

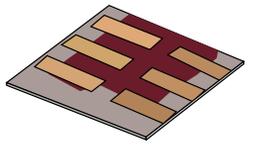
An introduction to modeling solar cells

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Autumn 2019

<https://www.gpvdm.com>

Released under
BY-CC

What is this tutorial?

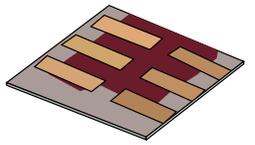


- A (very) brief introduction to modeling solar cells.
- Understanding how solar cells work is important for future engineers because solar energy will play an ever increasing role in our lives.
- The tutorial is aimed to give you some general ideas about their operation.

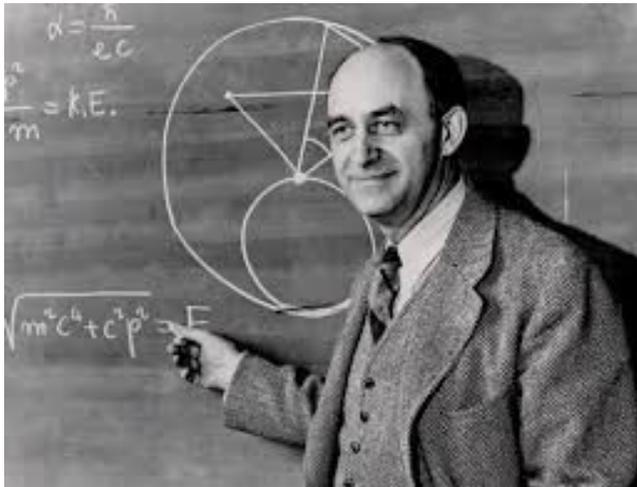


Isofoton.es

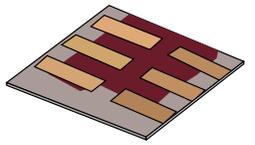
What is this tutorial *not*?



- This is not a semiconductor physics lecture.
- We will not even mention Fermi levels...

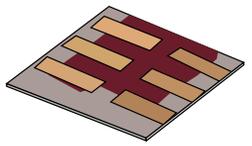


Isofoton.es

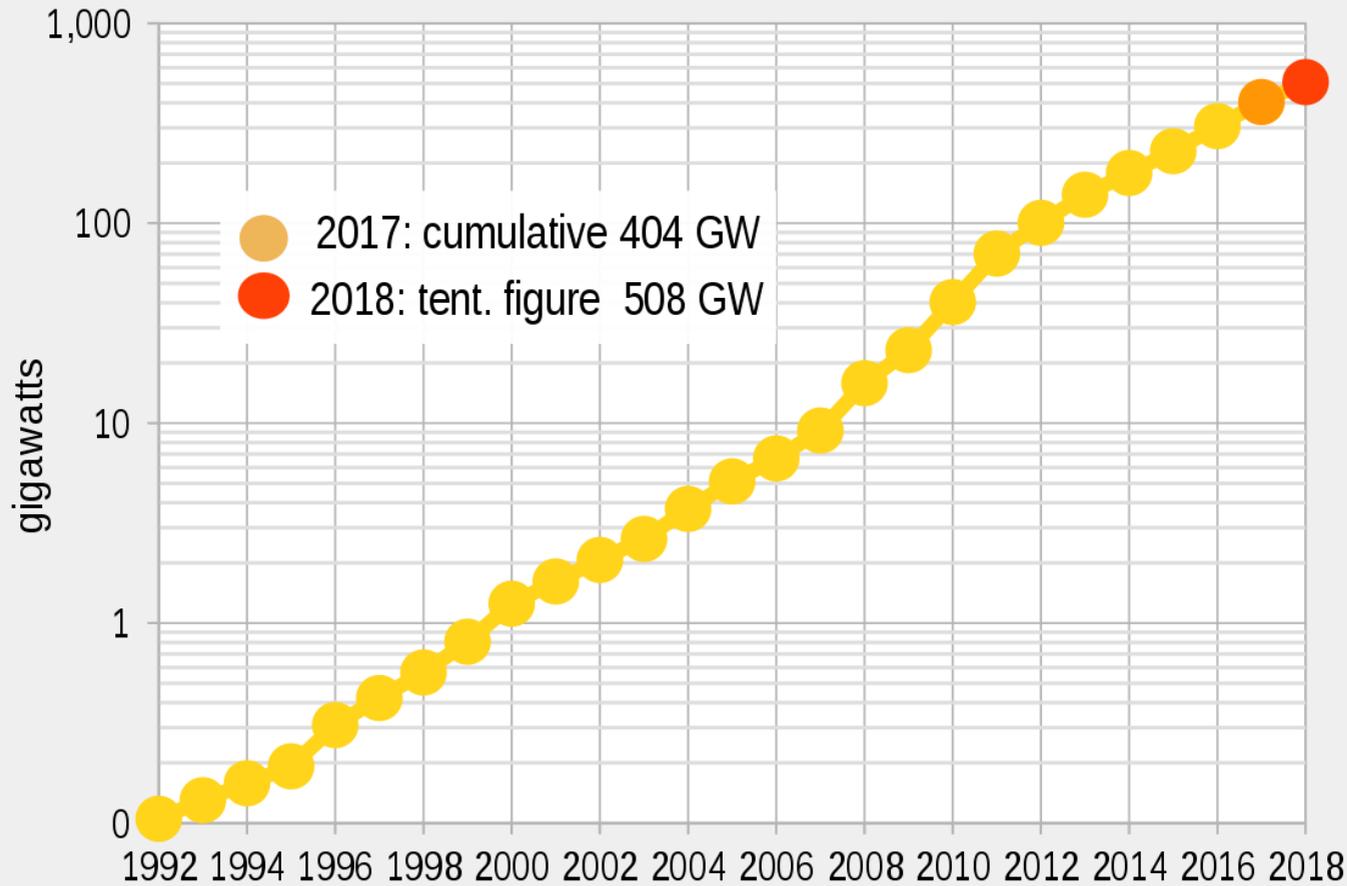


- **Motivation – why learn this?**
- The basic structure of 3rd generation solar cells.
- Downloading/Installing a solar cell CAD tool.
- Your first simulation
- Affect of varying layer thicknesses.
- The solar spectrum and material choice
- Performing optical simulations
- Recombination
- Charge carrier mobility
- The $\mu \cdot \tau$ product
- Parasitic resistances in a solar cell.
- Charge carrier traps.

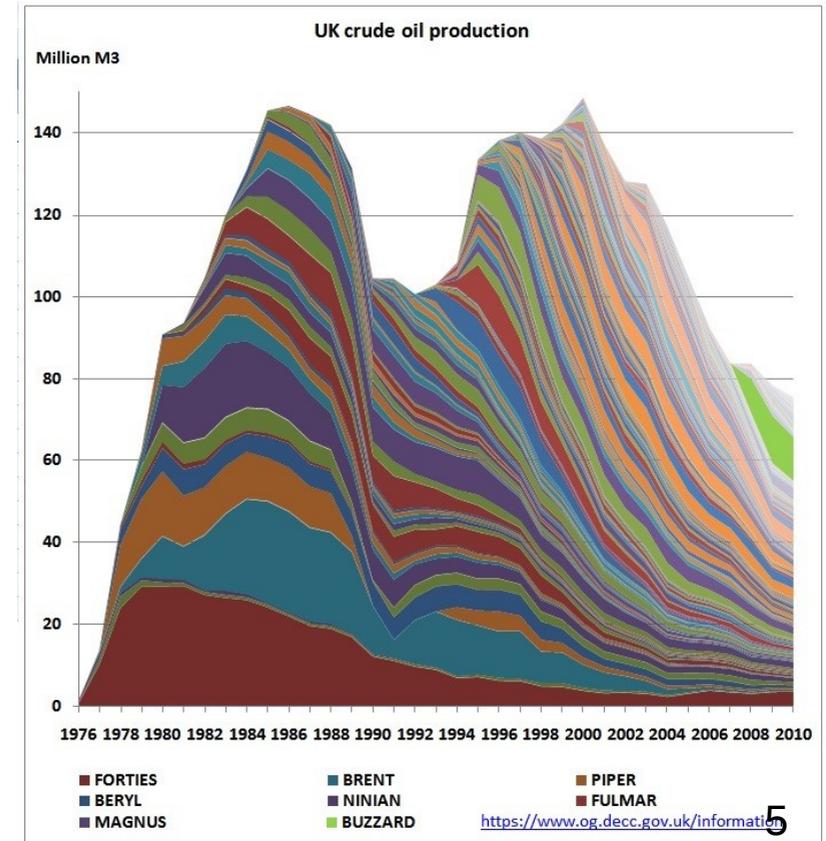
Why do I need to know about solar cells?

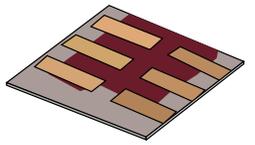


Exponential Growth of Solar PV (in GW)



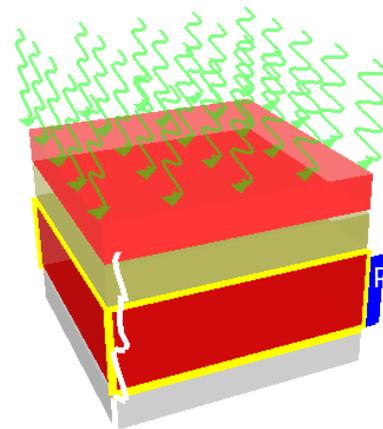
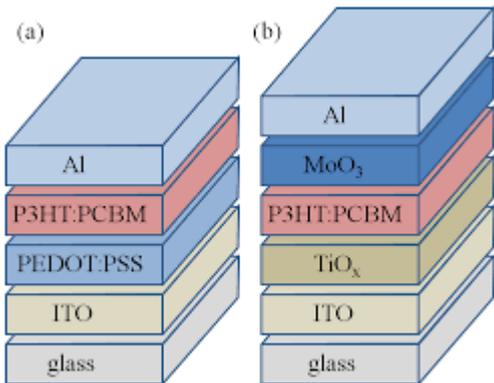
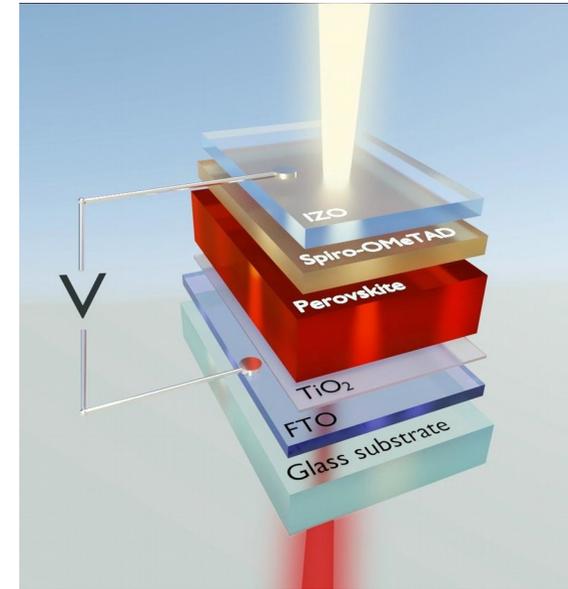
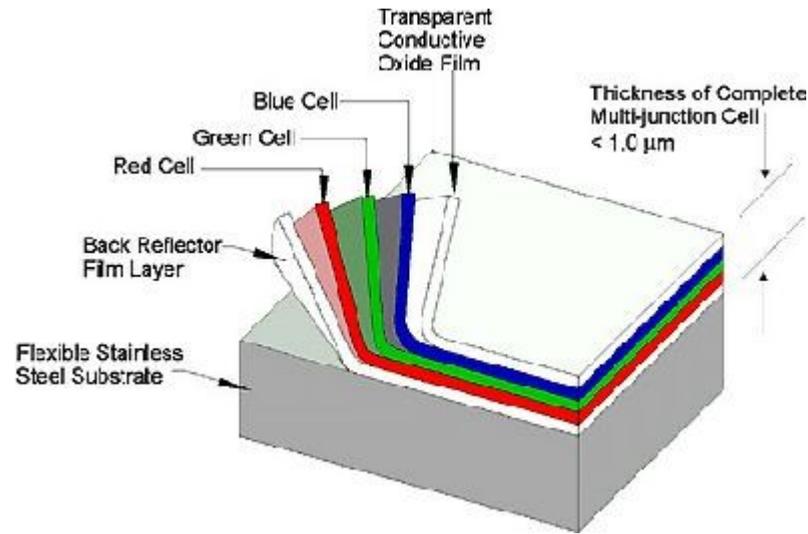
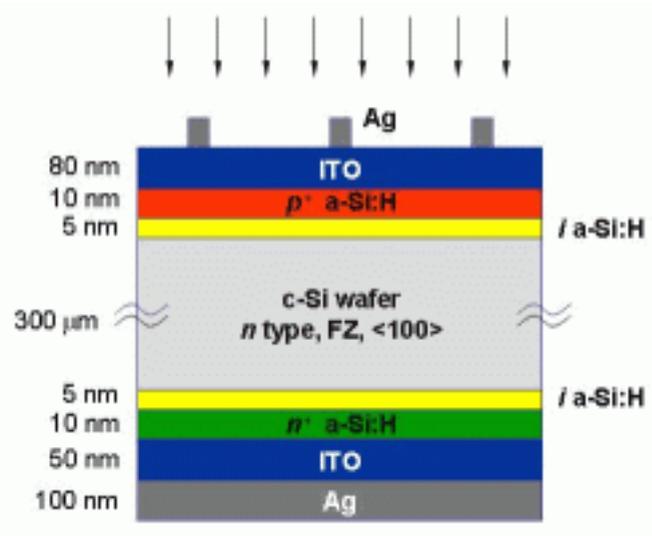
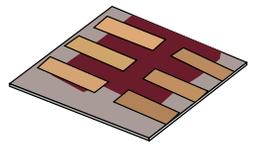
- Solar cells are going to be part of our lives if we like it or not...





