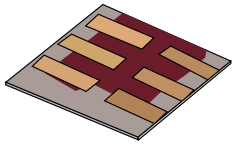

Adding materials to gpvdm

This tutorial covers adding extra materials to the gpvdm materials database.

Dr. Roderick MacKenzie
roderick.mackenzie@nottingham.ac.uk
Autumn 2021

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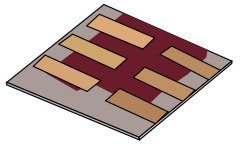
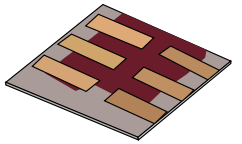
https://www.gpvdm.com

Outline

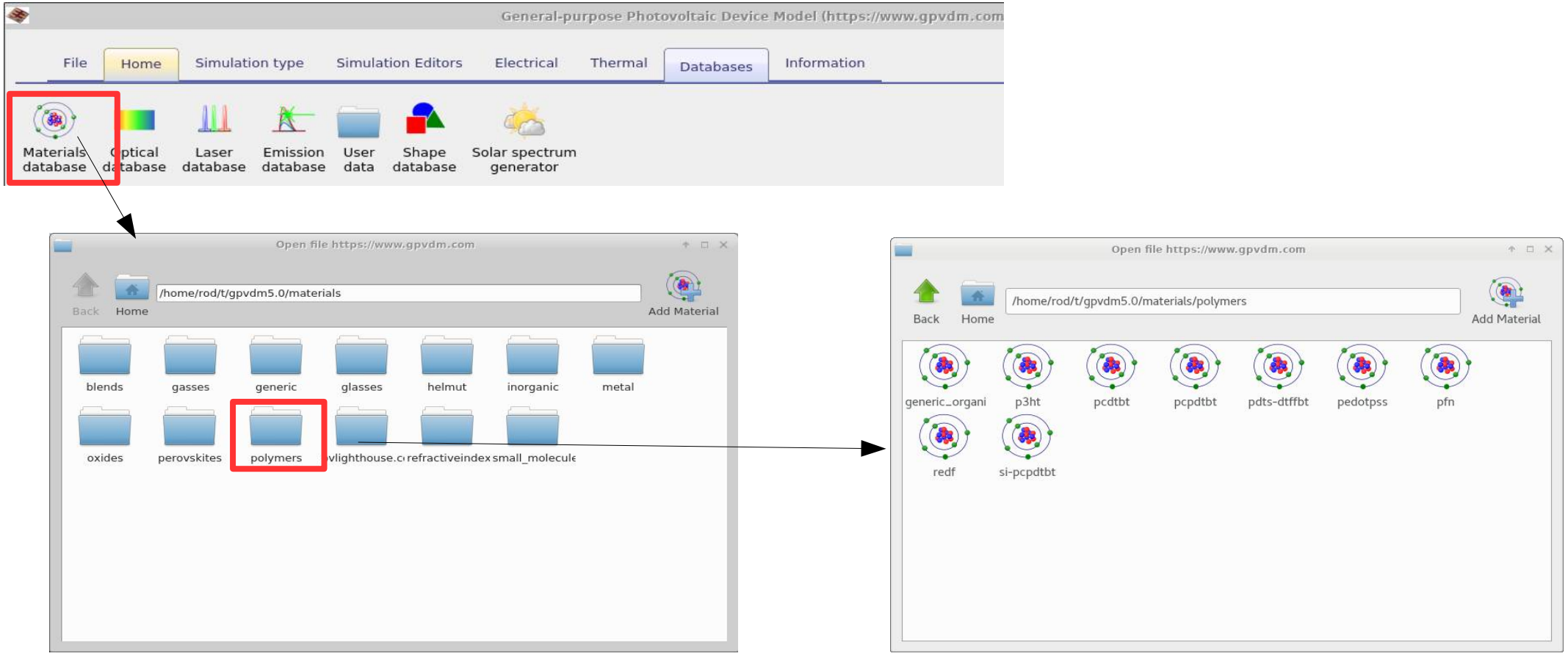


- **Introduction to the materials database in gpvdm**
- Where is the materials database stored?
- What format is the materials database stored in?
- Adding your own material the hard way.
- Where do I get refractive index information from?
- Extracting n/k data from the literature.
- Using the graphical interface to import data.
- Other information contained within the materials database.

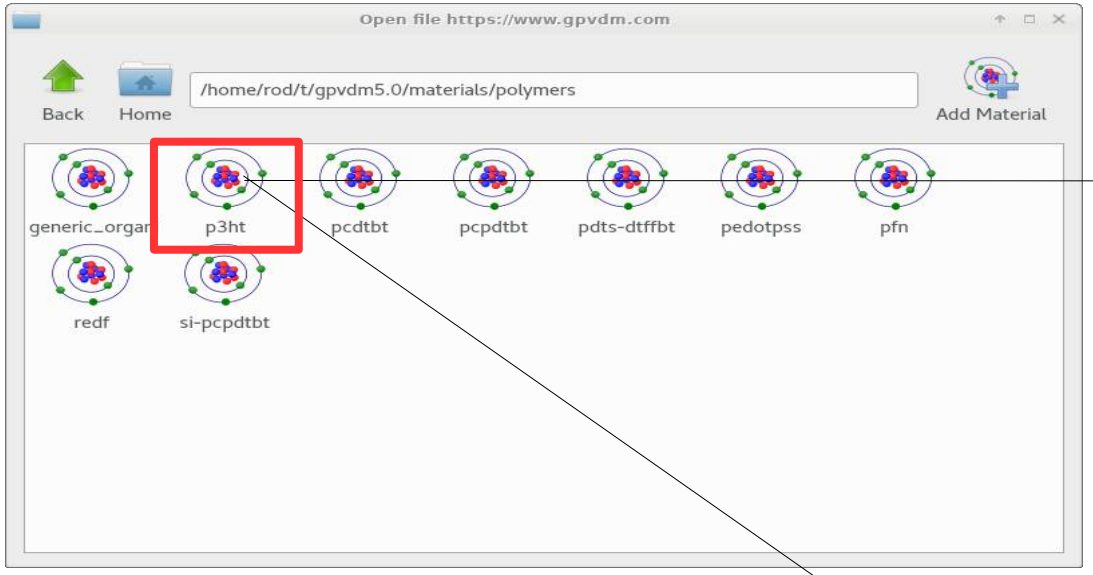
Introduction 1/3

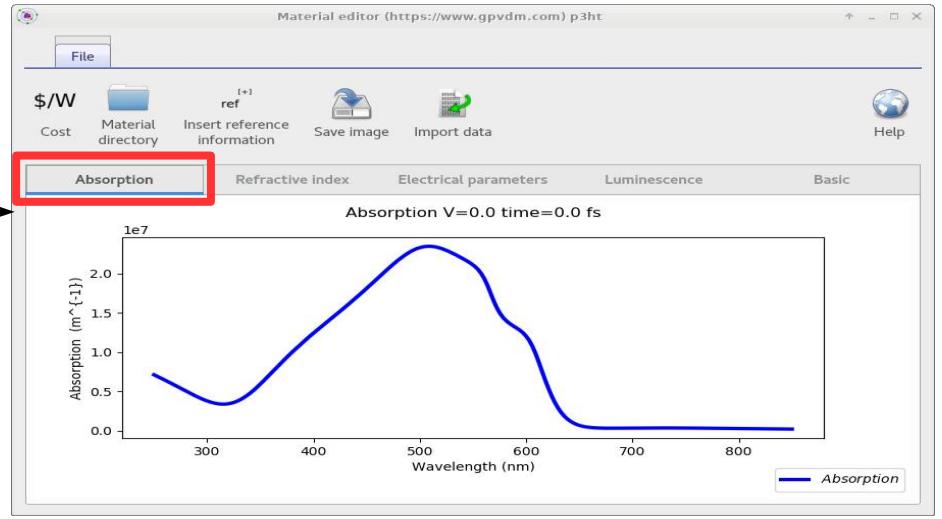


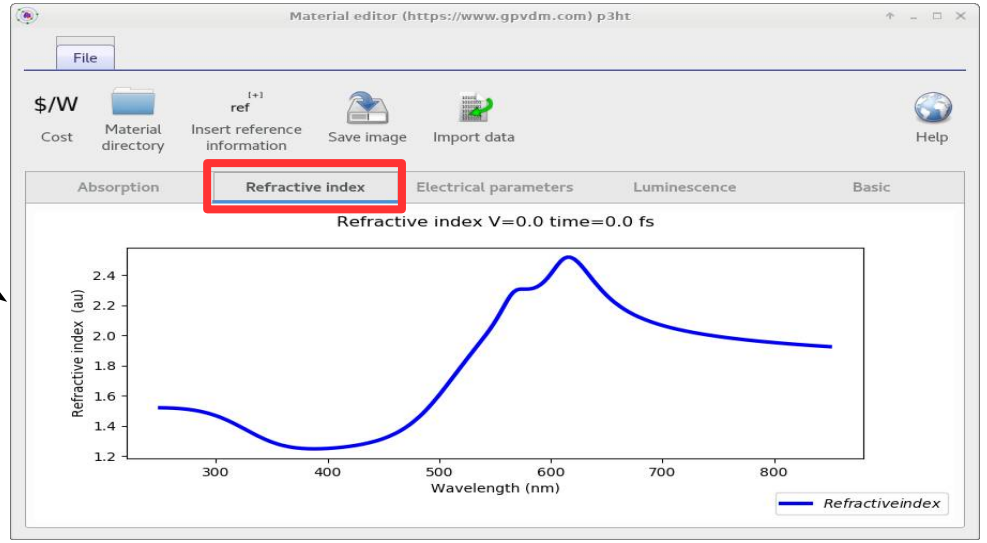
•The materials database stores mainly the optical (n/k) data for the materials used in gpvdm simulations. You can access it from the database tab.



