the optical simulation window and click "Run optical simulation"

Look at the generation rate in the device:





•This cell is excited with an LED, so you will see a very narrow region of excitation at 515 nm.

•The generation rate tab shows the generation profile in the device with all wavelengths jointed together.

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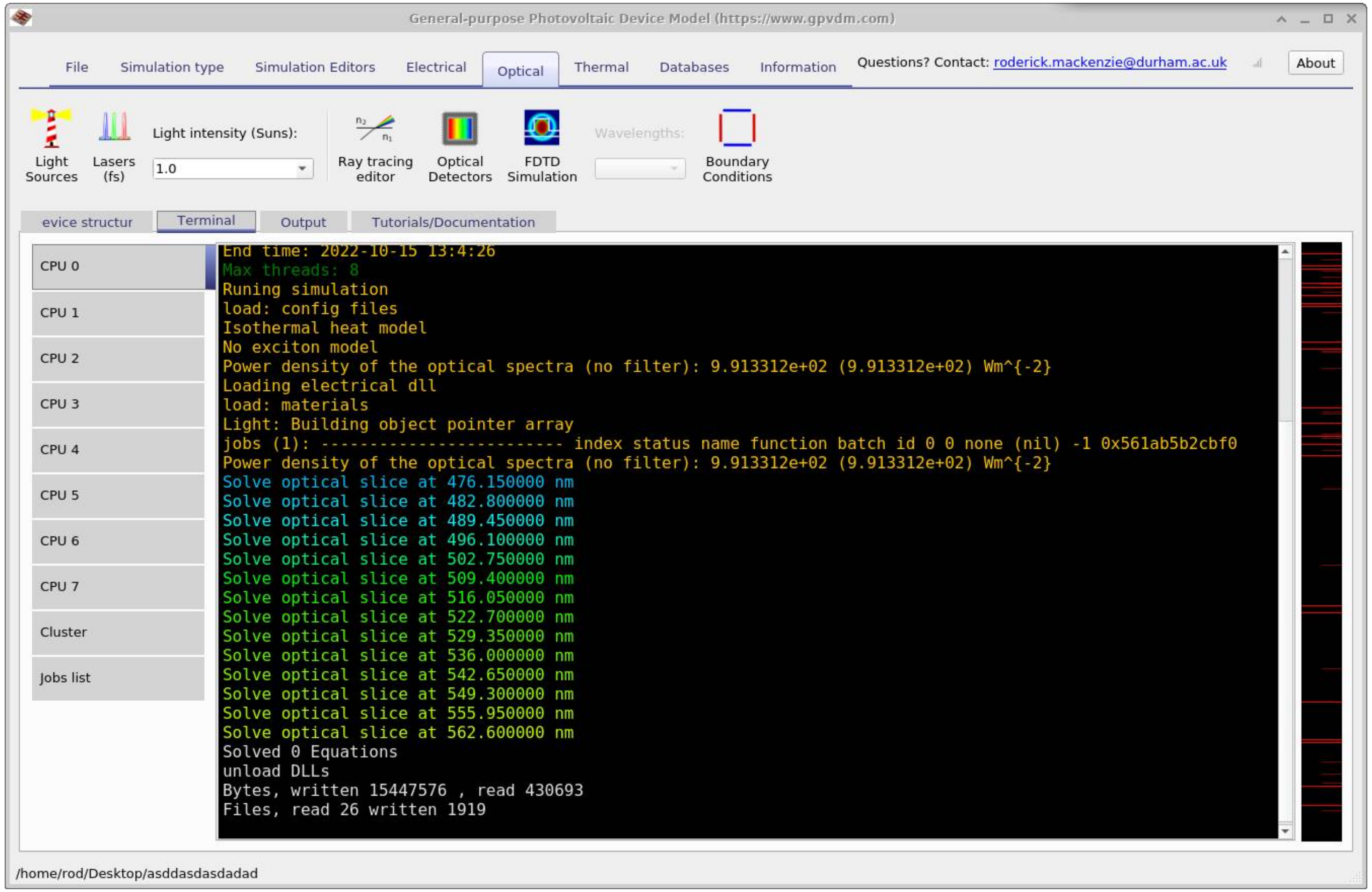
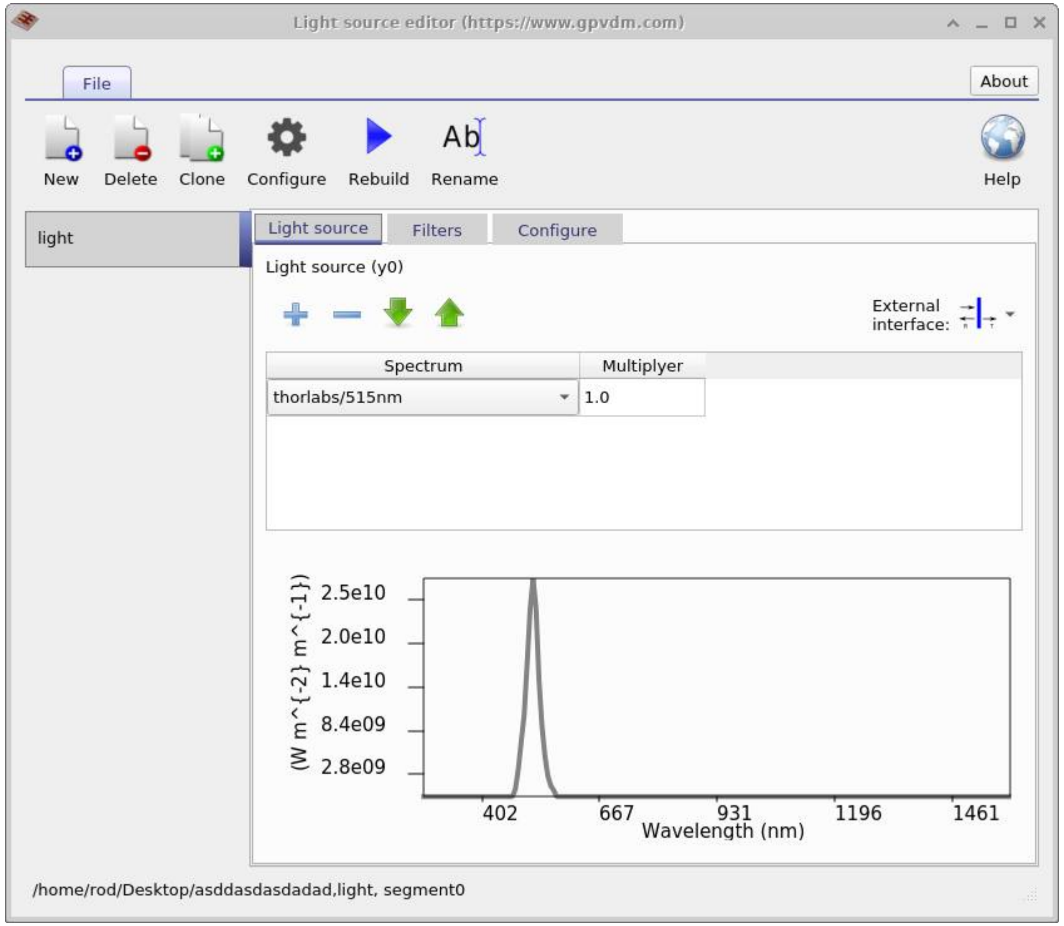
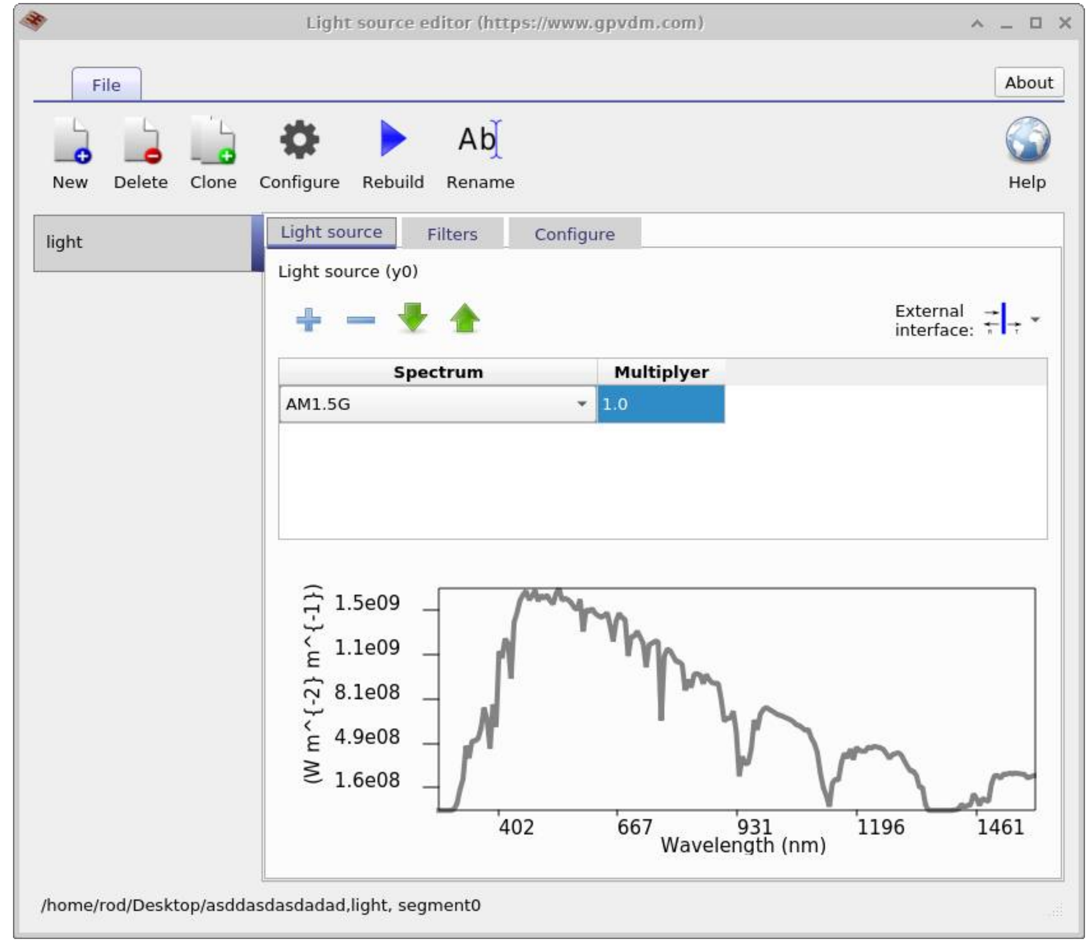
Light sources