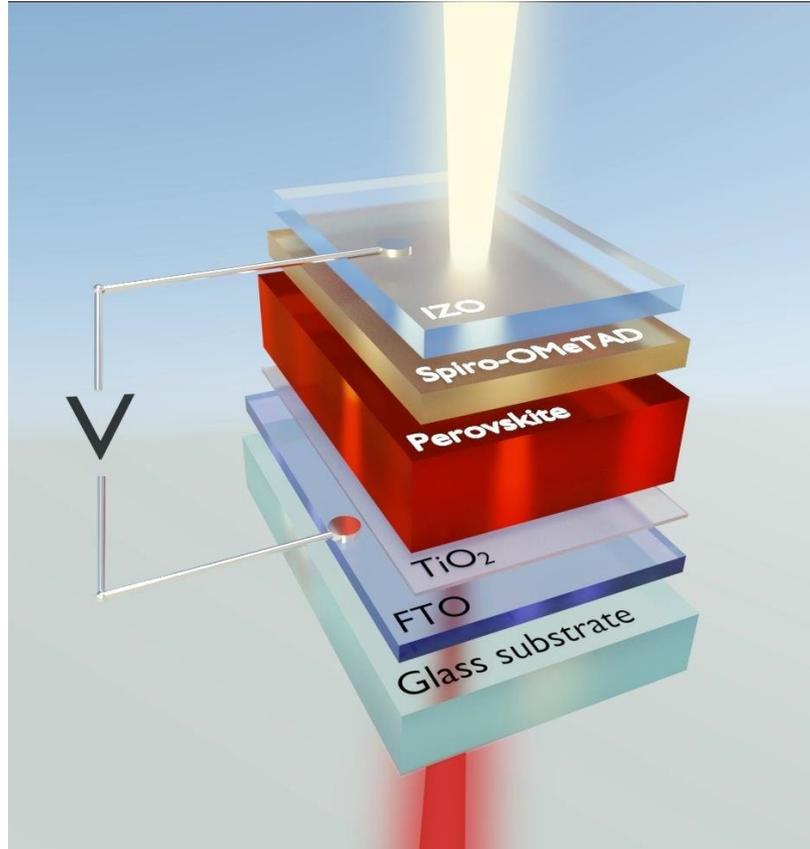
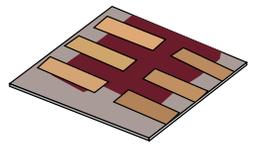
- Motivation – why learn this?
- **The structure of modern solar cells.**
- Downloading/Installing a solar cell CAD tool.
- Your first simulation
- Affect of varying layer thicknesses.
- The solar spectrum and material choice
- Performing optical simulaions
- Recombination
- Charge carrier mobility
- The $\mu \cdot \tau$ product
- Parasitic resistances in a solar cell.
- Charge carrier traps.

The structure of modern solar cells.



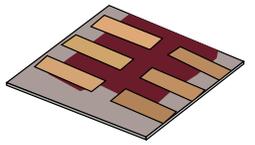
- The layers are optimized to do different things.

This is a perovskite solar cell

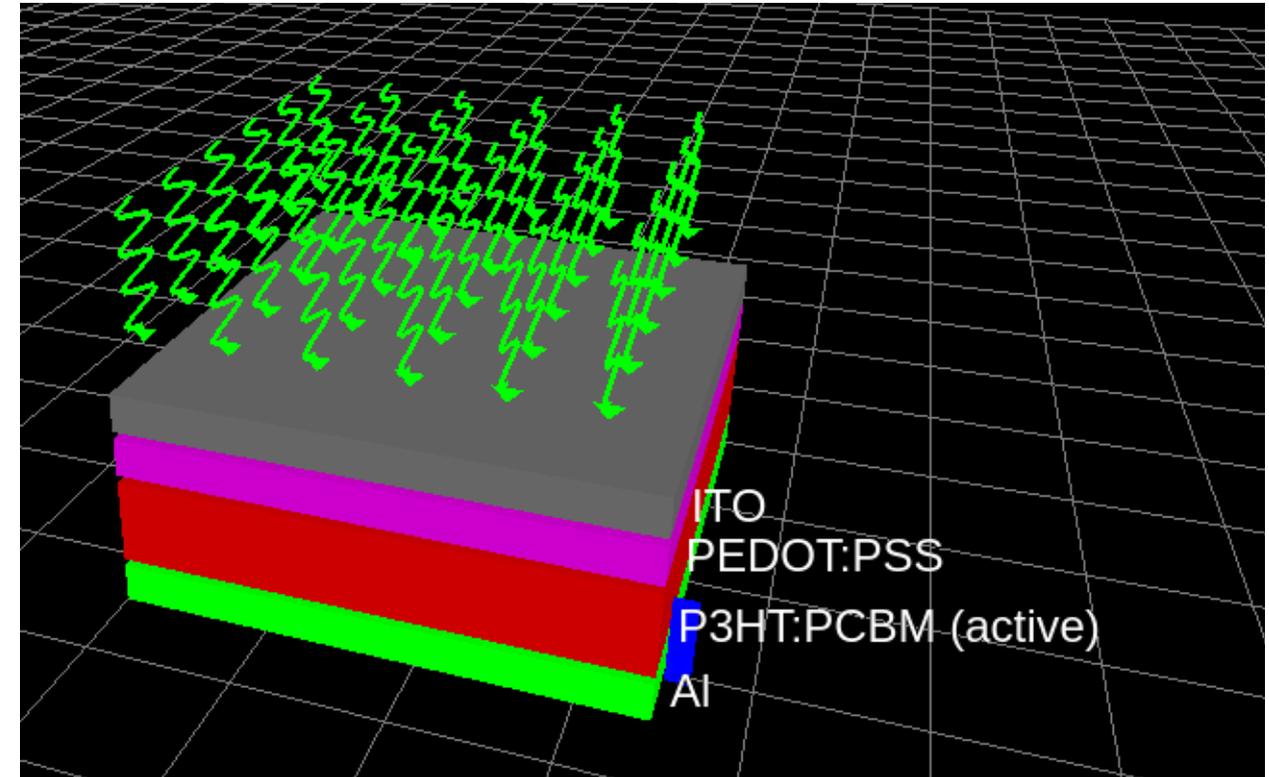


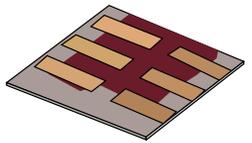
- The layers are optimized to do different things.
 - Absorb light (the active layer)
 - Act as contacts (Metal oxides/metals)
 - Reflect light (metals)
 - Act as a stiff substrate (Glass)
- Exactly what each layer does will depend on the exact design of the solar cell.

Question 1:



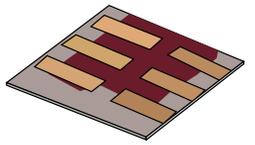
If you look at the image of the solar cell, you can see that it is split into 4-5 layers. Each layer has a name associated with it (ITO/PEDOT:PSS etc..). Write down, what does each layer of the solar cell do and what do the initials stand for? Where possible find images of the chemical structures and place this information in your report. You will be able to find this information in the internet.





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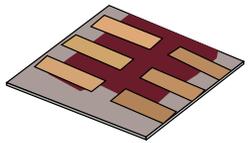
Downloading gpvdm



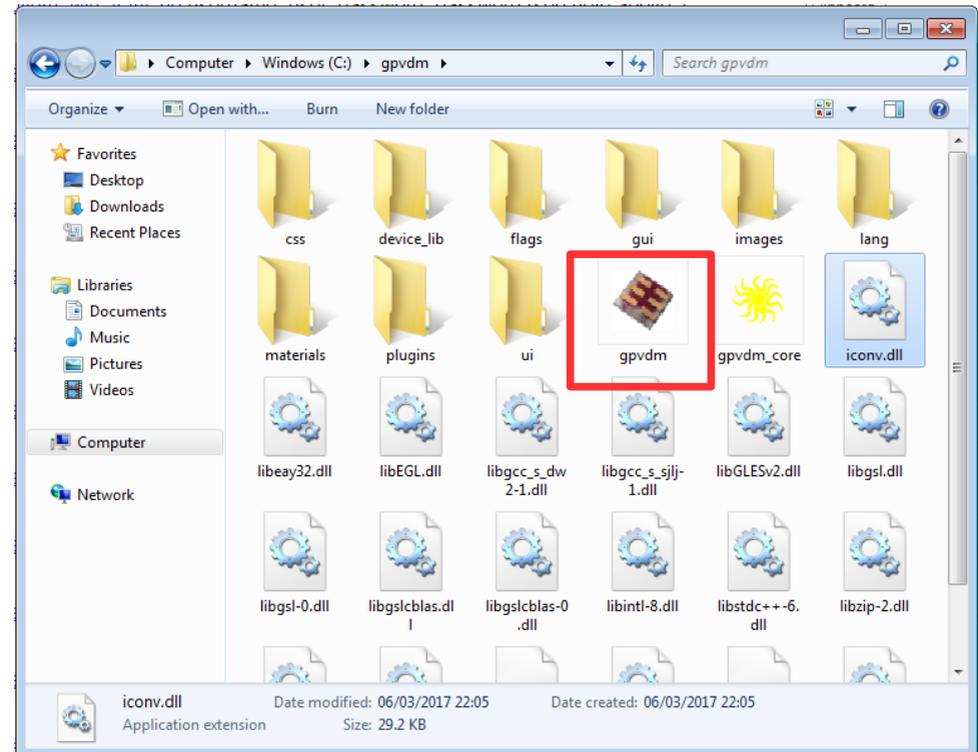
- Please download gpvdm from here:
<https://sandbox.gpvdm.com/downloads/winzip/>

NB: This is a new link to what I gave out during the class, just download the zip file just as you did in class.

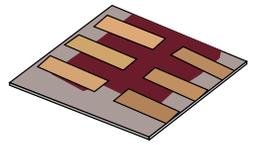
Installing gpvdm



- Once you have downloaded the zip file extract it to the Desktop
- Rename the directory *pub* to *gpvdm*.
- If you open it you should see a directory structure like this...
- Double click on the *gpvdm.exe*.



Register the software



Registration window (www.gpvdm.com)

Please register to use gpvdm. Thanks!

Name:

Company/University:

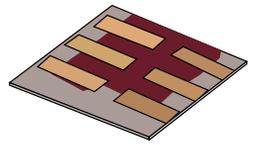
E-mail:

Confirm e-mail:

Register

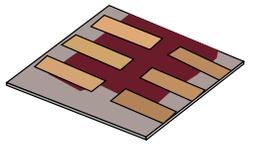
- You have to fill in all the boxes for it to work.
- Under Company, just put the University of Nottingham.

It will then ask you for a license key



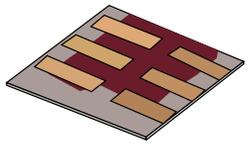
Your key is: **uon**

(lower case, no spaces
no numbers...)



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Making a new simulation



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

File Home Simulations Configure Device Information

New simulation Open simulation Export data

1.

General-purpose photovoltaic device model

(www.gpvdm.com)

To make a new simulation click *New Simulation* in the menu or 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.

Rod
18/10/13

New simulation (https://www.gpvdm.com)

Which type of device would you like to simulate?

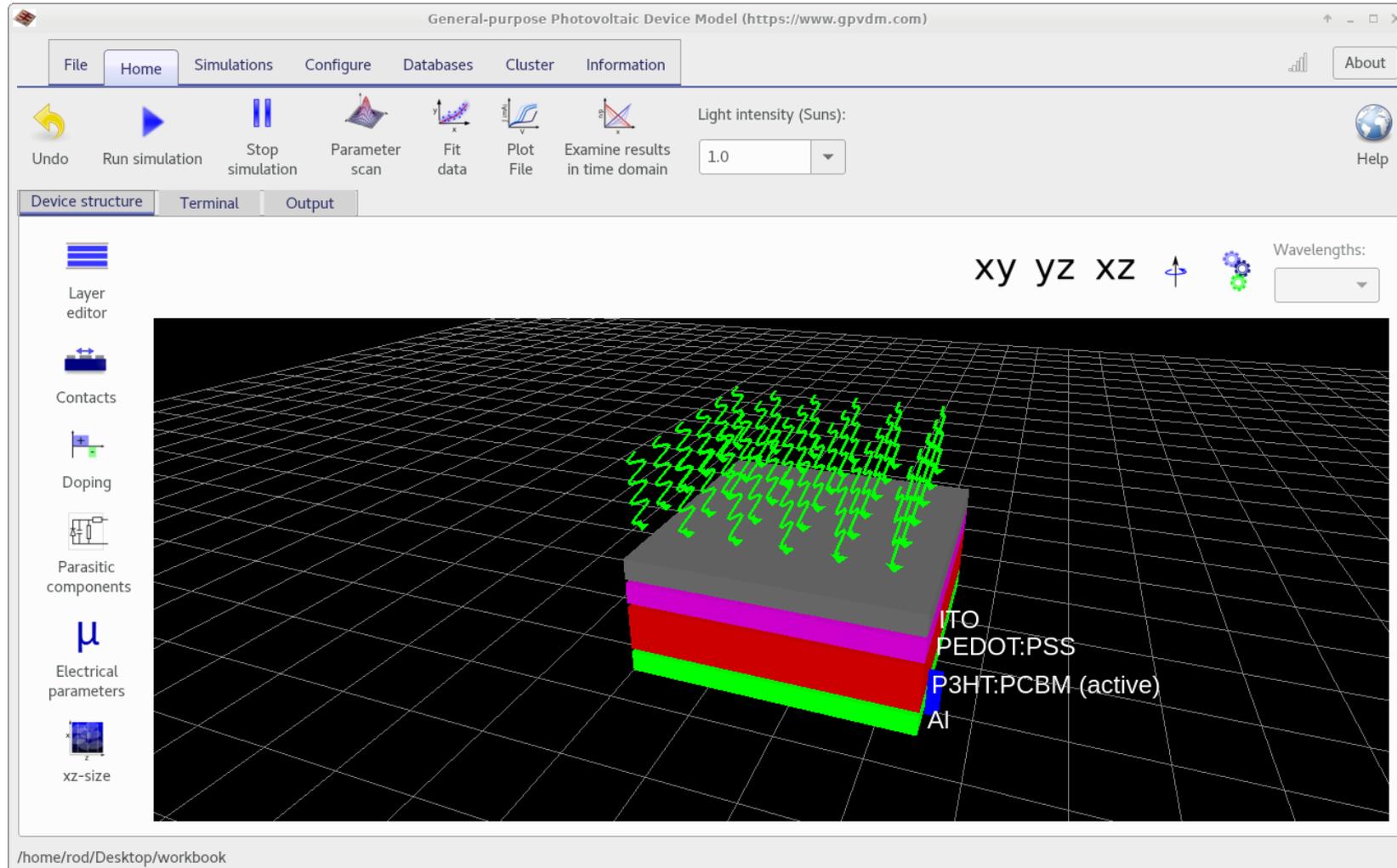
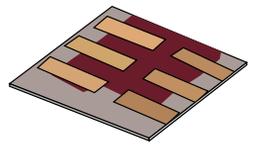
2.