Introduction 2/3

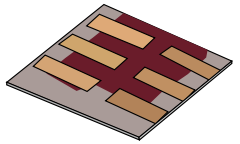






- Each material has n/alpha data stored for it.

Introduction 3/3

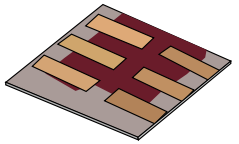


- Although the materials database does store some electrical parameters and thermal parameters ***these are not used in the simulations.***

- This is because gpvdm is mainly used for simulating thin film devices, and the material parameters change a lot between fabrication runs/labs/material batches. Therefore electrical/thermal parameters have to be set in the simulation it's self.

- **The materials database is mainly used for storing n/k data which is used in simulations.**

Outline



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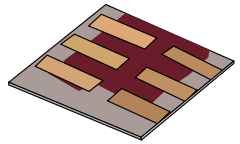
Where is the materials database stored on my computer?



- The materials database is stored in your home directory within the gpvdm_local folder. So for the user ‘Rod’ it would be stored in:

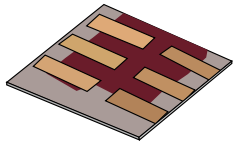
c:\Users\Rod\gpvdm_local\materials

- If your home directory is stored on a network or somewhere else the materials directory would be stored in:

‘the path to your home folder’\gpvdm_local\materials

Where ‘the path to your home folder’ would represent the path to your home folder whereever it may be stored.

Outline



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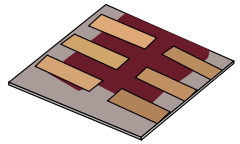
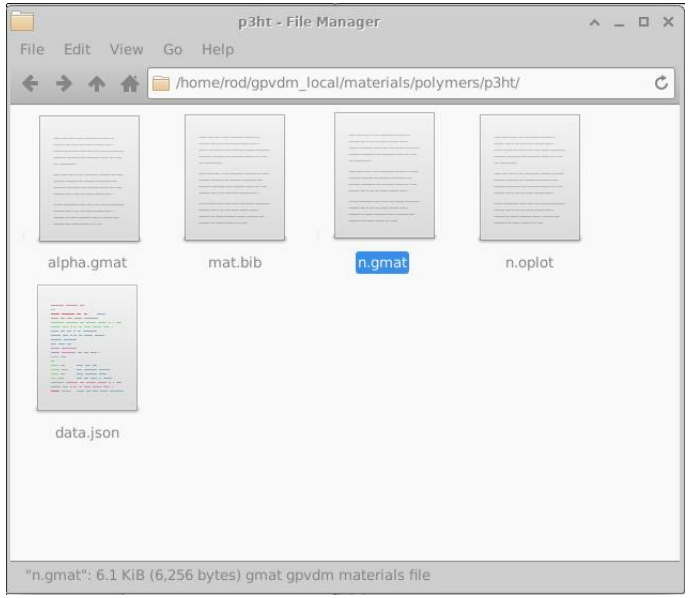
What format are the materials stored in?



•Each material is stored in it's own directory in the materials directory, so for example p3ht is stored in the directory p3ht:

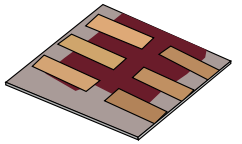
•In each materials directory there are 4 files:

•**alpha.gmat**: Contains the optical absorption information
•**n.gmat**: contains the real part of the refractive index
•**bat.bib**: Is a bib file containing references.
•**data.json** contains all other information about the material in JSON format.

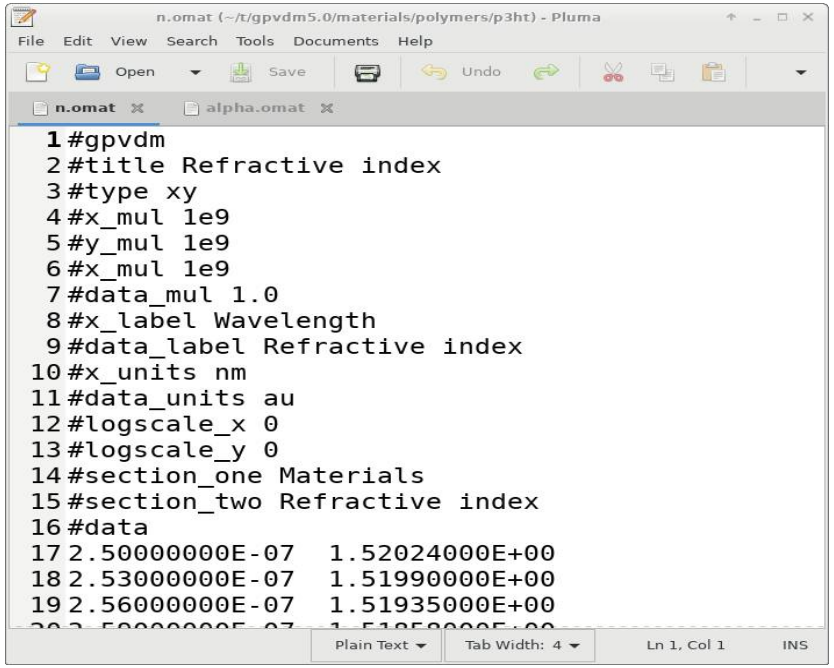


•**These are all text files you can edit them directly with a text editor.**

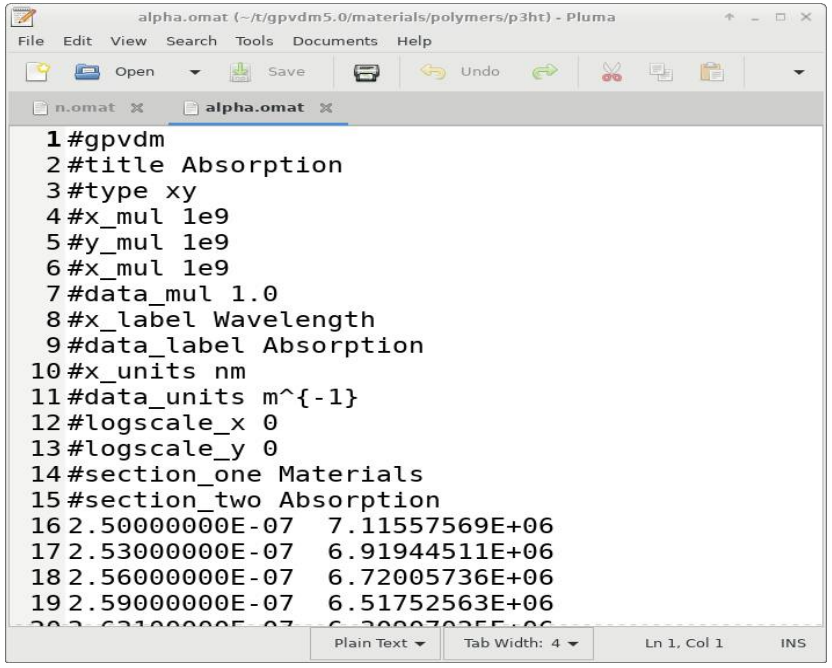
n.omat and alpha.omat files look like this...



- n.omat



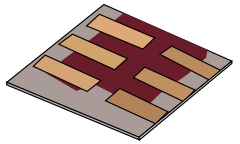
- alpha.omat



There is a header which you can leave alone, then there are two columns:
n.omat: wavelength (meters) / refractive index
alpha.omat: wavelength (meters) / Absorption in (m^{-1})

- **Again these are text files you can edit them by hand.**

Outline



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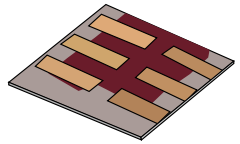
Adding your own material the hard way...



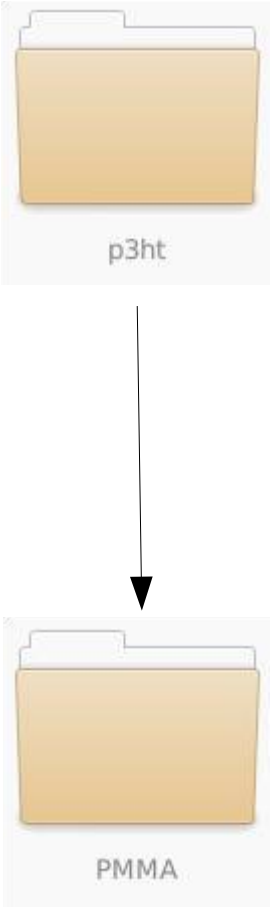
- Simply copy an existing material directory to a new one say copy p3ht to a new directory called PMMA.

- Then copy and paste the refractive index/absorption information into alpha.gmat and n.gmat.

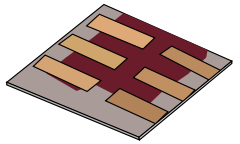
- Make sure you use the correct units i.e. wavelength (m) and absorption in m^{-1}.

- That's it.

- **It will not work if you use cm or um for wavelength, and absorption must be in m^{-1}.**



Outline



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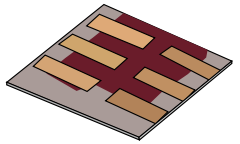
Getting hold of refractive index absorption data.