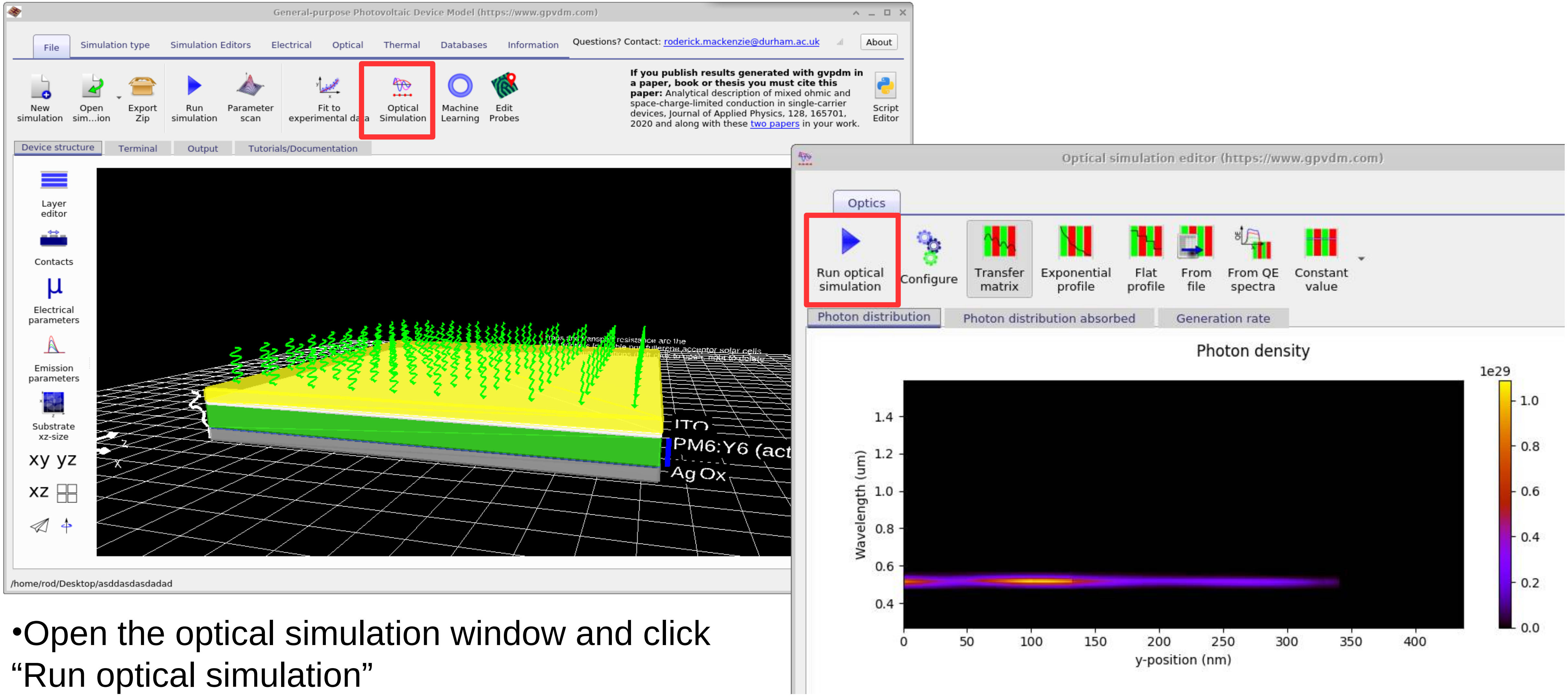
- You will





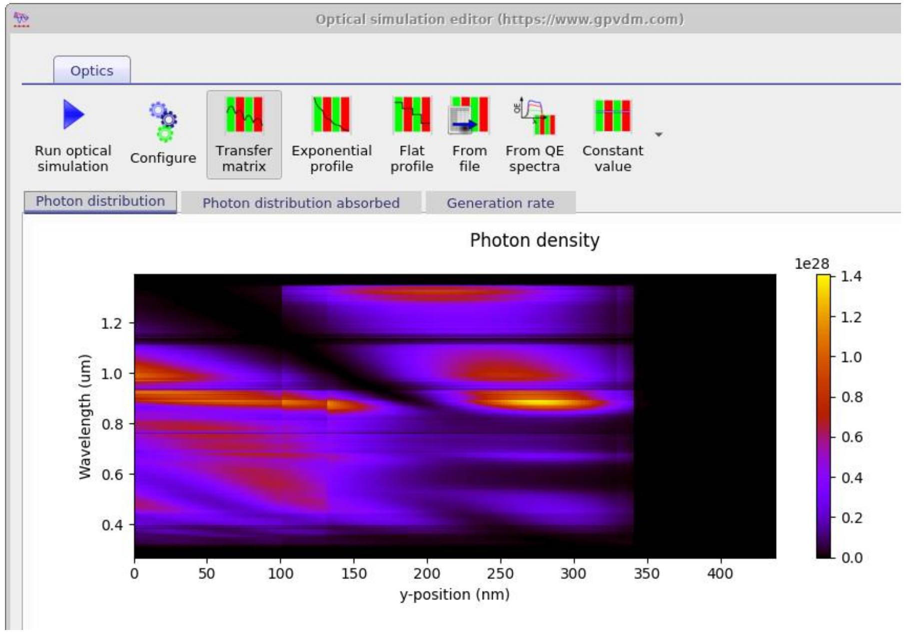
- **Note:** You can also mix various spectra and apply filters using this window.