- Organic solar cell (p3htpcbm.gpvdm)
- Organic LED (oled.gpvdm)
- Crystalline silicon solar cell (silicon.gpvdm)
- CIGS Solar cell (cigs.gpvdm)
- a-Si solar cell (a-silicon.gpvdm)
- polycrystalline silicon (silicon.gpvdm)
- OFET (ofet.gpvdm)

3.

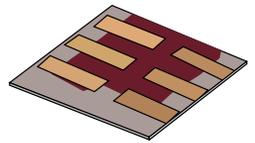
Cancel Next

You should get a window which looks like this



Try using the mouse to look around the picture of the cell and look at its layer structure.

Click the play button



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

File Home Simulations Configure Databases Information About

Undo Run simulation Stop simulation Parameter scan Fit data Plot File Examine results in time domain Light intensity (Suns): 1.0 Help

Device structure Terminal Output

Layer editor

Contacts

Doping/Ions

Parasitic components

Electrical parameters

xz-size

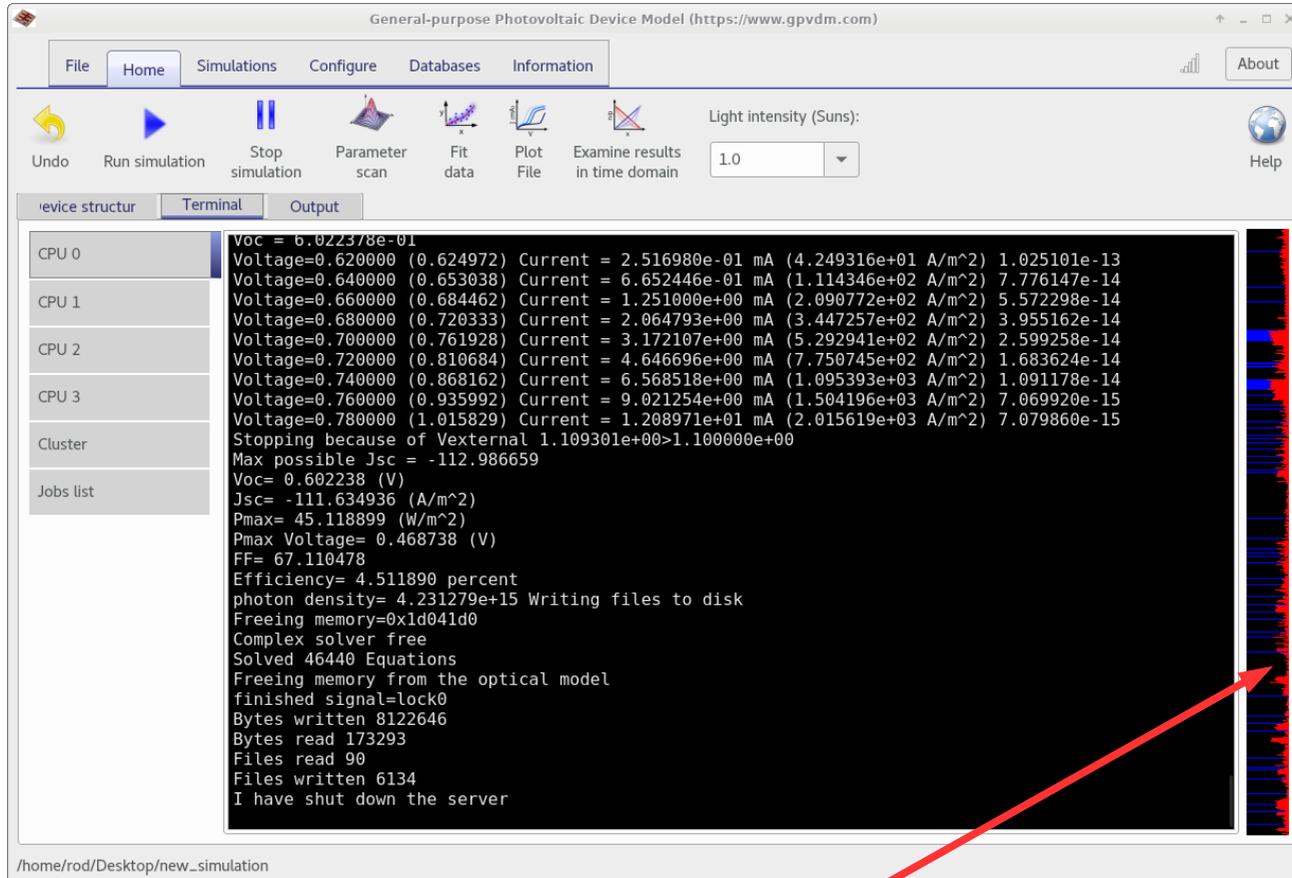
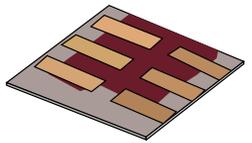
xy yz xz

Wavelengths:

ITO
PEDOT:PSS
P3HT:PCBM (active)
Al

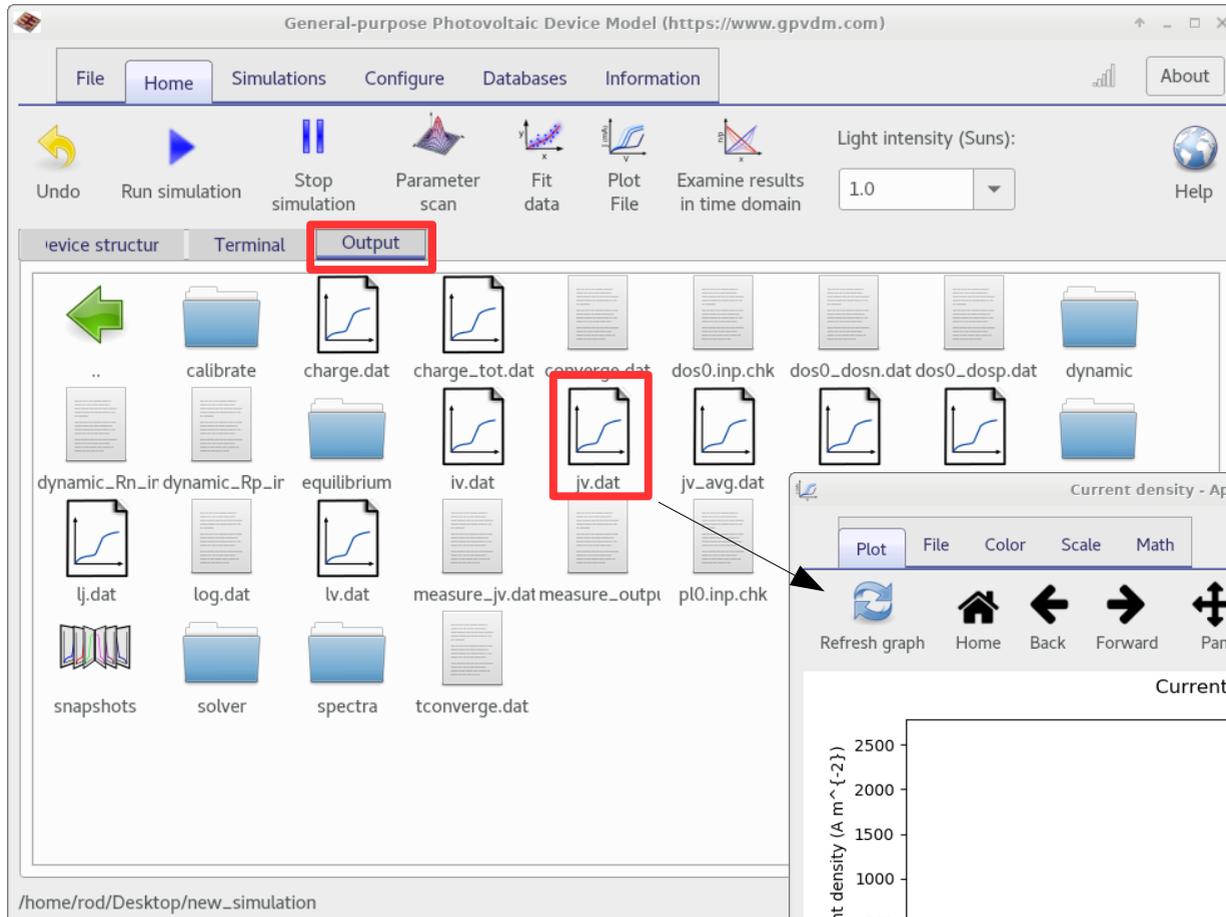
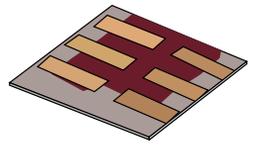
/home/rod/Desktop/new_simulation

The core solver will be run on CPU 0

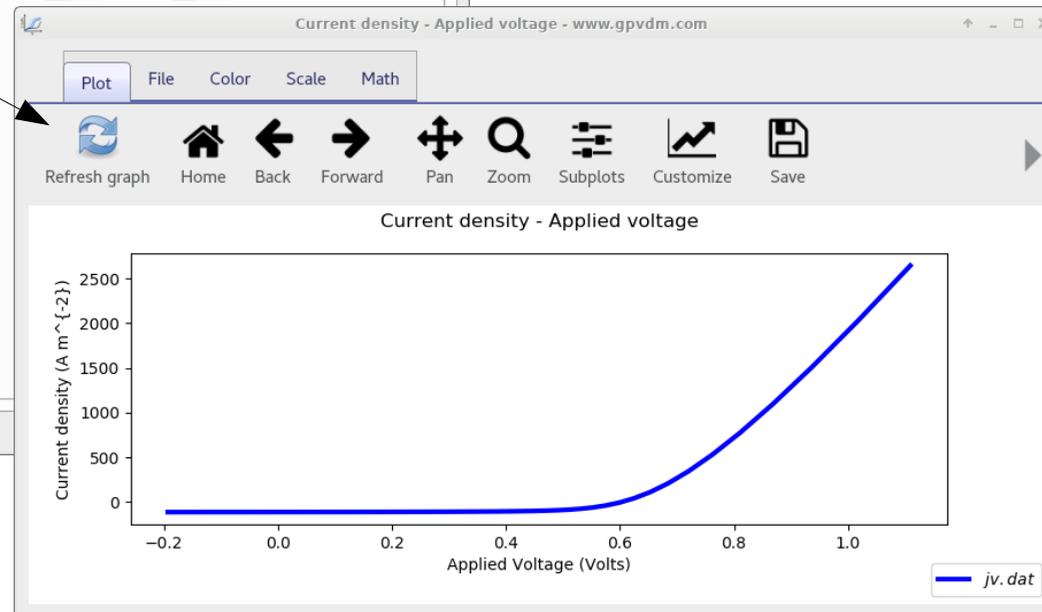


• Blue is CPU usage, red is disk usage, if you simulation is running slowly, writing to the HDD is **always** the bottleneck, SSDs highly recommended.