- There are lots of places to get hold of refractive index data:

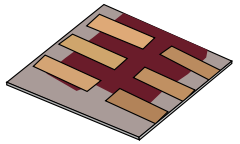
1. Your own experiments – this is the best option.

2. https://refractiveindex.info This is a very good site containing lots of refractive index information.

3. https://www.pvlighthouse.com.au/ another good site with n/k data.

4. Extract the n/k data from the literature.

Outline



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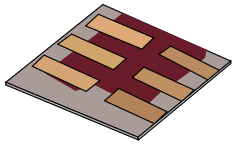
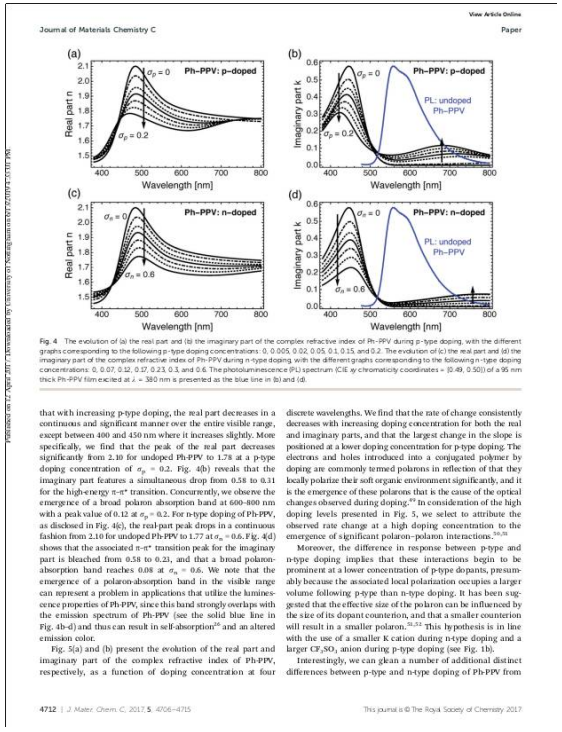
Extracting n/k data from the literature



- **Step 1:** Find a paper with the refractive index/absorption data in it (hint: Try google image search for this)

- **Step 2:** Take a screenshot of the graph you want to import, and save it as a .png file.

Pdf of paper


View Article Online

Journal of Materials Chemistry C

Paper

Fig. 4 The evolution of (a) the real part and (b) the imaginary part of the complex refractive index of Ph–PPV during p–type doping, with the different graphs corresponding to the following p–type doping concentrations: 0, 0.005, 0.02, 0.05, 0.1, 0.15, and 0.2. The evolution of (c) the real part and (d) the imaginary part of the complex refractive index of Ph–PPV during n–type doping, with the different graphs corresponding to the following n–type doping concentrations: 0, 0.07, 0.12, 0.17, 0.23, 0.3, and 0.6. The photoluminescence (PL) spectrum (CIE xy chromaticity coordinates = [0.49, 0.50]) of a 95 nm thick Ph–PPV film excited at λ = 380 nm is presented as the blue line in (b) and (d).

that with increasing p-type doping, the real part decreases in a continuous and significant manner over the entire visible range, except between 400 and 450 nm where it increases slightly. More specifically, we find that the peak of the real part decreases significantly from 2.10 for undoped Ph-PPV to 1.78 at a p-type doping concentration of σ_p = 0.2. Fig. 4(b) reveals that the imaginary part features a simultaneous drop from 0.58 to 0.11 for the high-energy π–π* transition. Concurrently, we observe the emergence of a broad polaron absorption band at 600–800 nm with a peak value of 0.12 at σ_p = 0.2. For n-type doping of Ph-PPV, as disclosed in Fig. 4(c), the real-part peak drops in a continuous fashion from 2.10 for undoped Ph-PPV to 1.77 at σ_n = 0.6. Fig. 4(d) shows that the associated π–π* transition peak for the imaginary part is bleached from 0.58 to 0.23, and that a broad polaron-absorption band reaches 0.08 at σ_n = 0.6. We note that the emergence of a polaron-absorption band in the visible range can represent a problem in applications that utilize the luminescence properties of Ph-PPV, since this band strongly overlaps with the emission spectrum of Ph-PPV (see the solid blue line in Fig. 4b-d) and thus can result in self-absorption[26] and an altered emission color.

Fig. 5(a) and (b) present the evolution of the real part and imaginary part of the complex refractive index of Ph-PPV, respectively, as a function of doping concentration at four discrete wavelengths. We find that the rate of change consistently decreases with increasing doping concentration for both the real and imaginary parts, and that the largest change in the slope is positioned at a lower doping concentration for p-type doping. The electrons and holes introduced into a conjugated polymer by doping are commonly termed polarons in reflection of that they locally polarize their soft organic environment significantly, and it is the emergence of these polarons that is the cause of the optical changes observed during doping.[49] In consideration of the high doping levels presented in Fig. 5, we select to attribute the observed rate change at a high doping concentration to the emergence of significant polaron–polaron interactions.[50,51]

Moreover, the difference in response between p-type and n-type doping implies that these interactions begin to be prominent at a lower concentration of p-type dopants, presumably because the associated local polarization occupies a larger volume following p-type than n-type doping. It has been suggested that the effective size of the polaron can be influenced by the size of its dopant counterion, and that a smaller counterion will result in a smaller polaron.[52,53] This hypothesis is in line with the use of a smaller K cation during n-type doping and a larger CF_3SO_3 anion during p-type doping (see Fig. 1b).

Interestingly, we can glean a number of additional distinct differences between p-type and n-type doping of Ph-PPV from

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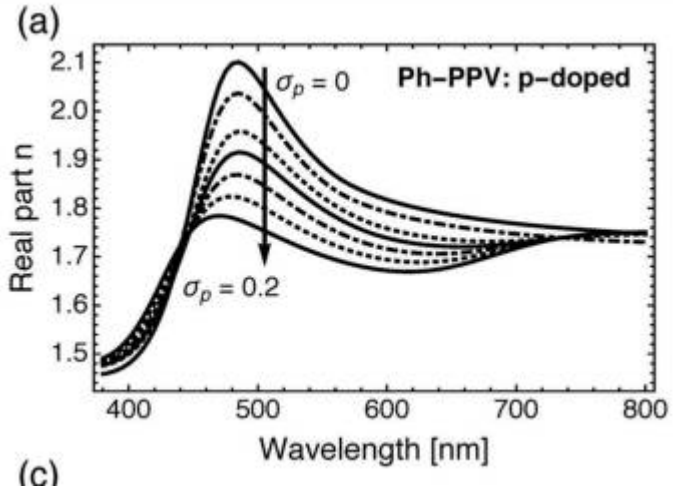
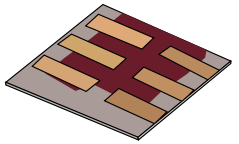
Graph saved as png.

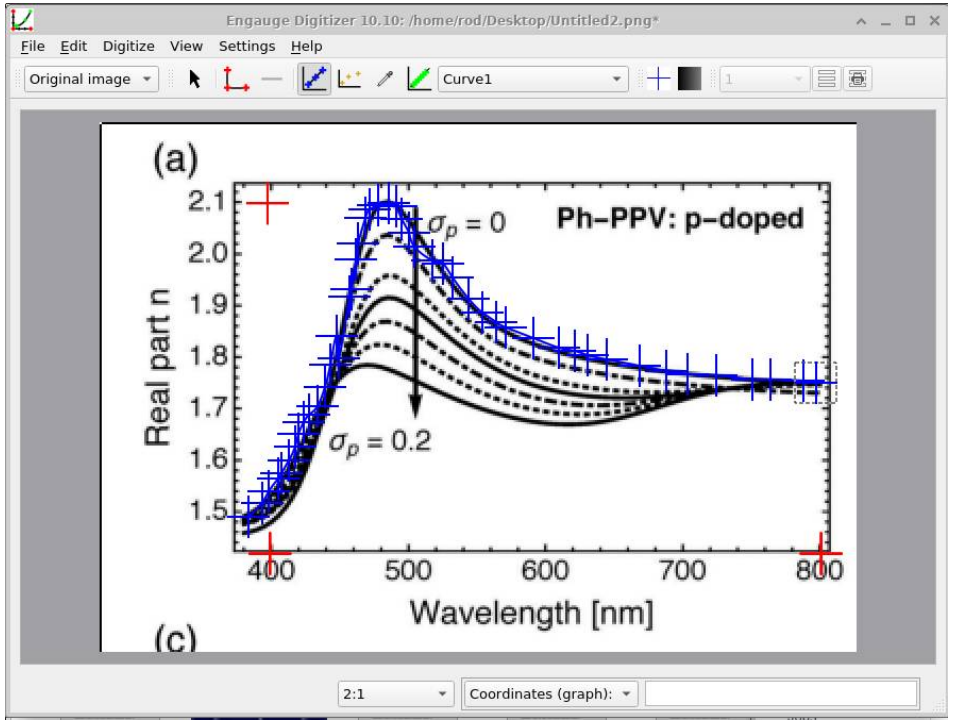


Extracting n/k data from the literature



- **Step 3:** Download Engauge Digitizer from the internet:
  - http://markummitchell.github.io/engauge-digitizer/

- **Step 4:** Set up the axies (red crosses), then by hand draw points on the the data you want to extract.



Step 5: Save this data as:

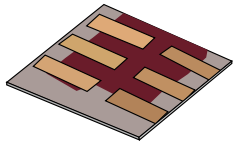
Wavelength(m) v.s. n

or

Wavelength(m) v.s. absorption (m^{-1})

Step 6: Copy and paste this data into your n.gmat or alpha.gmat files.