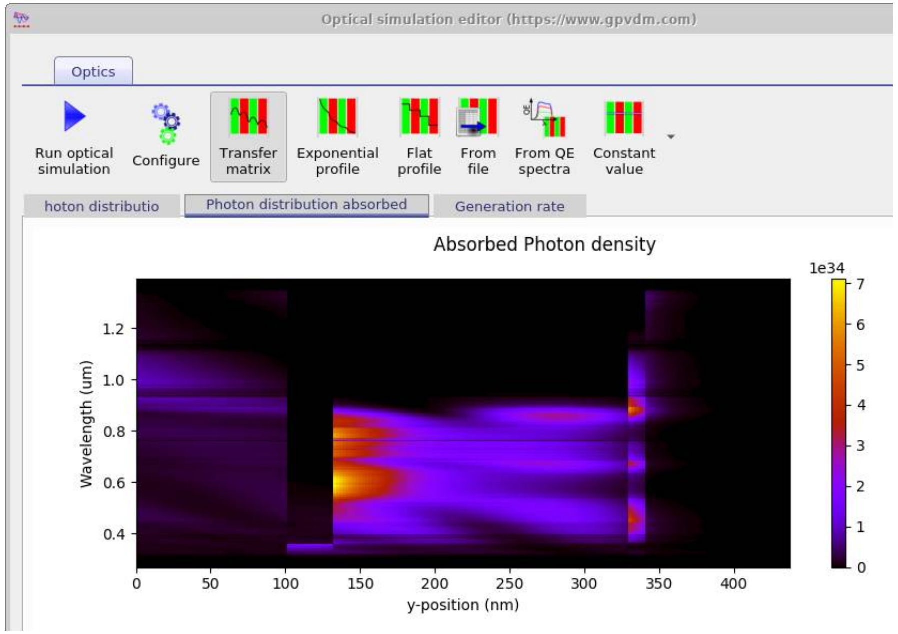
Now go back and rerun the optical simulation

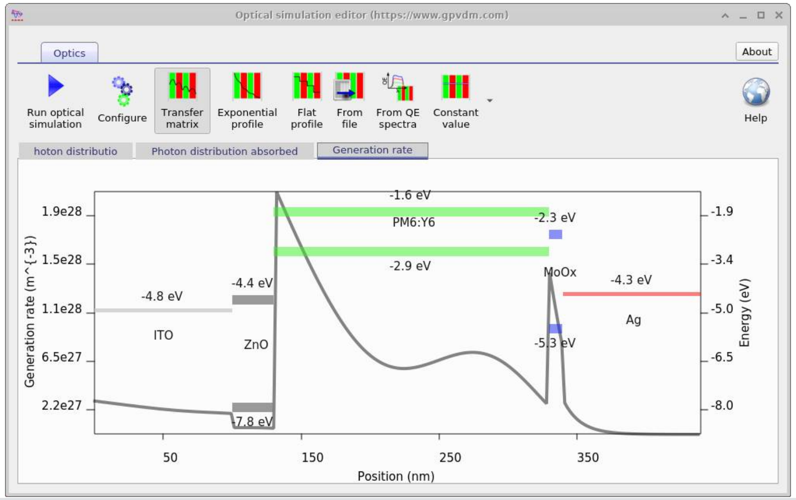


- Open the optical simulation window and click "Run optical simulation"