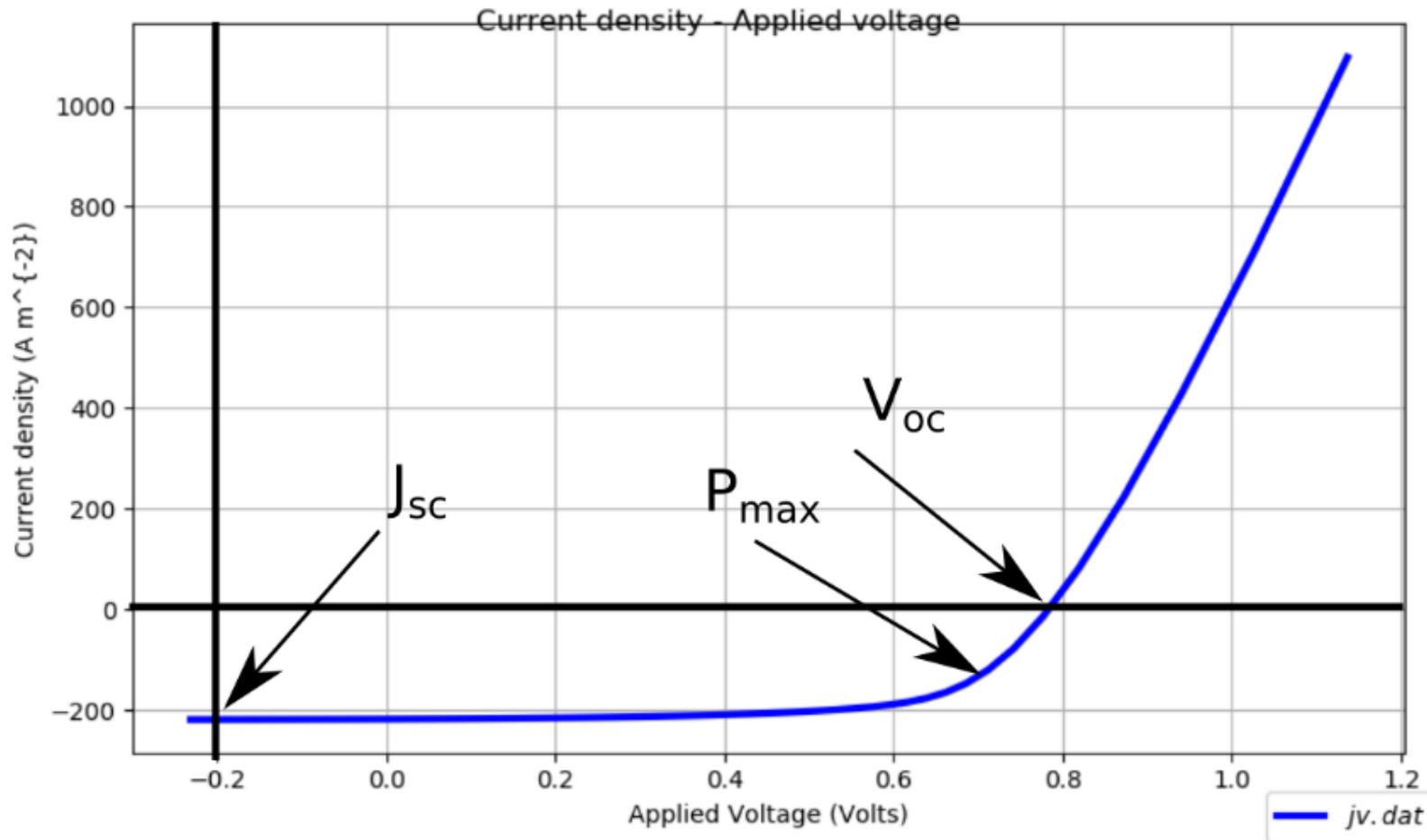
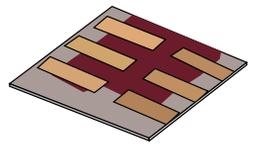
Examining the results.



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



Let's look at this in more detail

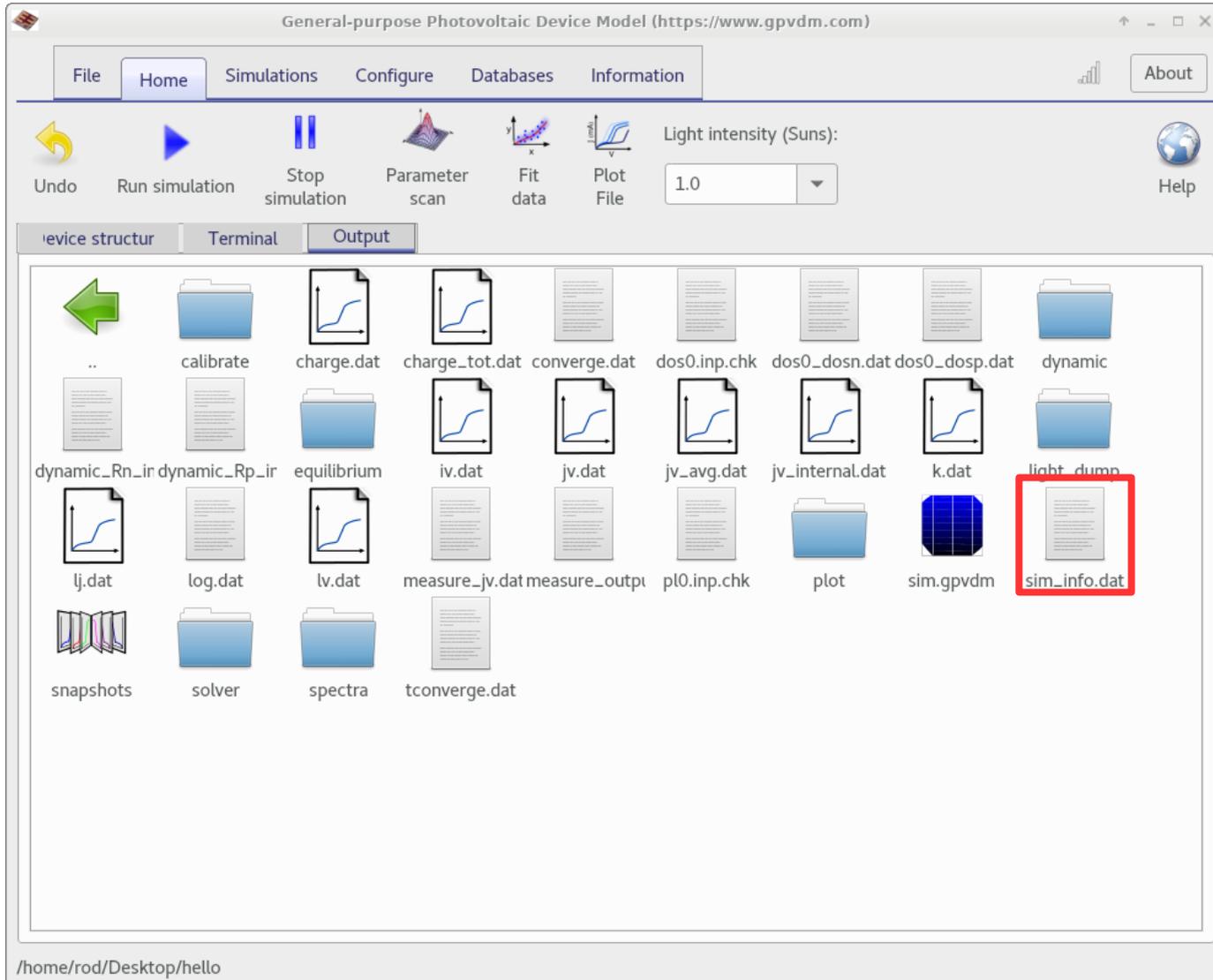
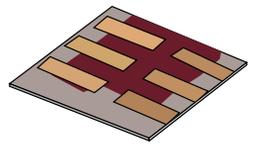


- V_{oc} : Maximum voltage a cell can produce

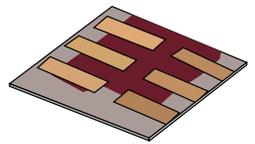
- J_{sc} : The maximum current a cell can produce.

- P_{max}

You can get the values of FF, Voc and Jsc from the file `sim_info.dat`



- Double click on it to open it.



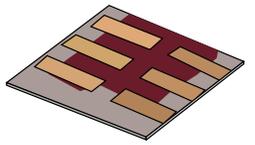
Simulation information (www.gpvd.com)

Simulation Information

Fill factor	0.671105	a.u.
Power conversion efficiency	4.511890	Percent
Max power	45.118899	Watts
V _{oc}	0.602238	V
Recombination time constant at Voc	1.025421e-05	s
Recombination rate at Voc	4.270122e+27	m ⁻³ s ⁻¹
Average carrier density at P _{max}	1.756484e+22	m ⁻³
Recombination time constant	3.897166e-05	m ⁻¹
Trapped electrons at Voc	3.041562e+22	m ⁻³
Trapped holes at Voc	4.409148e+22	m ⁻³
Free electrons at Voc	2.574245e+22	m ⁻³
Free holes at Voc	1.832887e+22	m ⁻³
J _{sc}	-1.116349e+02	A m ⁻²
Total carriers (n+p)/2 at Voc	4.777811e+22	m ⁻³

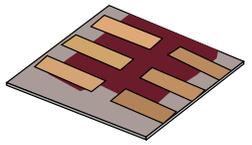
- The values of Voc, Jsc, and FF are in this file.

Question 2:

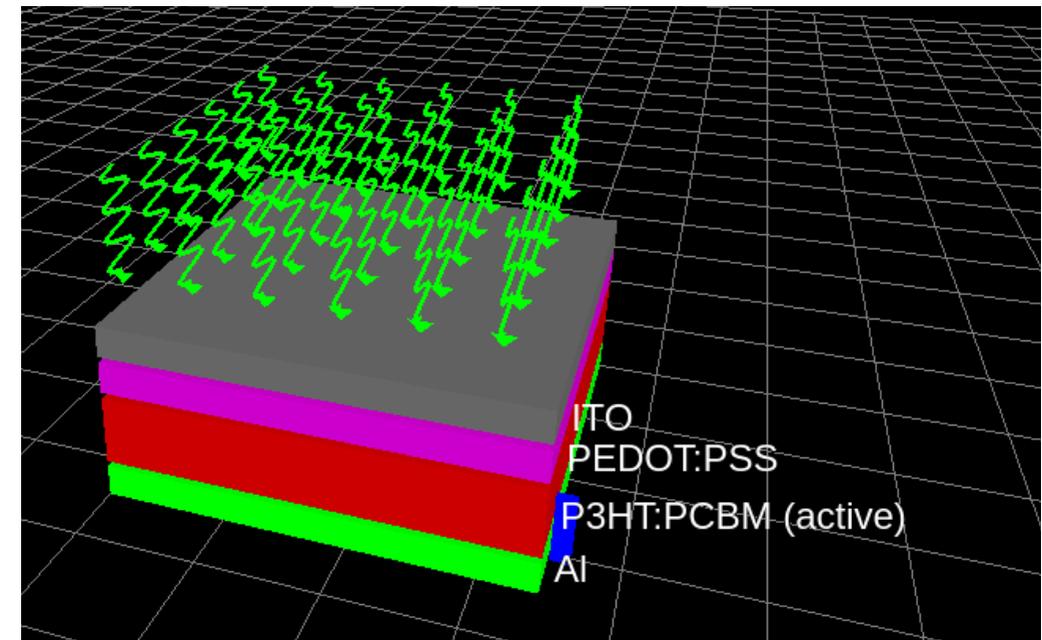


What is the J_{sc} , V_{oc} and Fill Factor (FF) of this solar cell? How do these number compare to a typical Silicon solar cell? (Use the internet to find typical values for a Silicon solar cell.)]

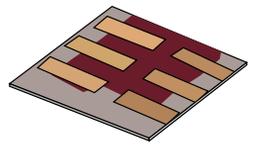
Overview



- Motivation – why learn this?
- The structure of modern solar cells.
- Downloading/Installing a solar cell CAD tool.
- Your first simulation
- **Varying the active layer thicknesses.**
- The solar spectrum and material choice
- Performing optical simulations
- Recombination
- Charge carrier mobility
- The $\mu \cdot \tau$ product
- Parasitic resistances in a solar cell.
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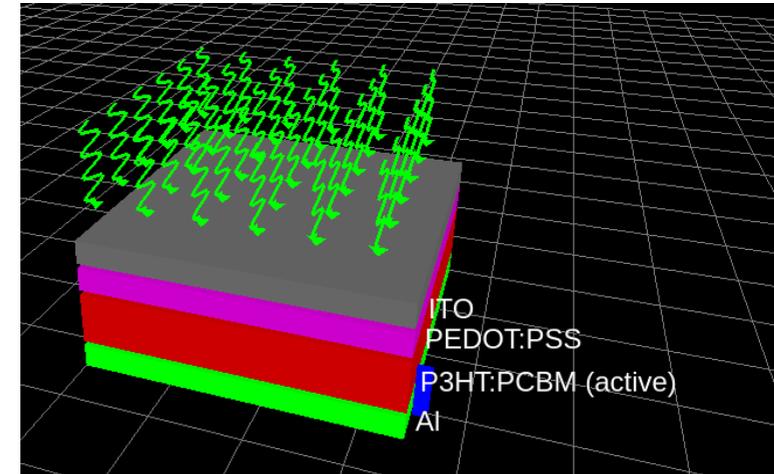


The layer editor used for changing the thicknesses of layers in a cell.

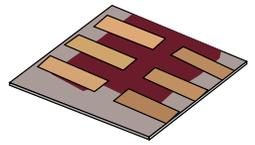


The screenshot shows the main window of the General-purpose Photovoltaic Device Model (GPVDM) software. The 'Layer editor' window is open, displaying a table of layer properties. The 'Layer editor' icon in the left sidebar is highlighted with a red box. The main window also shows a 3D view of the device structure and various simulation controls.

Layer name	Thickness	Optical material	Layer type
ITO	1e-07	oxides/ito	contact
PEDOT:PSS	1e-07	polymers/pedotpss	other
P3HT:PCBM	2.2e-07	blends/p3htpcbm	active layer
Al	1e-07	metal/al	contact



You can change the thicknesses of the layers here..