Outline



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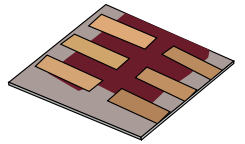
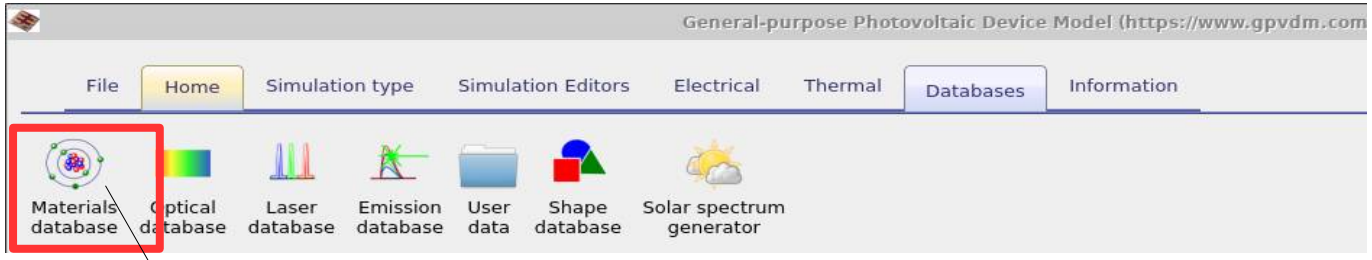
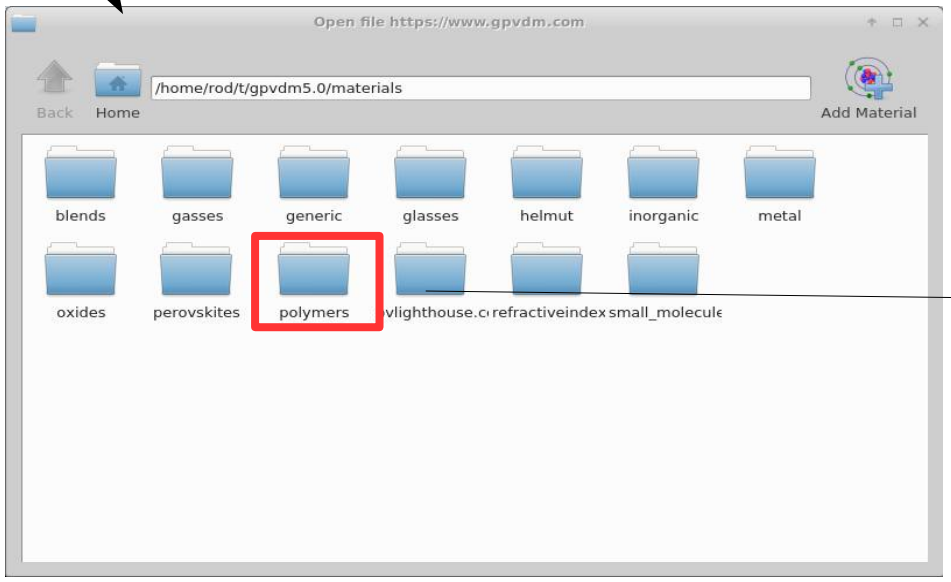
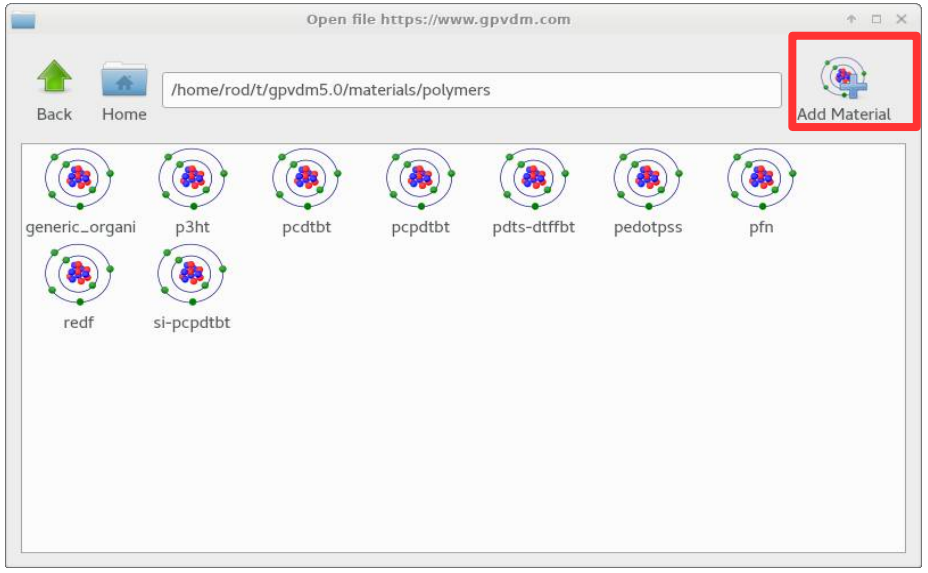
Adding a material using the graphical interface



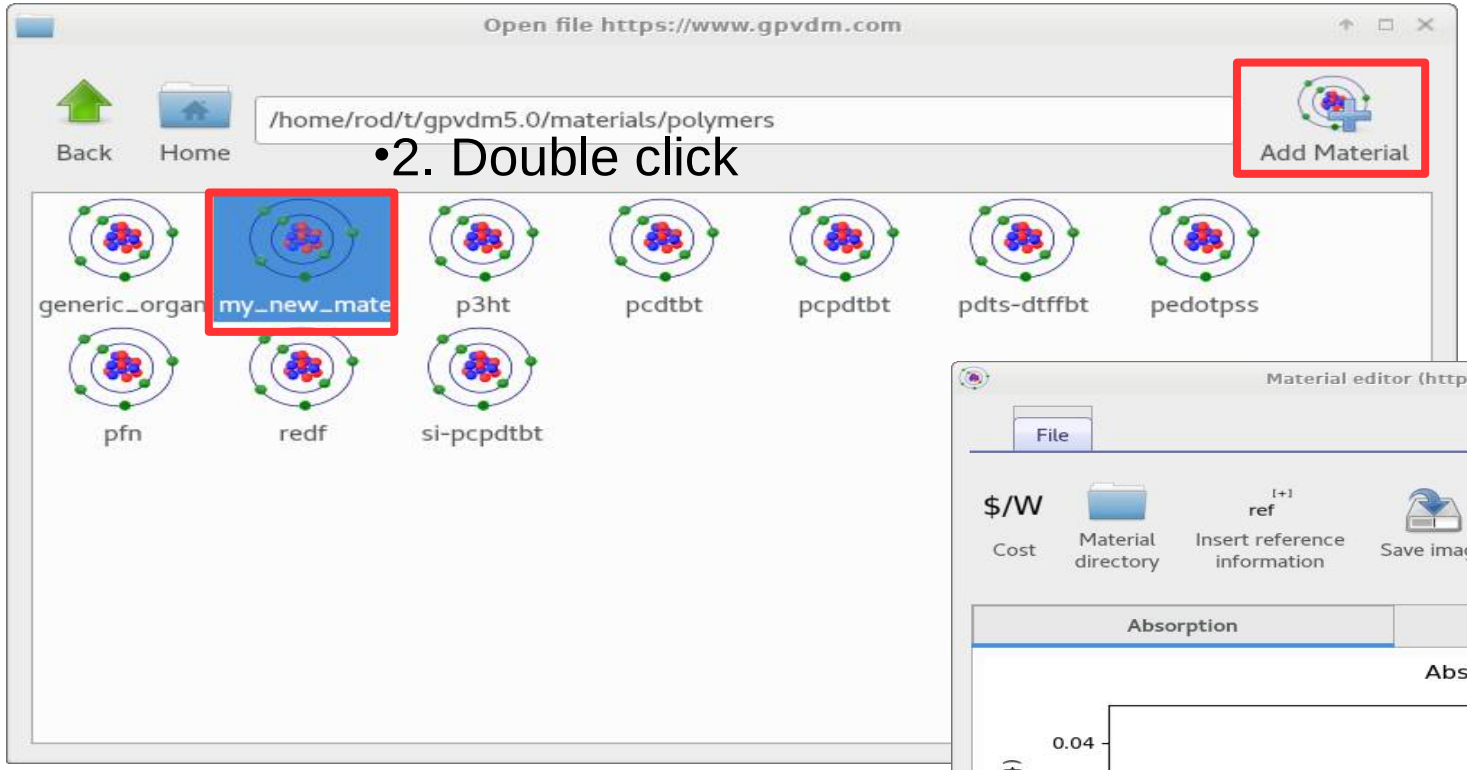
- Select the materials directory to which you want to add a material to then click Add material.