Now go back and rerun the optical simulation







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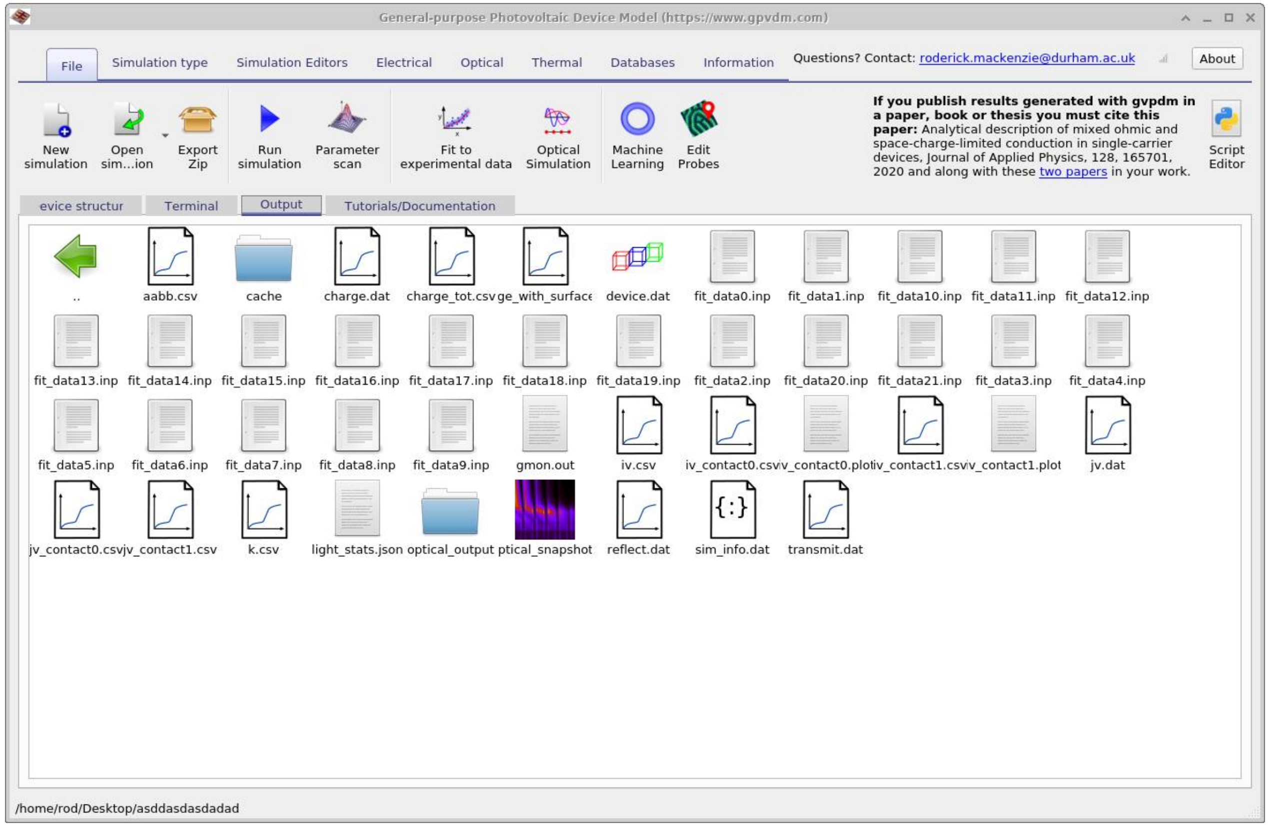
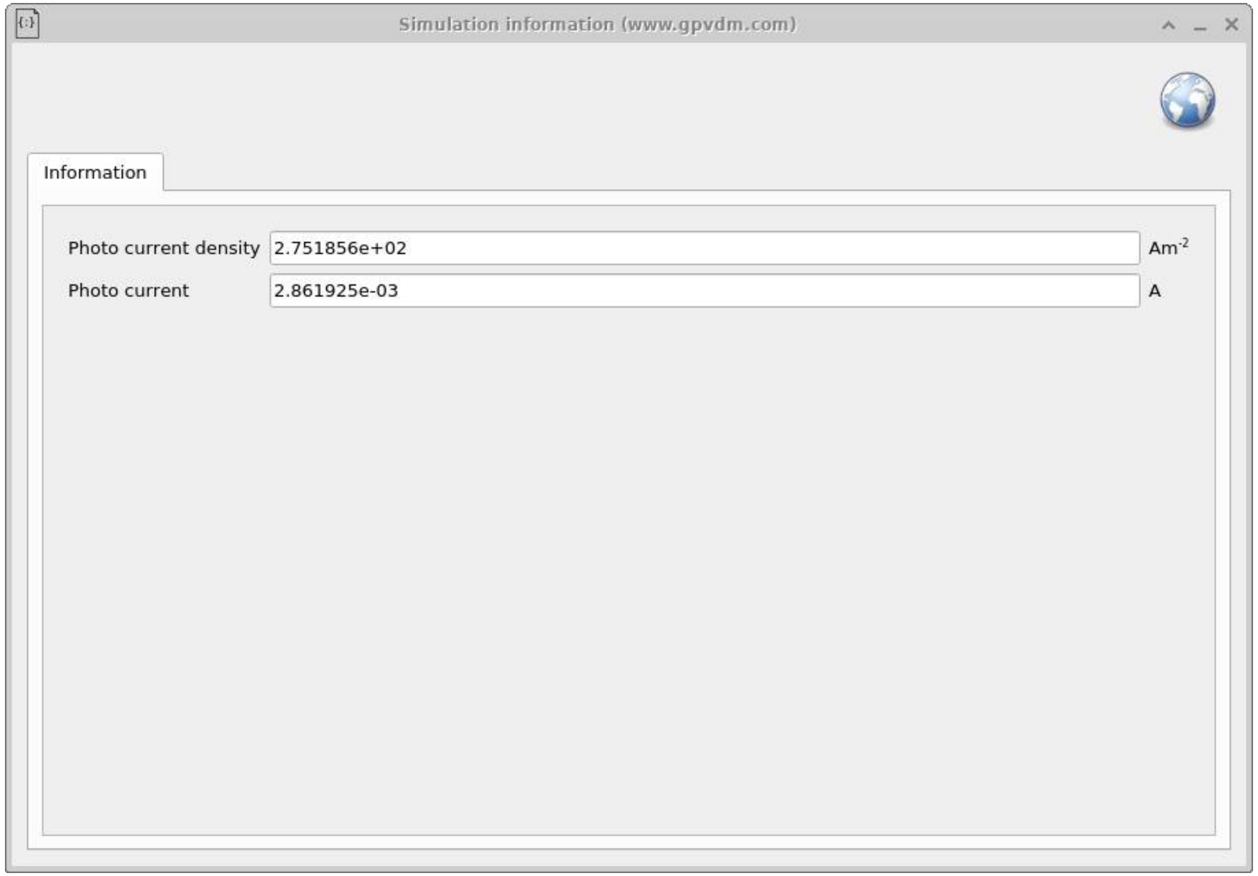
Outputs:
Optical snapshots