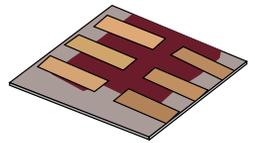
Layer editor <https://www.gpvd.com>

+ - ↓ ↑

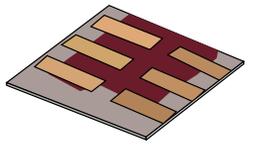
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P3HT:PCBM	2.2e-07	blends/p3htpcb	active layer
Al	1e-07	metal/al	contact

- All values are in meters
- Think about how thick these layers are compared to the width of a human hair. (17 μm to 181 μm)

Question 3:

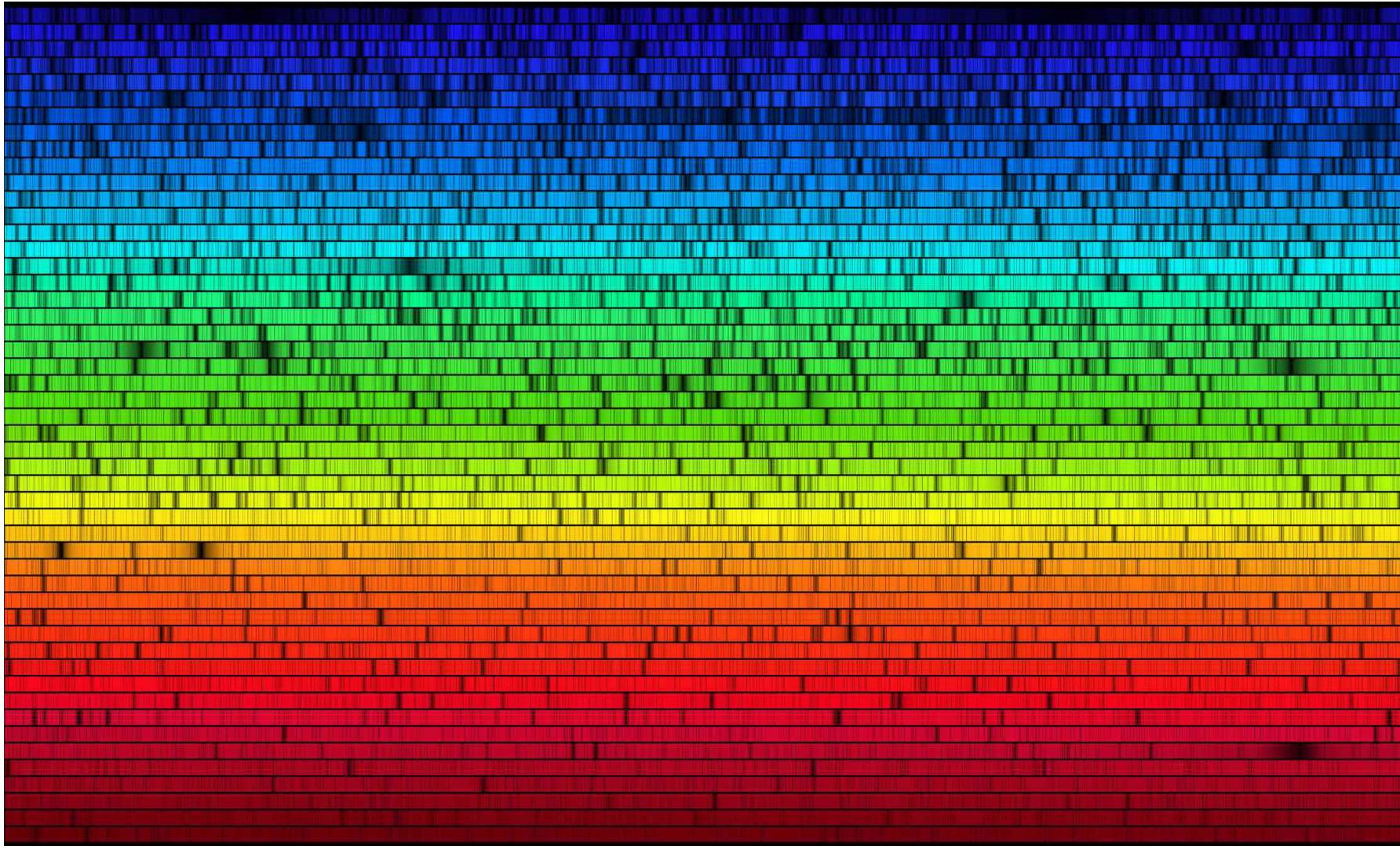
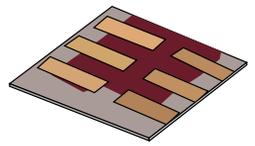


Plot a graph (using excel or any other graphing tool), of device efficiency v.s. thickness of the active layer. What is the optimum efficiency/thickness of the active layer? Also plot graph V_{oc} , J_{sc} and FF as a function of active layer thickness. J_{sc} is generally speaking the maximum current a solar cell can generate, try to explain your graph of J_{sc} v.s. thickness, [Hint, the next section may help you answer this part of the question.]



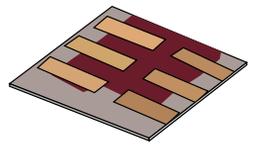
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Let's first look at what the sun's spectrum looks like before we consider material choices to absorb it's energy.



- That looks cool, I wonder which material will best absorb that light?

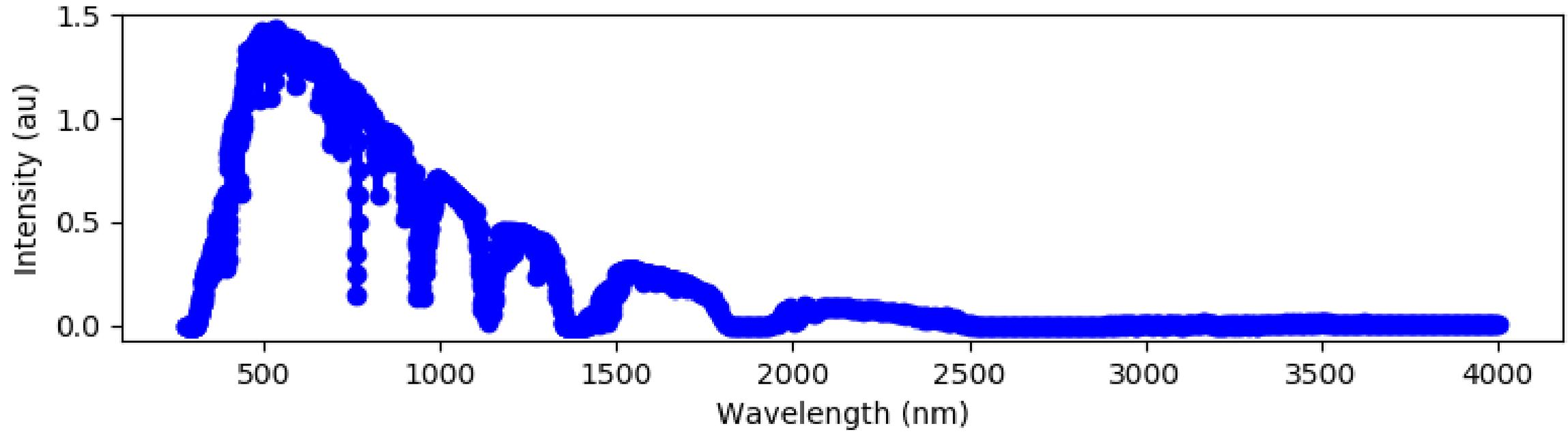
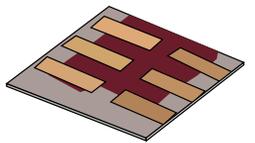
Let's plot that in a more conventional way.



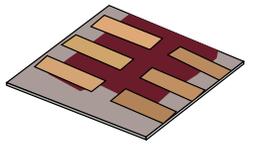
The screenshot shows the 'General-purpose Photovoltaic Device Model' software interface. The 'Databases' menu is highlighted in red. Below it, the 'Optical database' icon is also highlighted in red. A file explorer window shows a directory of spectral files, with 'sun' highlighted in red. An 'Optical spectrum editor' window displays a plot of Intensity (au) vs. Wavelength (nm) for the 'sun' source, showing a peak around 500 nm.

Wavelength (nm)	Intensity (au)
400	0.0
500	1.4
600	1.0
700	0.5
800	0.2
1000	0.1
1500	0.05
2000	0.02
3000	0.01
4000	0.0

The solar spectrum...

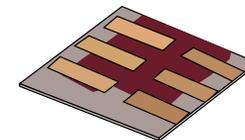


Question 4:



Describe the main differences between the light which comes from the LED and the sun. Rather than referring to the various regions of the spectrum by their wavelengths, refer to them using English words, such as infrared, Ultra Violet, Red, and Green etc... you will find which wavelengths match to each color on the internet. If you were designing a material for a solar cell, what wavelengths would.

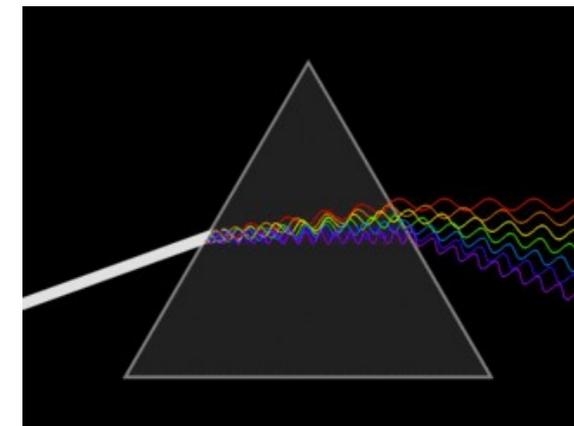
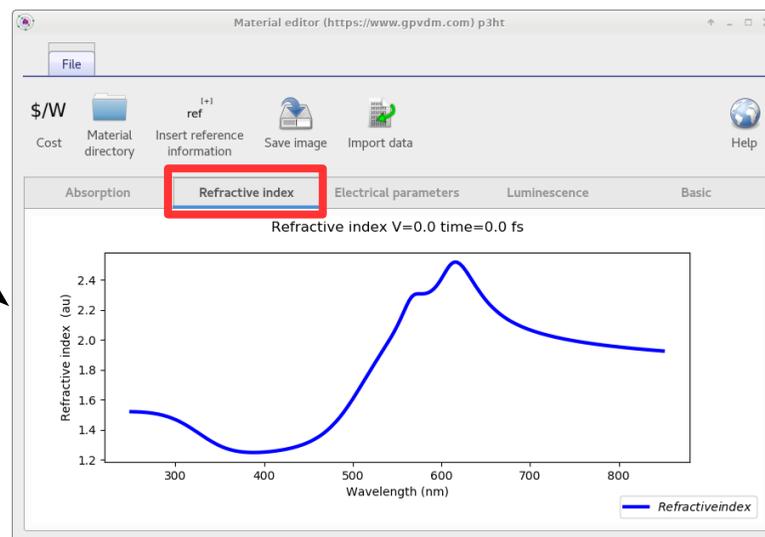
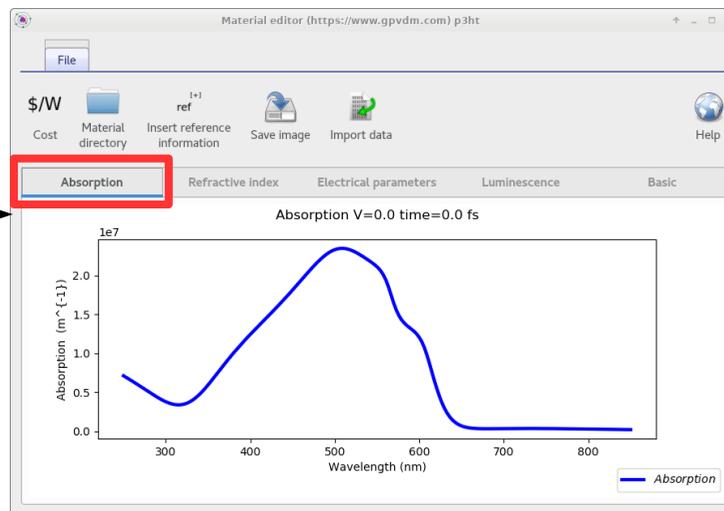
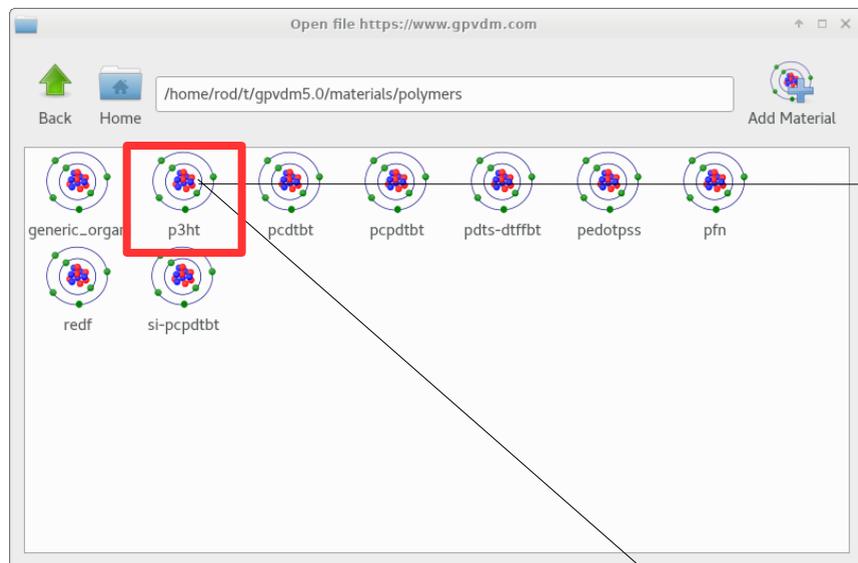
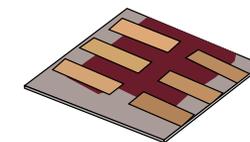
The materials from which solar cells are made.