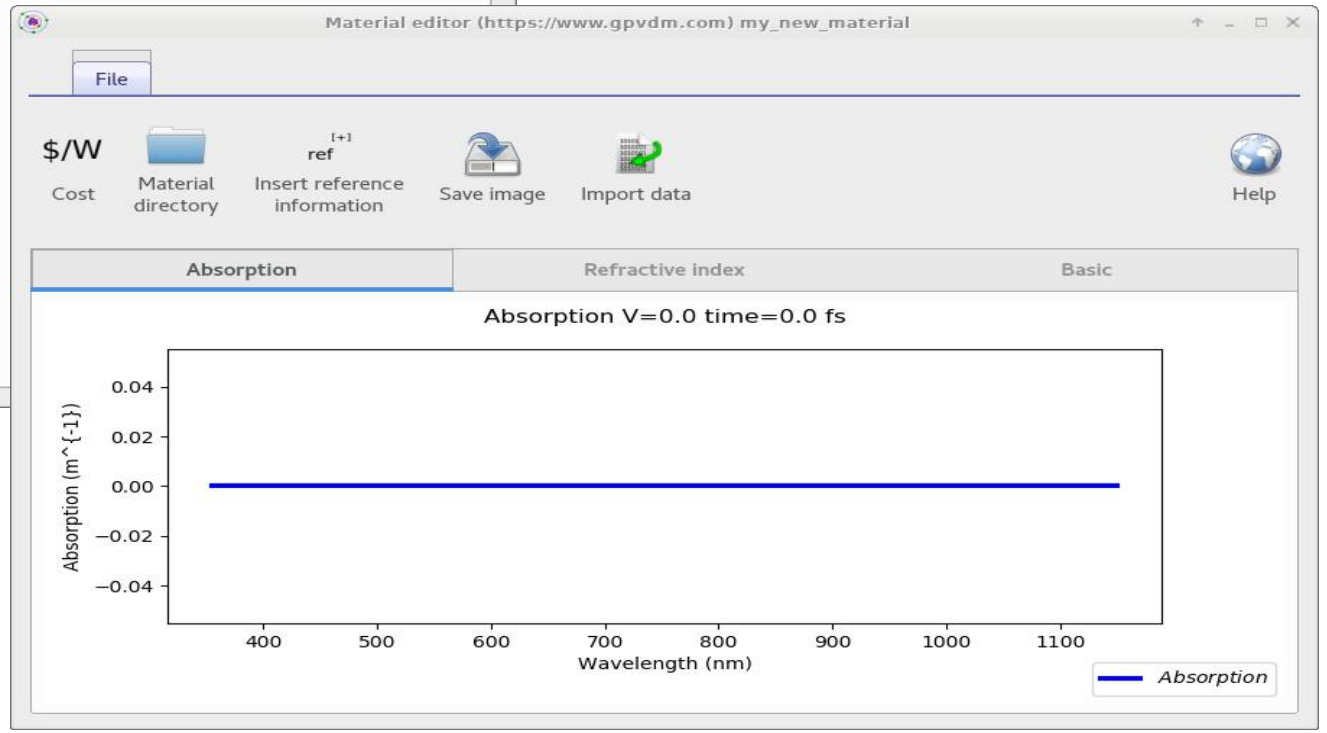


Making a new material the easy way...



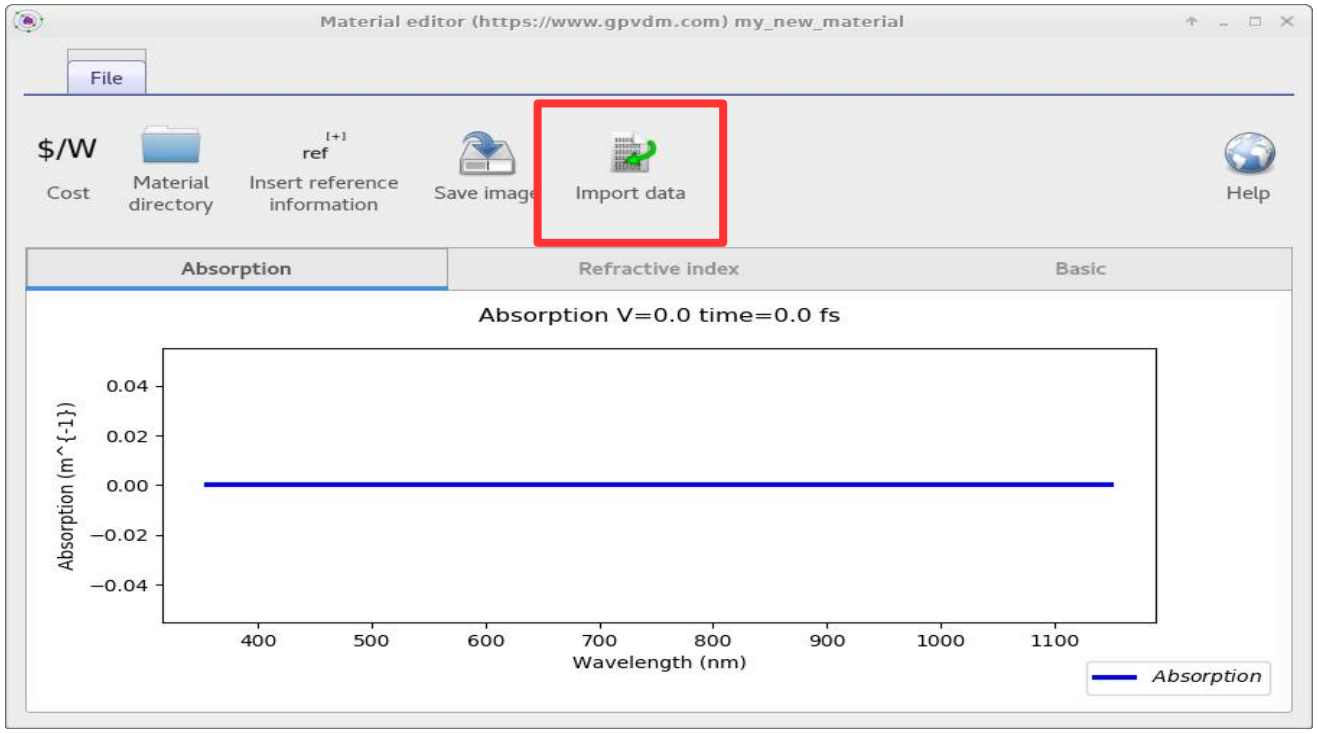
•1. Click

•2. Double click



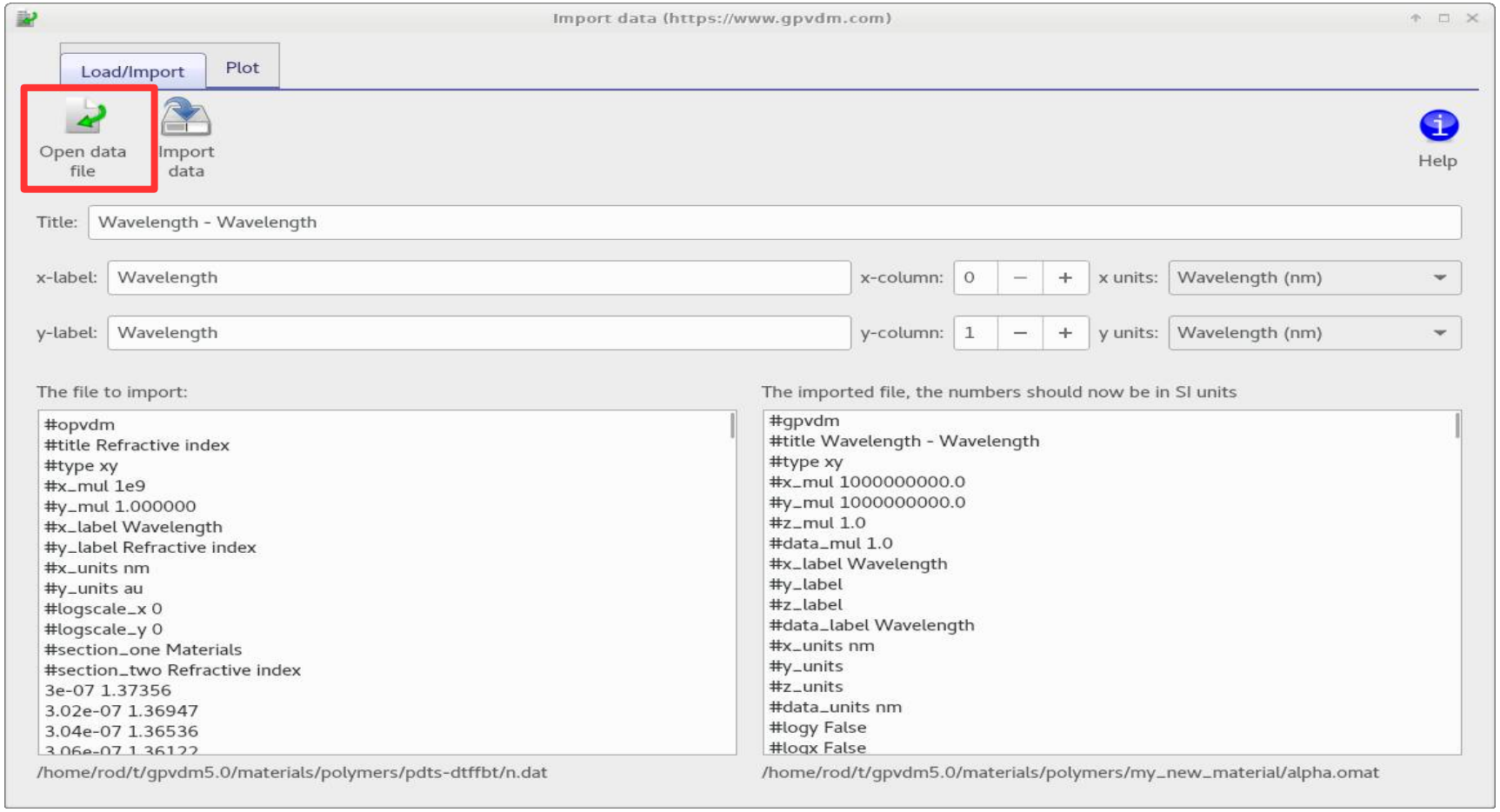
•The material file has no data….