Simulation information: sim_info.dat



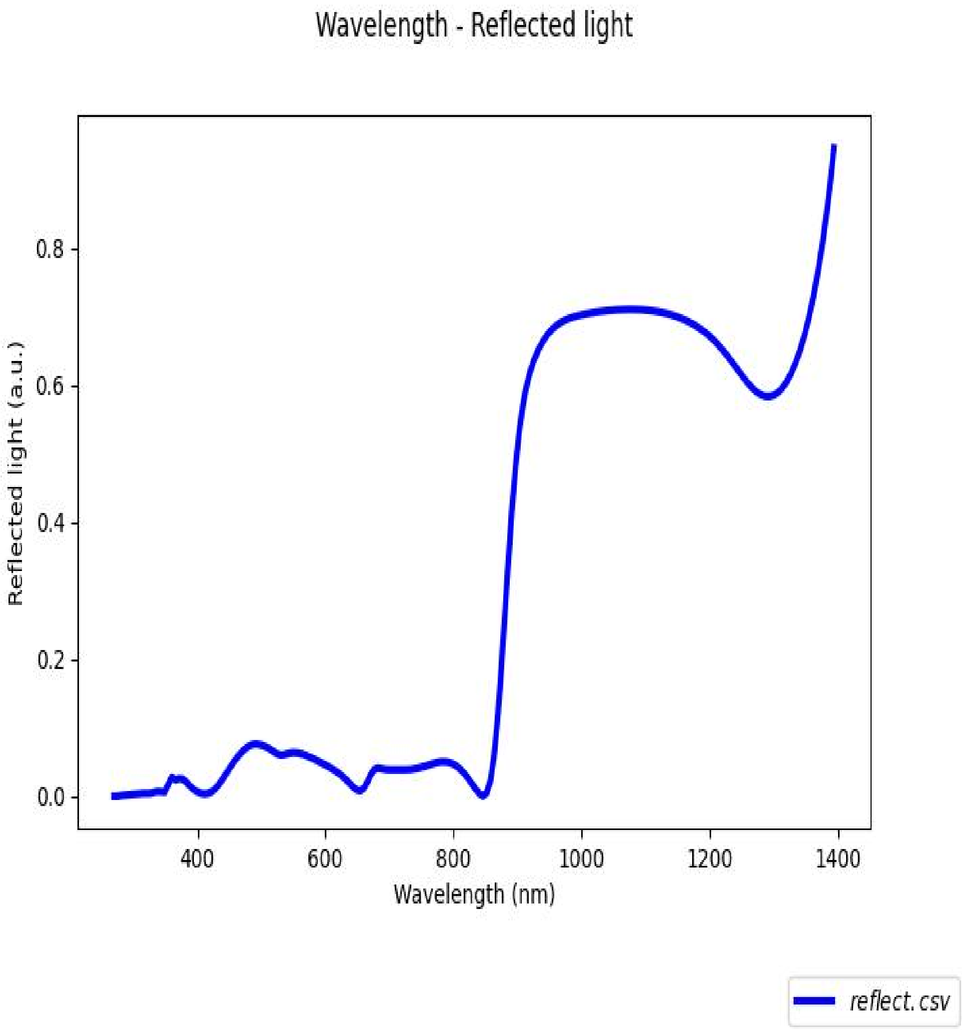
- This file contains the maximum photocurrent one would get out of the device.

Statistics: light_stats.json


```
{
    "layers" : 5,
    "layer0": {
        "light_frac_photon_generation": 1.103641e-01
        },
    "layer1": {
        "light_frac_photon_generation": 8.650944e-03
        },
    "layer2": {
        "light_frac_photon_generation": 8.050166e-01
        },
    "layer3": {
        "light_frac_photon_generation": 5.804029e-02
        },
    "layer4": {
        "light_frac_photon_generation": 1.792815e-02
        }
}
```


- This file contains a breakdown of which layers absorb what fraction of light in the material.

Optical transmission/reflection transmit.csv, reflect.csv



- Transmission reluctance

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Summary

- In this talk we covered the basics of modeling light in thin films.

- This should be useful sensors, solar cells, filters and many other classes of opto-electronic devices.