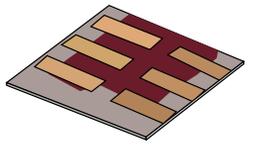
The image illustrates the navigation process in the General-purpose Photovoltaic Device Model (GPVDM) software to access material databases. It consists of three overlapping window screenshots:

- Top Window:** The main application interface with the menu bar. The 'Databases' menu item is highlighted with a red box. Below the menu, the 'Materials database' icon is also highlighted with a red box.
- Middle Window:** A file explorer window titled 'Open file https://www.gpvd5.0.com' showing the directory path `/home/rod/t/gpvd5.0/materials`. The 'polymers' folder is highlighted with a red box.
- Bottom Window:** A file explorer window titled 'Open file https://www.gpvd5.0.com' showing the contents of the 'polymers' folder. The path is `/home/rod/t/gpvd5.0/materials/polymers`. It displays several material icons with labels: 'generic_organ', 'p3ht', 'pcdtbt', 'pcpdtbt', 'pdts-dtffbt', 'pedotps', 'pfn', 'redf', and 'si-pcpdtbt'.

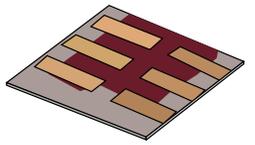
Have a look at the absorption and refractive index.



Question 5:

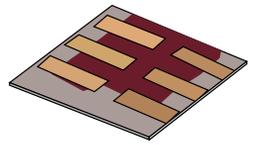


What color of light does the polymer p3ht absorb best? Which material in the polymers directory do you think will absorb the suns light best?



- Motivation – why learn this?
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- Recombination
- Charge carrier mobility
- The $\mu \cdot \tau$ product
- Parasitic resistances in a solar cell.
- Charge carrier traps.

We can study how light interacts with our solar cell by using the optical simulation tool.



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

File Home **Simulations** Configure Databases Information

Time domain simulation editor. Steady state simulation editor. Suns Voc simulation editor. Simple diode model. Simulation mode: jv. Optical Simulation. Laser editor. FDTD Simulation. Measure. Calculate the cost.

Device structure Terminal Output

Layer editor. Contacts. Doping/Ions. Parasitic components. Electrical parameters. xz-size.

Optical simulation editor (https://www.gpvd.com)

Optics. Run optical simulation. Save graph. Wavelengths: all. Optical model: full. Solar spectrum: sun.

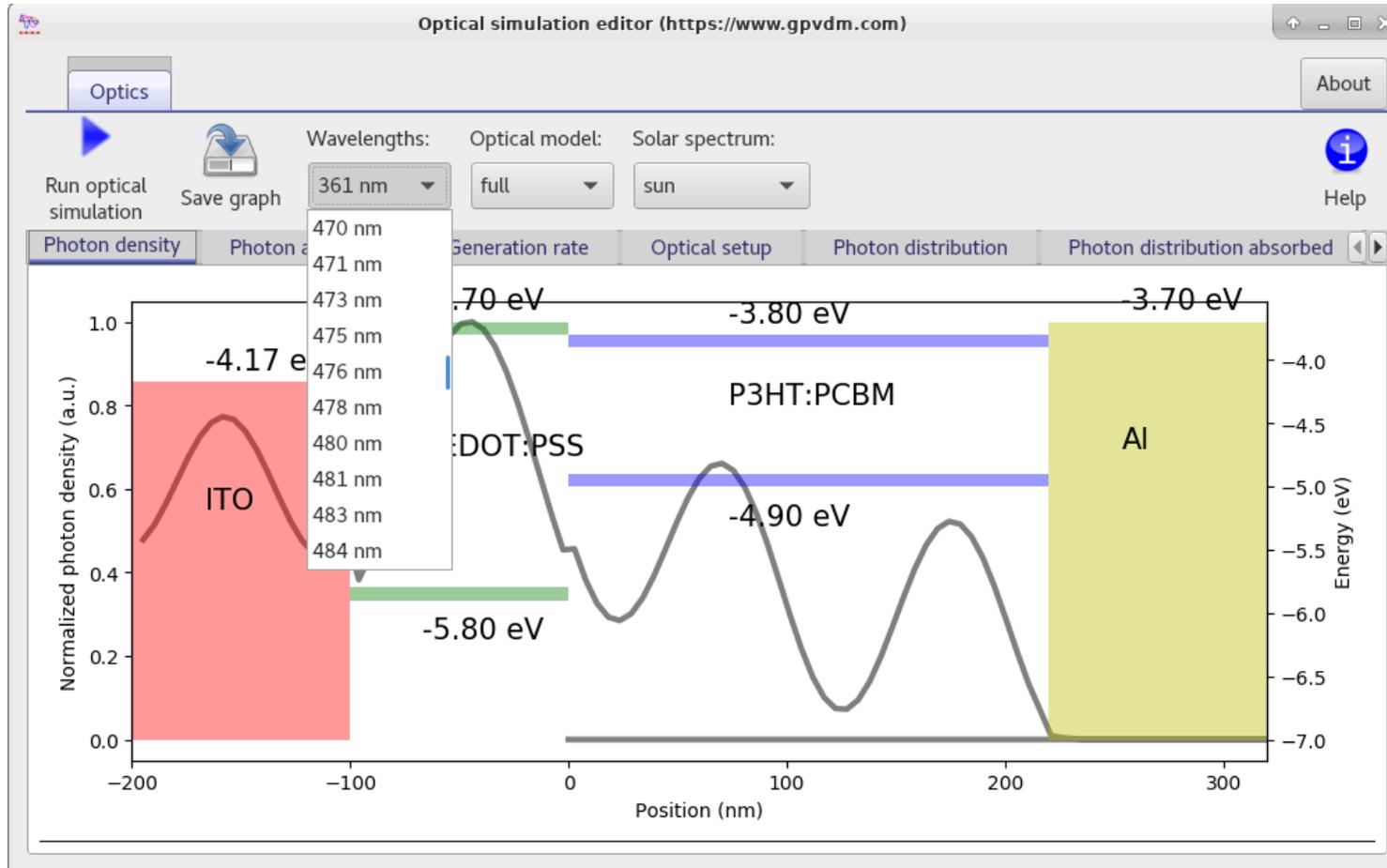
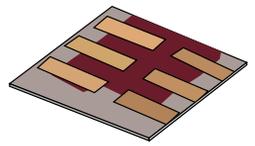
Photon density Photon absorbed Generation rate Optical setup Photon distribution Photon distribution absorbed

Photon density (a.u.) vs Position (nm) vs Energy (eV)

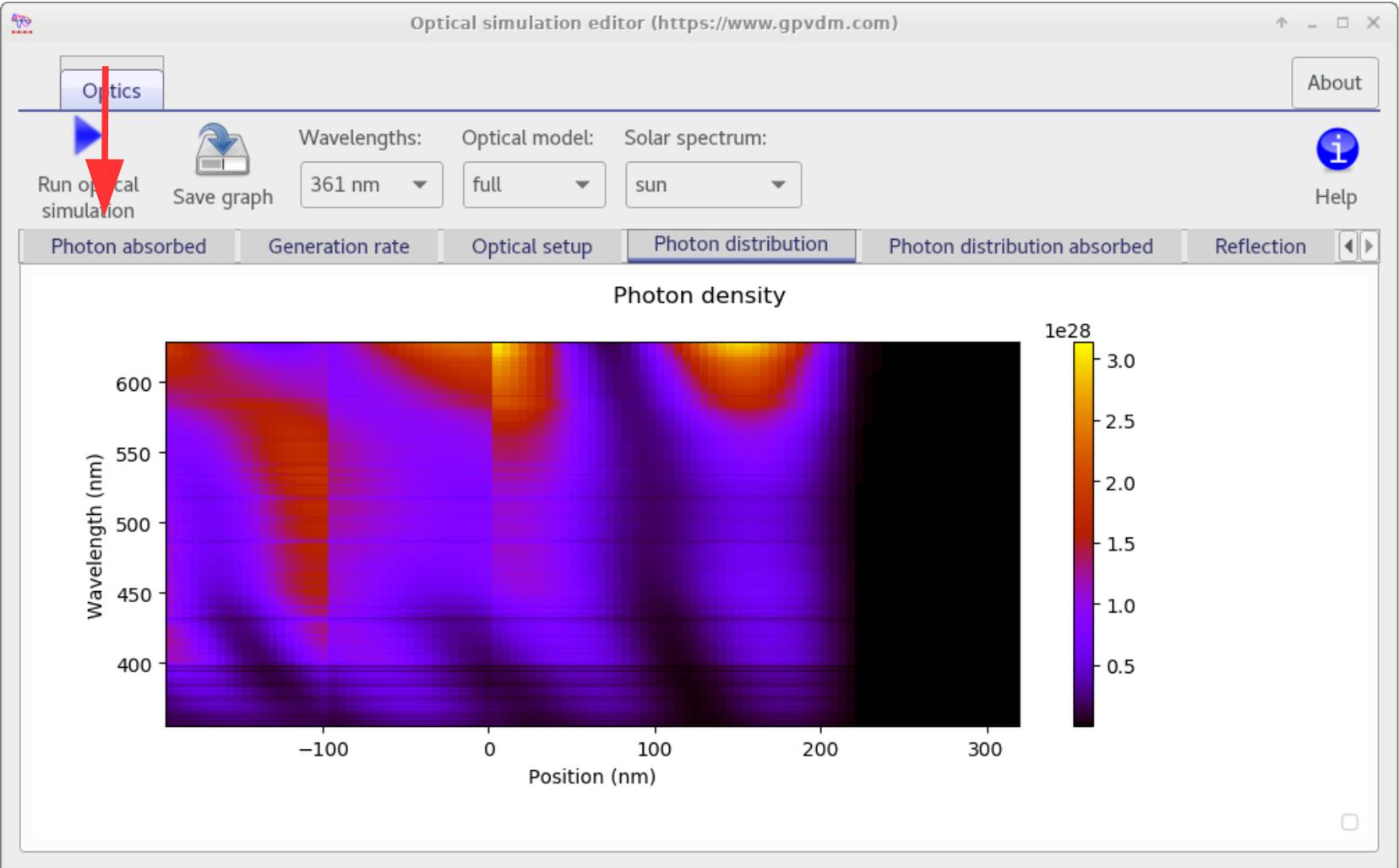
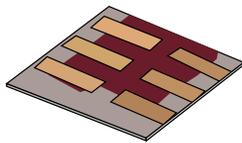
ITO: -4.17 eV, PEDOT:PSS: -5.80 eV, P3HT:PCBM: -4.90 eV, Al: -3.70 eV

•Click run....

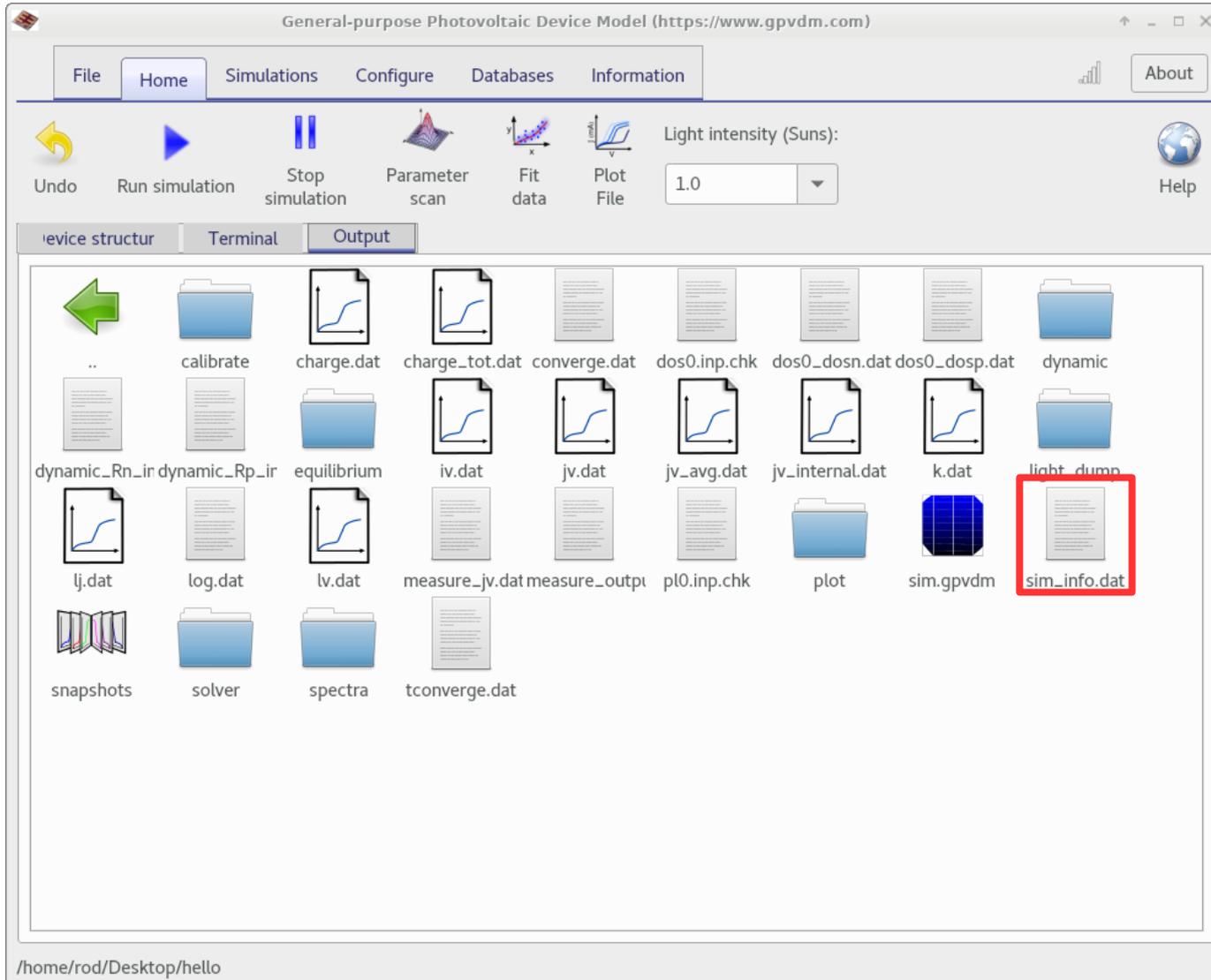
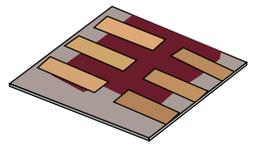
This shows us exactly where the light is being absorbed in the cell, think if it as ripples on a pond.