Adding a material using the graphical interface



- Click import data, and the data importer window will be displayed….

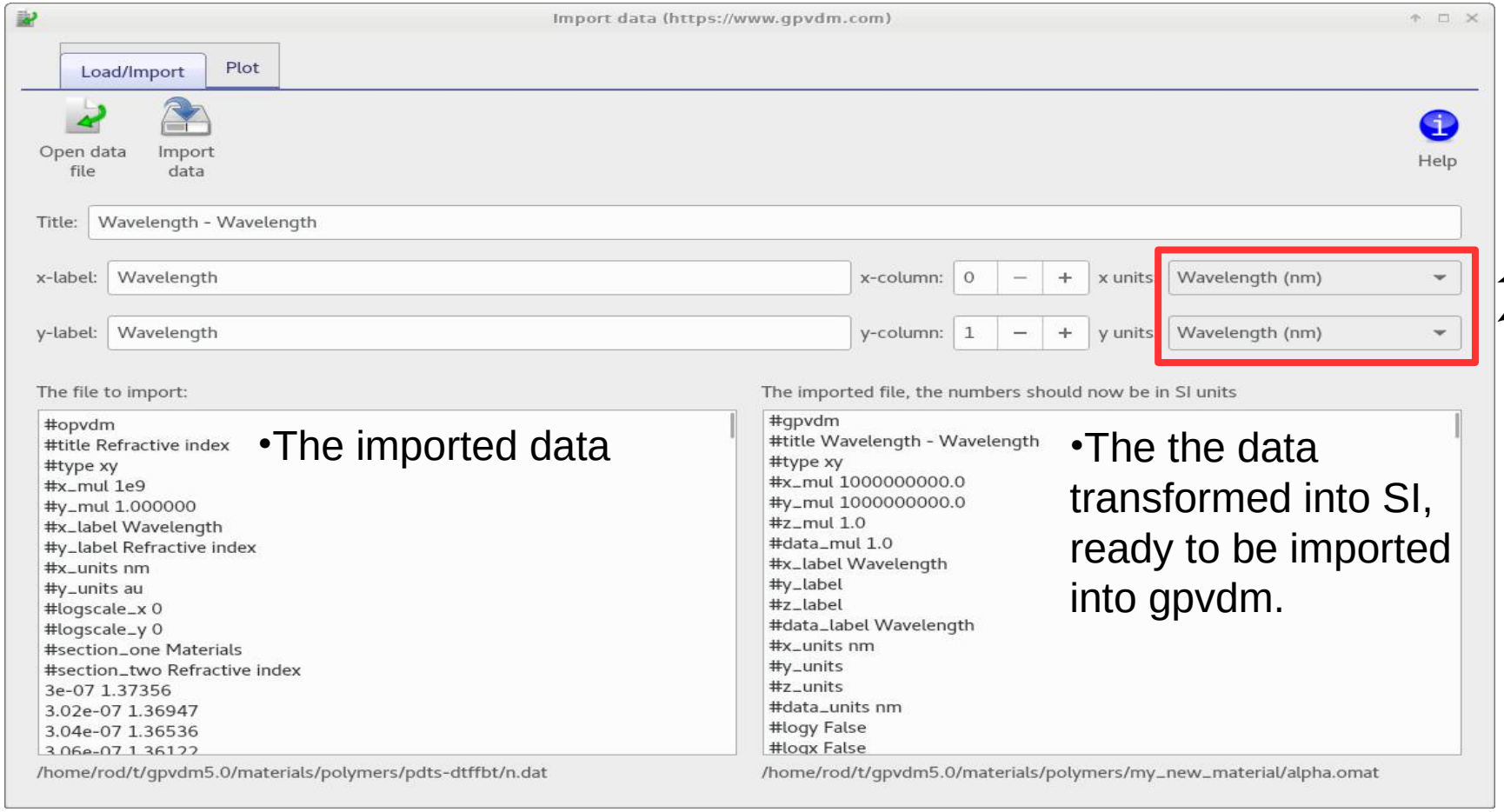
Click open data file...



- And select the data file containing your n/k data.

- See earlier on in the slide deck to find out how to get n/k data.

The import window used to convert data to SI



•The imported data

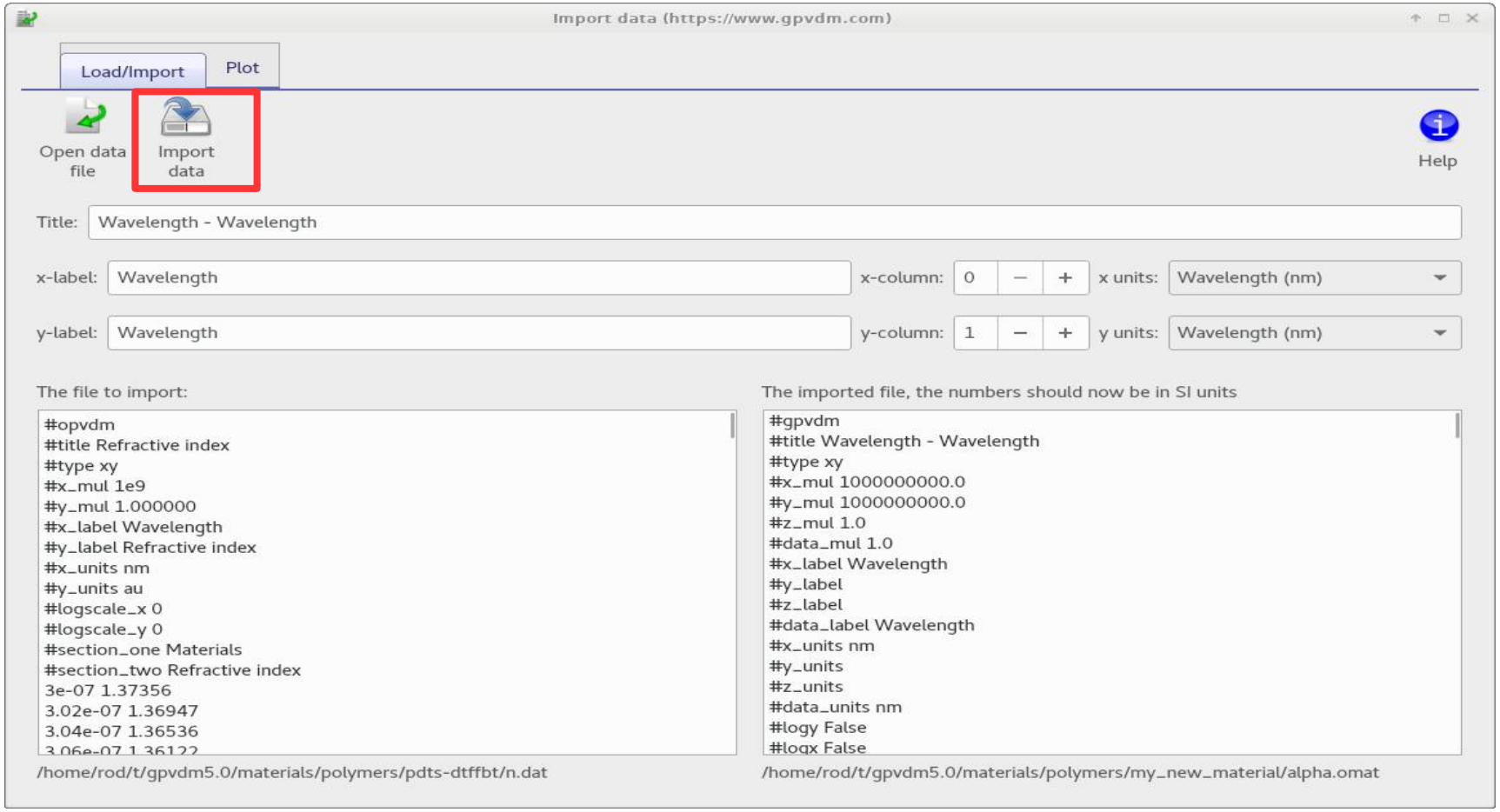
•The the data transformed into SI, ready to be imported into gpvdm.

•Set these to the units of the **input file**.

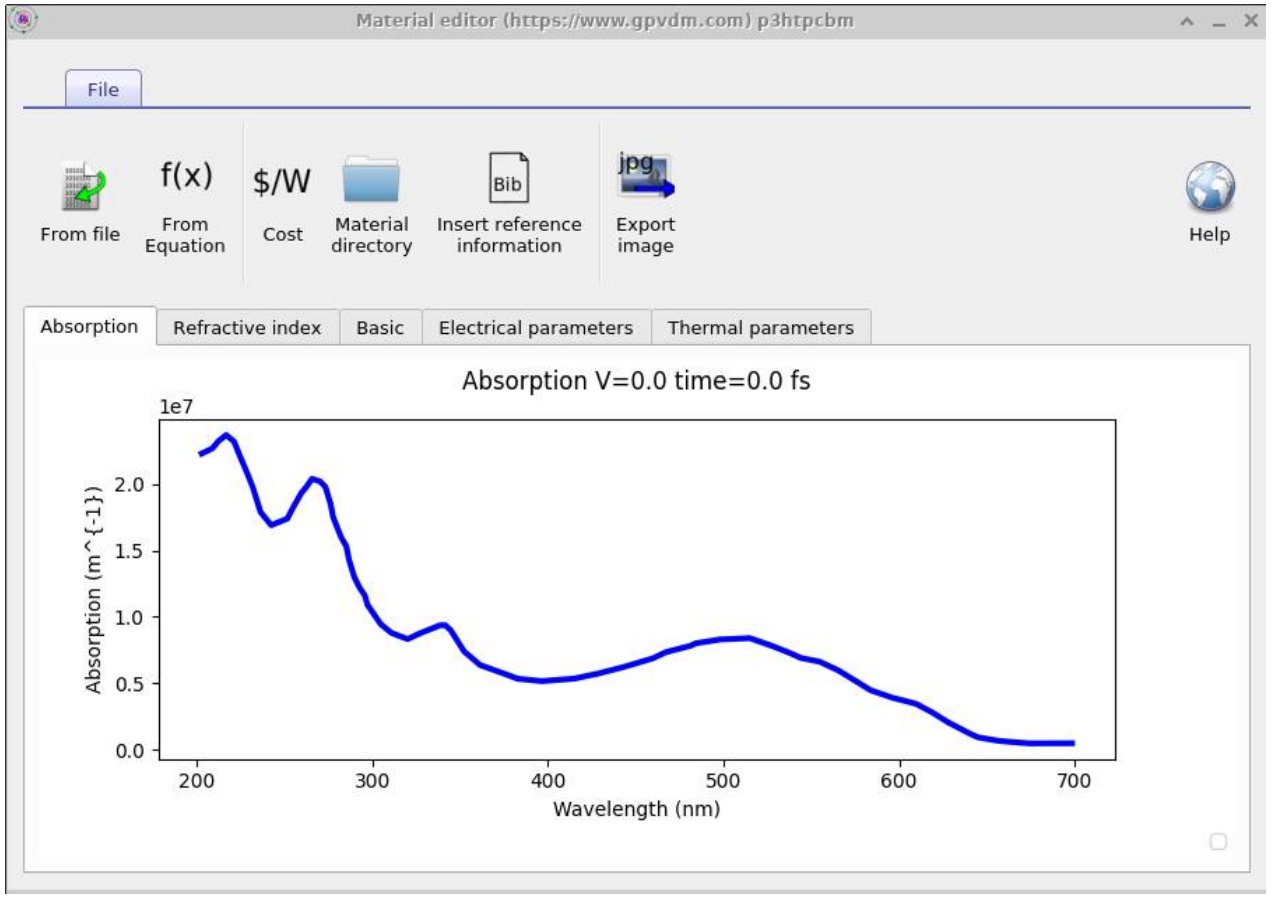
•Note this can transform between absorption units.

•So if your file were in units of wavelength nm and absorption ‘attenuation coefficient’, select those.

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

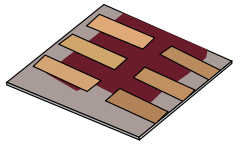


And you will have imported your data..



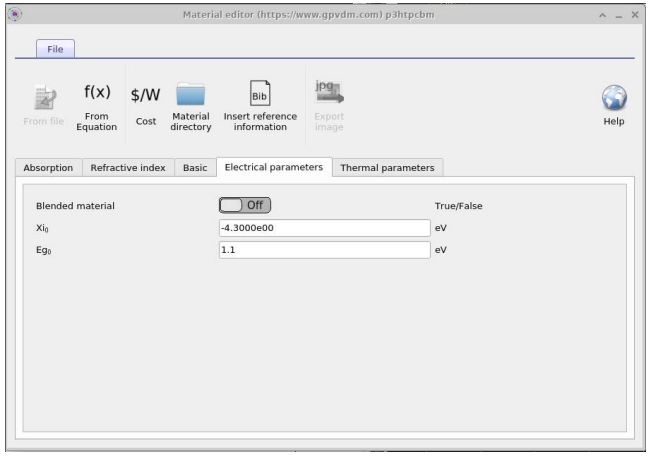
- You will need to do this for both the Absorption and the real part of the refractive index.

Overview

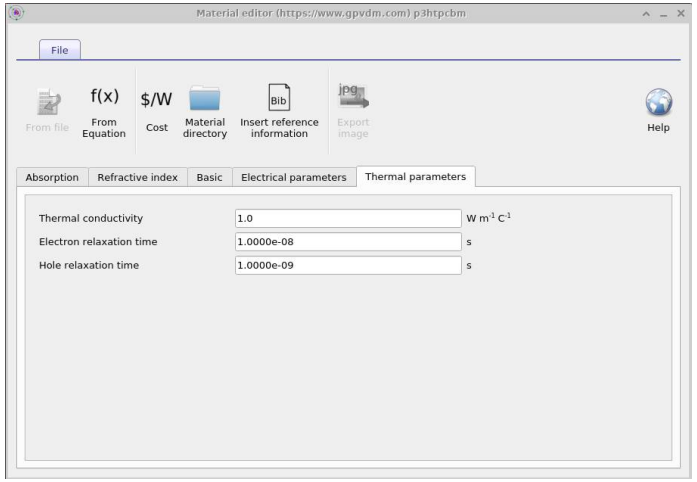


- Introduction to the materials database in gpvdm
- Where is the materials database stored?
- What format is the materials database stored in?
- Adding your own material the hard way.
- Where do I get refractive index information from?
- Extracting n/k data from the literature.
- Using the graphical interface to import data.
- **Other information contained within the materials database.**

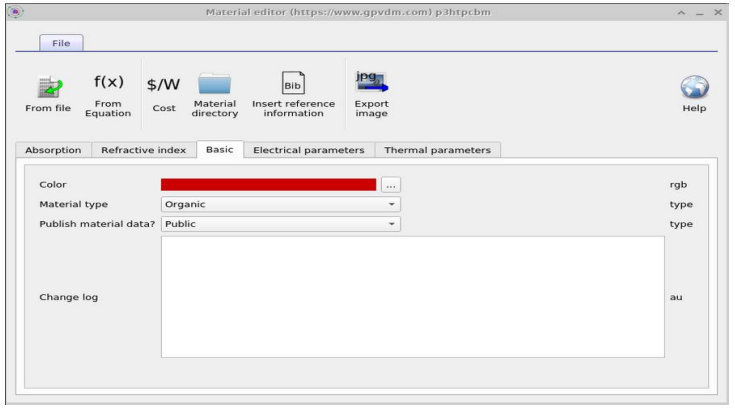
The materials database contains:



Basic Electrical information

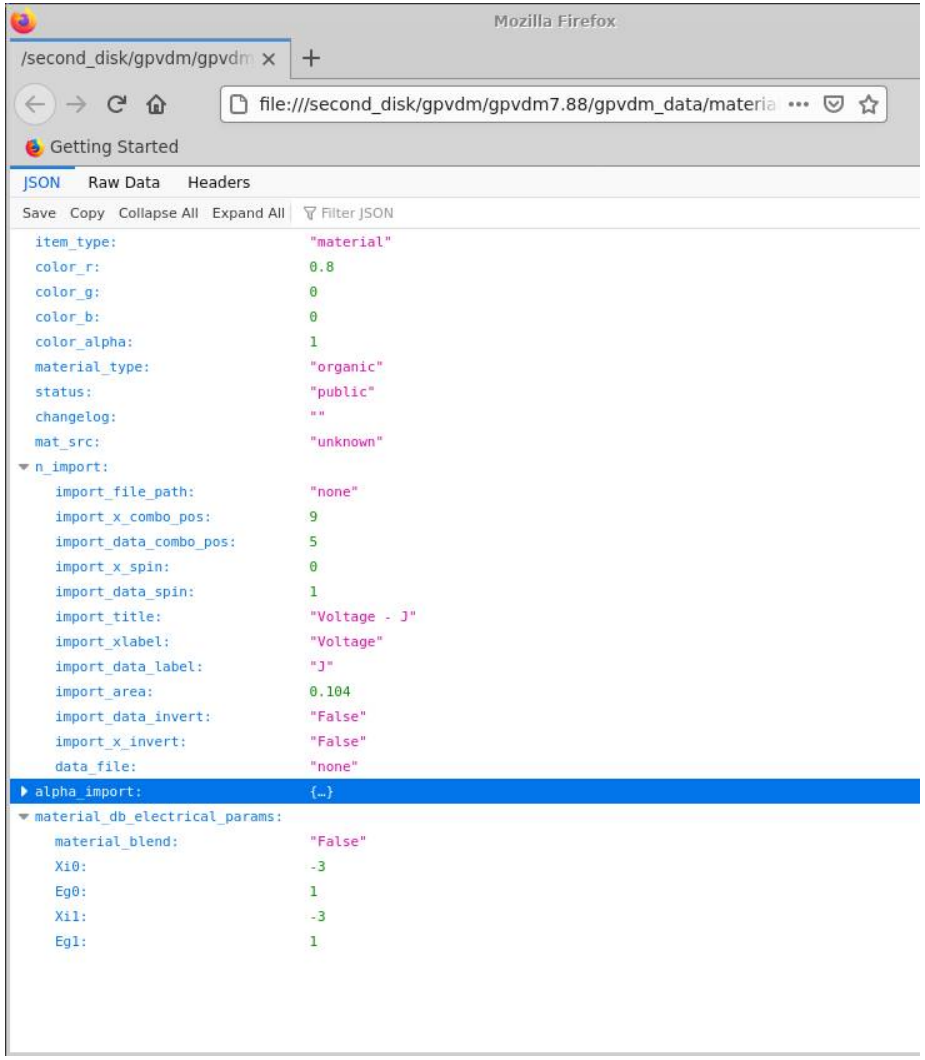


Thermal information



Basic information

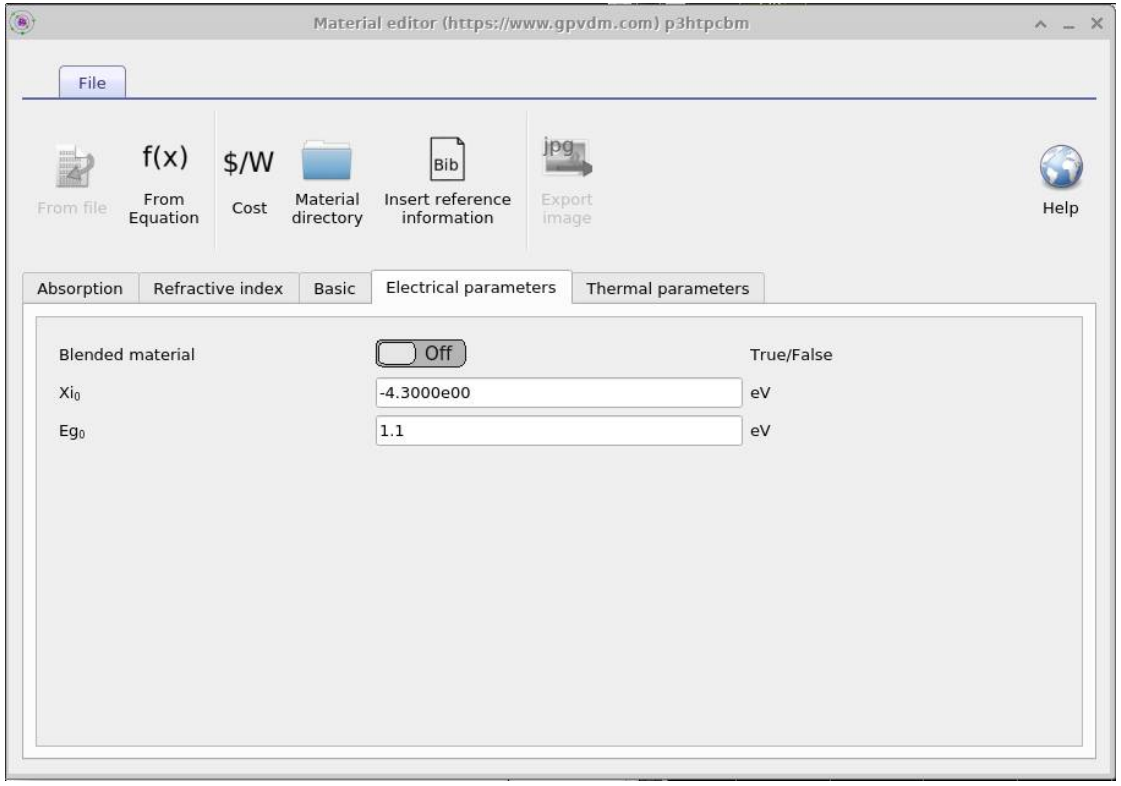
All other material data is stored in the data.json



- These are stored in the data.json file

- This can be viewed in firefox, or in a text editor.

Basic electrical information

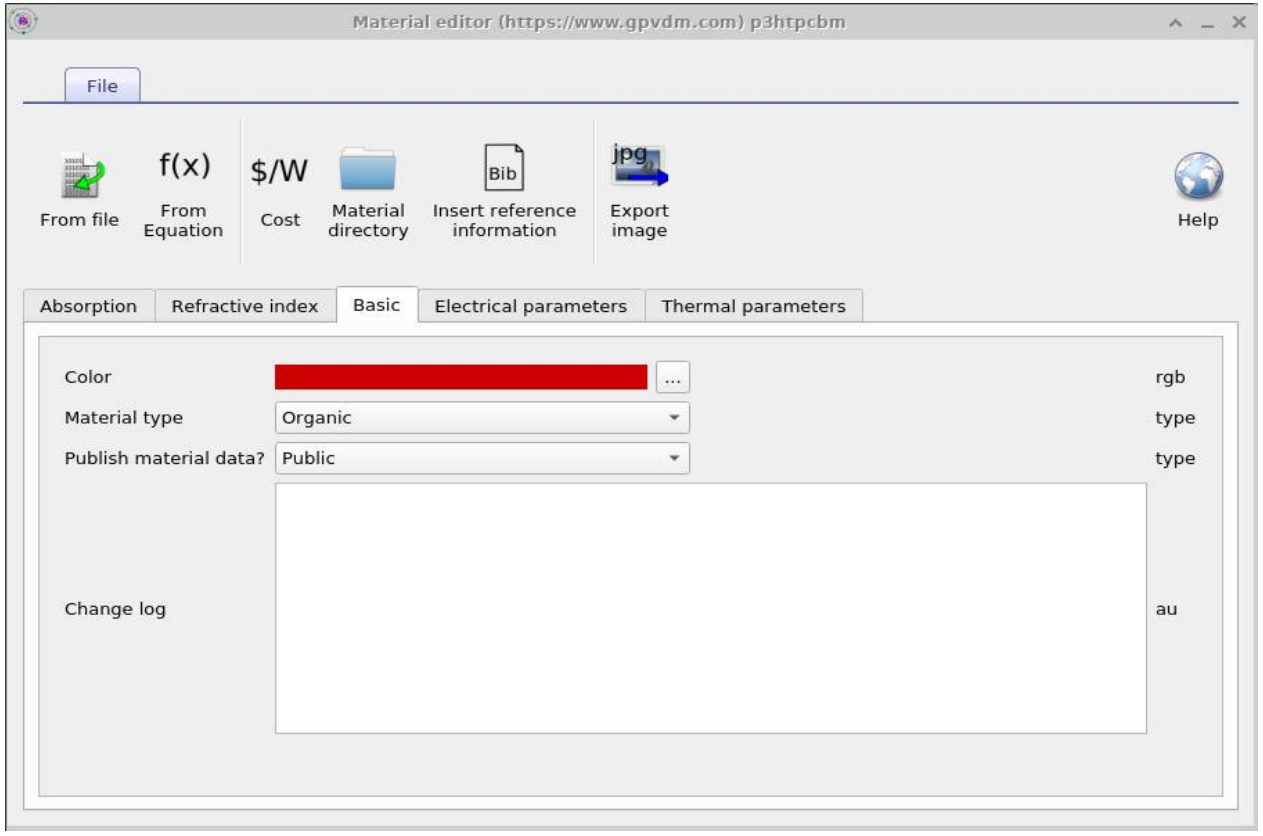


•Because gpvdm is mainly used to simulate thin film devices, and because the quality of thin films changes a lot between devices/labs/ fabrication runs, it does not make sense to have a database of electrical parameters for materials such as P3HT.

•Therefore the electrical parameters should be set in the electrical parameters window in your simulation, not in the materials database.

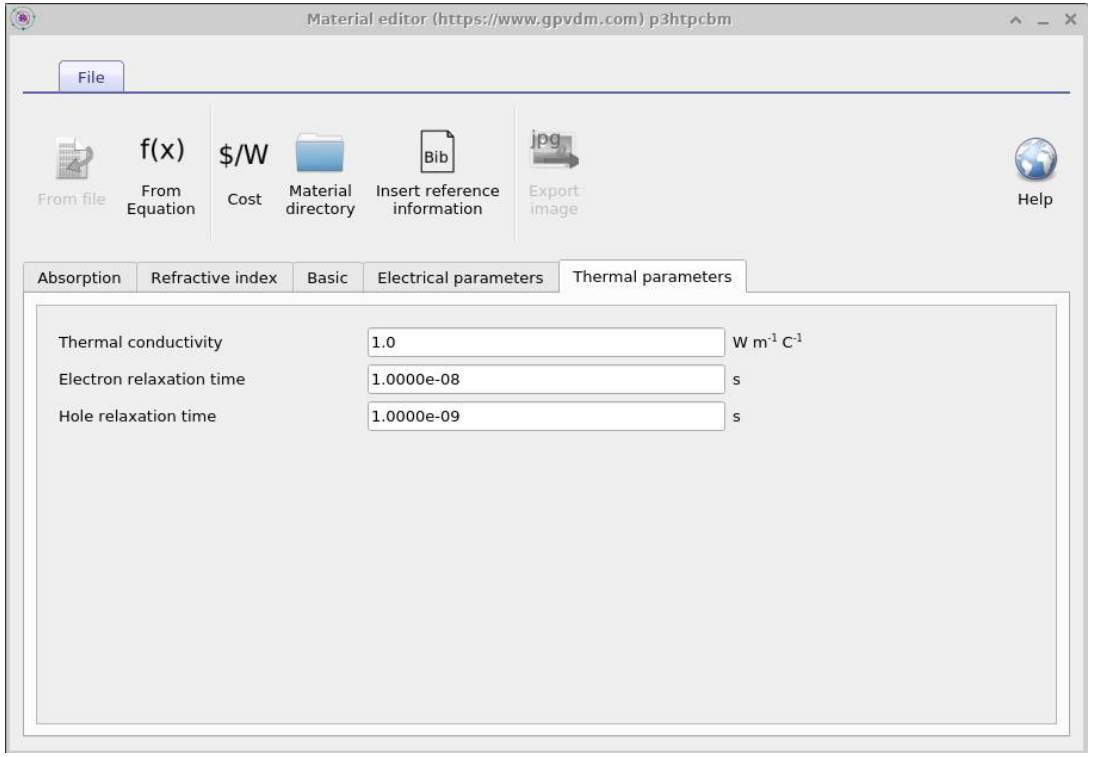
•The values in this window are simply use for drawing pretty band diagrams, and are not used in the simulation.

Basic information



- This contains basic information about the material, such as it's color and material type, metal/oxide/polymer etc...

Thermal information



- These values are used as the default values for thermal simulations.