Plot the photon density as a function of wavelength/position

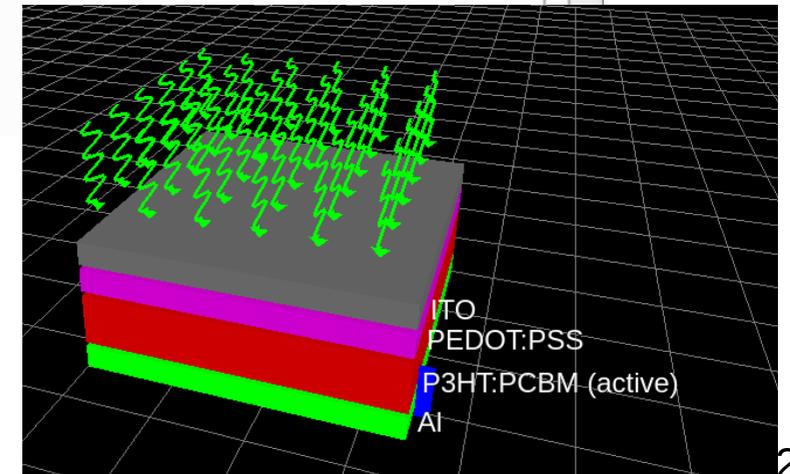
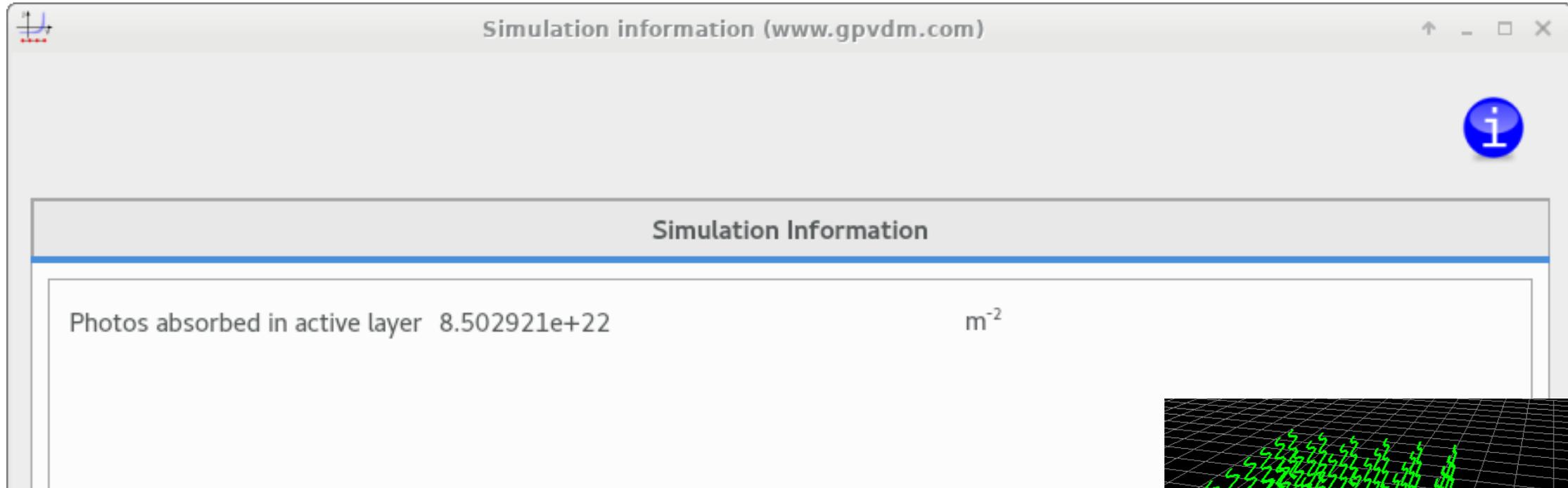
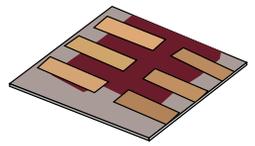


Let's look at sim_info.dat again, now we have run the optical simulation.

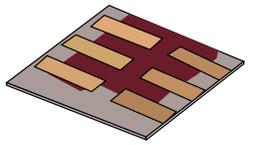


- Double click on it to open it.

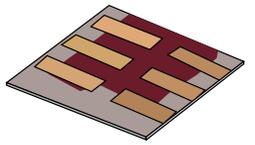
Photons absorbed in the active layer from sim_info.dat



Question 6:

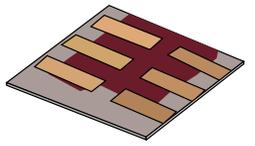


By running 5 or 6 with different active layer thicknesses, plot a graph of active layer thickness, v.s. the number of photons absorbed in the device. At what thickness do almost all photons get absorbed in the device? [Hint: I would run the simulations from 40nm to 200nm]



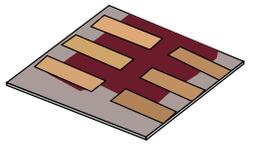
- Motivation – why learn this?
- The basic structure of 3rd generation solar cells.
- Downloading/Installing a solar cell CAD tool.
- Your first simulation
- Affect of varying layer thicknesses.
- The solar spectrum and material choice
- Performing optical simulations
- **Recombination**
- Charge carrier mobility
- The $\mu \cdot \tau$ product
- Parasitic resistances in a solar cell.
- Charge carrier traps.

So is a thicker solar cell always better? Well think about this....

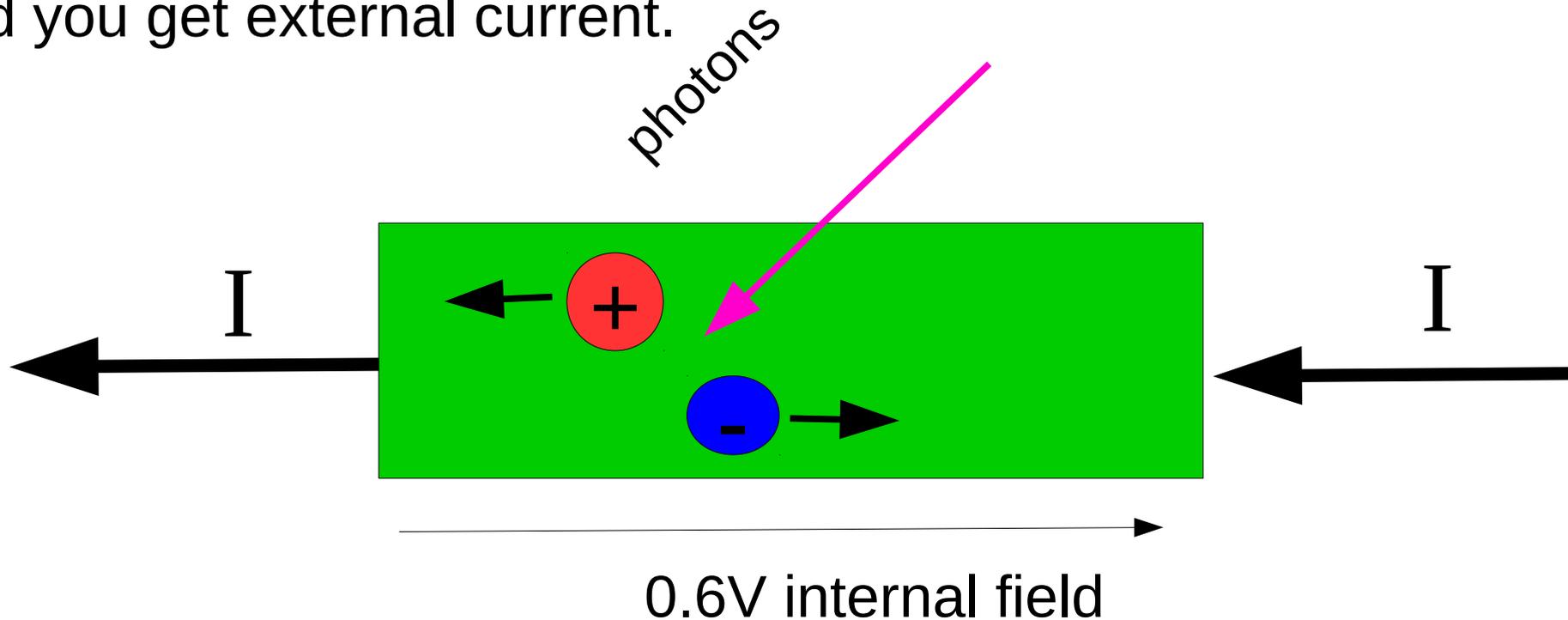


- Thicker means more material, so a more expensive device.
- It also means more energy (CO₂) has to be used to produce the devices as it's got more material in it.
- But more importantly....

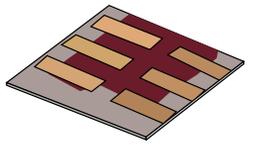
Recombination...



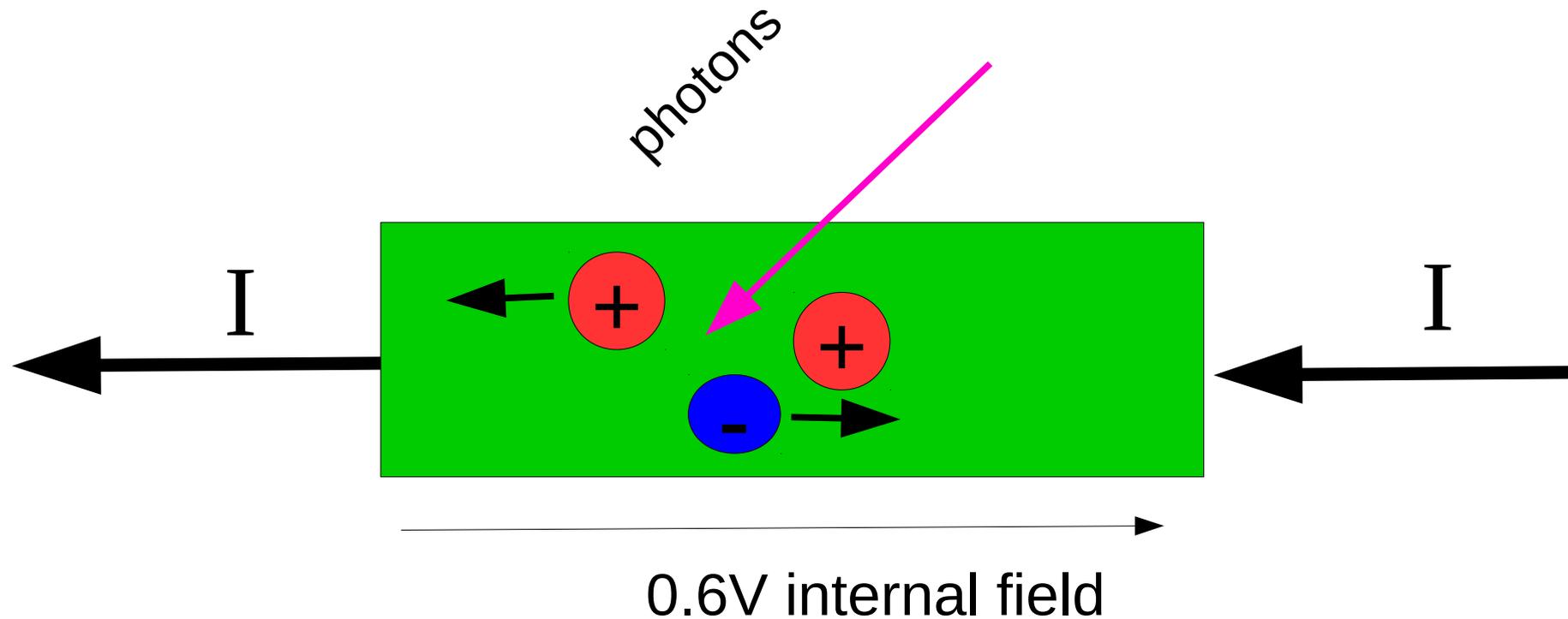
- Think about a photon generating a positive and negative charge in a solar cell.
- One charge gets dragged to one contact the other gets dragged to the other and you get external current.



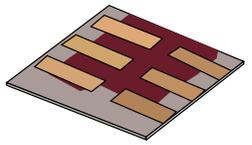
Recombination...



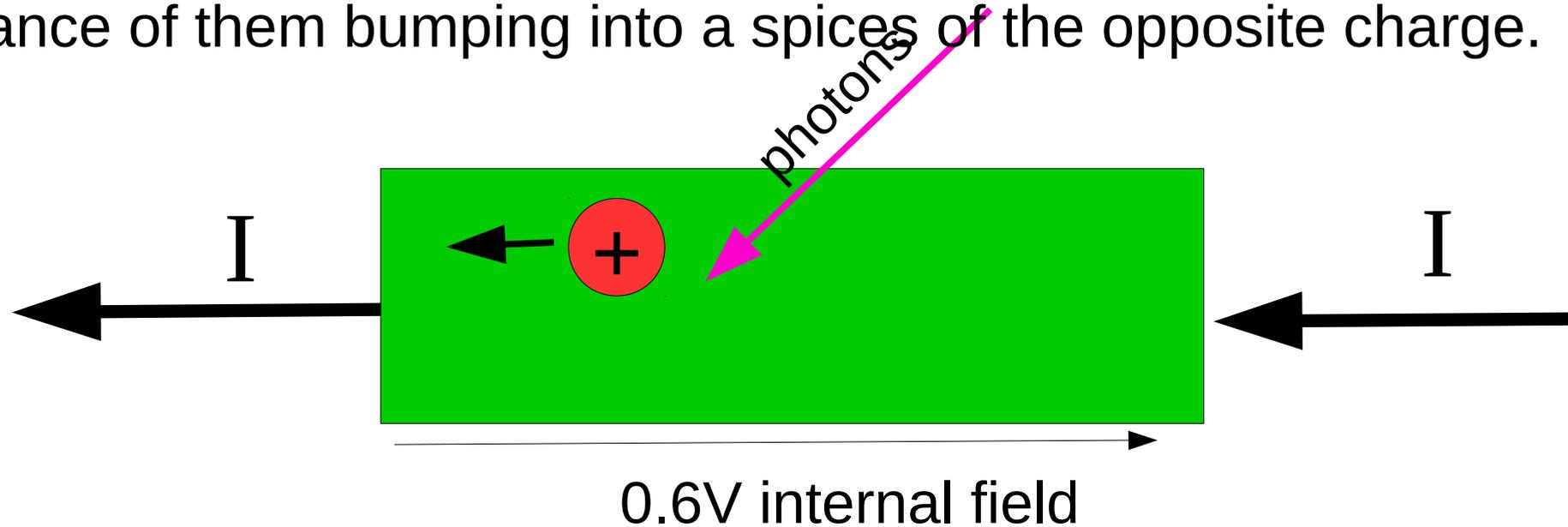
- But now imagine if one of these charge carriers meets a species of opposite charge on the way out...
- What will happen?



Recombination...

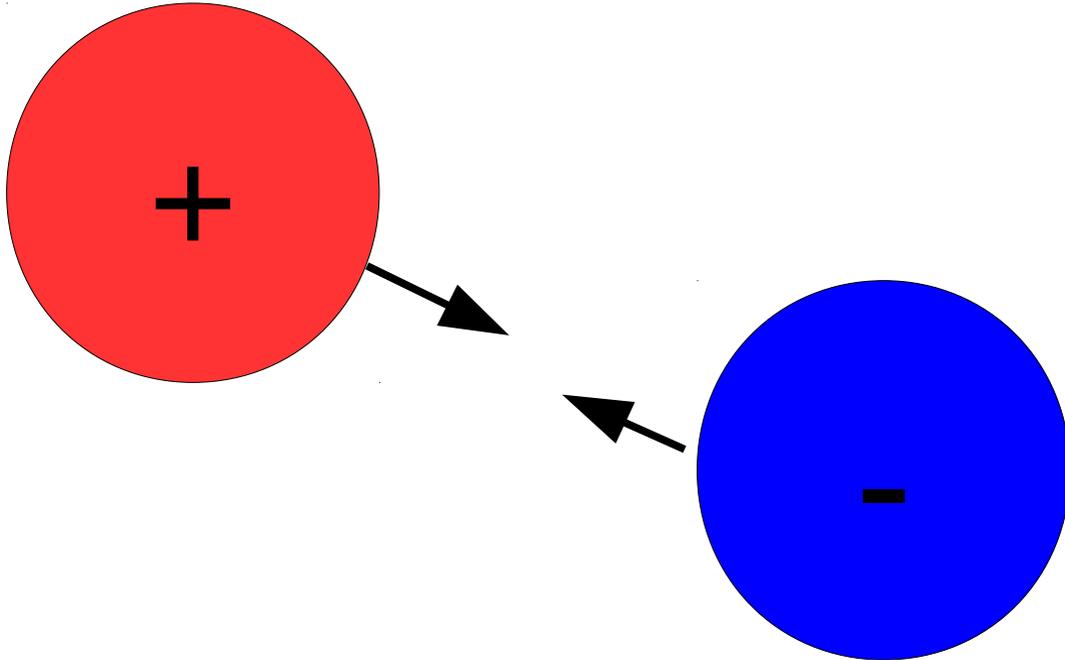
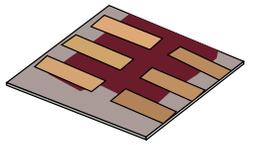


- Annihilation... so two charge carriers are lost..
- This seems bad. One way we can make this less likely to happen is to get the electrons/holes out of the device as quickly as possible so there is less chance of them bumping into a species of the opposite charge.



- So from a recombination stand point do we want a thick or thin device?

Recombination

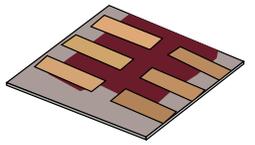


- The rate at which electrons/holes meet each other and get destroyed is given by this equation:

$$R(x) = k n(x) p(x)$$

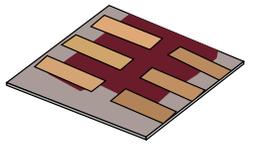
- Where, k is a constant, n is the density of electrons and p is the density of holes.

Question 7:

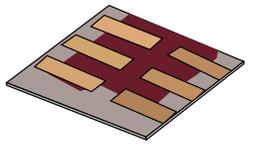


In no more than two sentences describe what an electron and hole are.

Question 8:

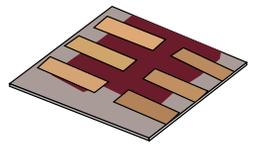


Plot a new graph of active layer thickness v.s. device efficiency. By looking at your graph, what is the optimum device thickness for a device with a recombination constant of $k = 1 \times 10^{-15}$?

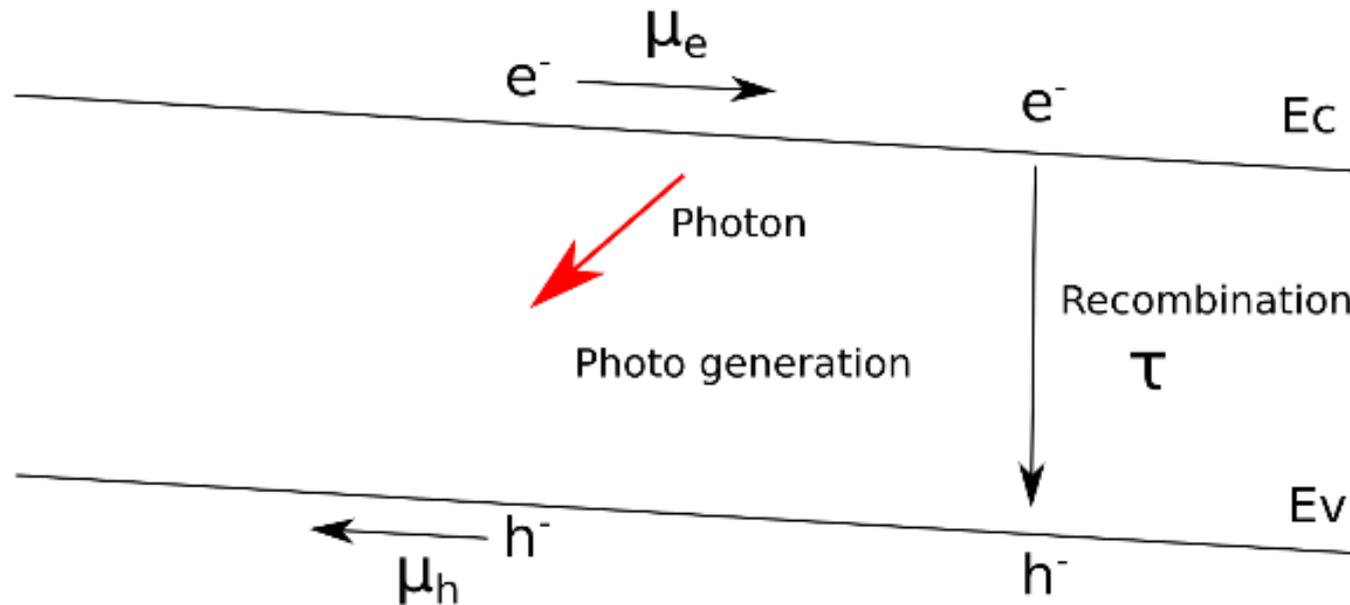


- Motivation – why learn this?
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- Recombination
- **Charge carrier mobility**
- The $\mu \cdot \tau$ product
- Parasitic resistances in a solar cell.
- Charge carrier traps.

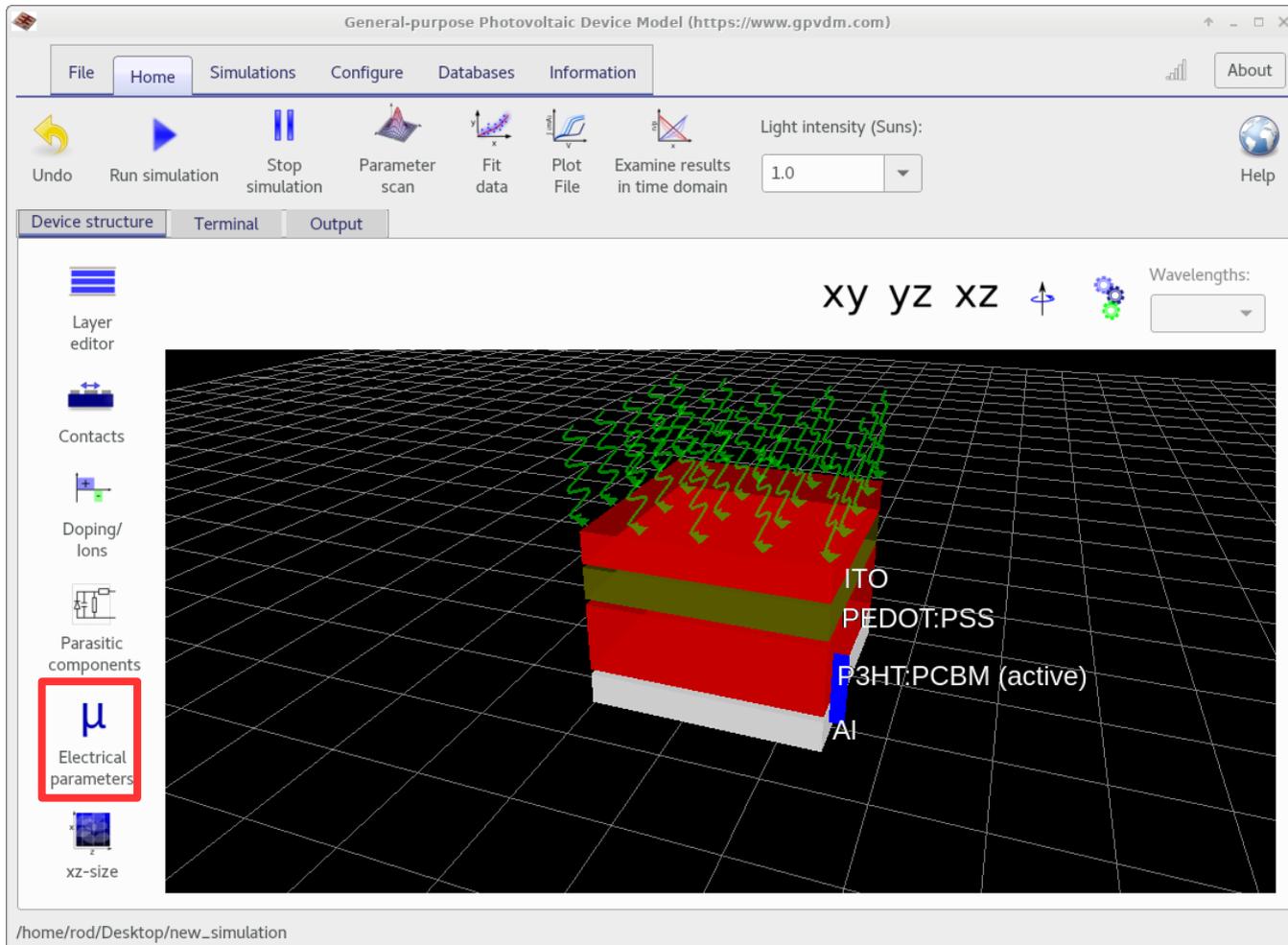
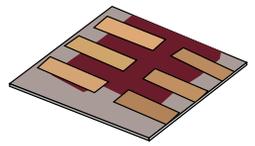
Mobility of charge carriers in solar cells.



- How fast electrons and holes can move in a solar cell is governed by a material property called charge carrier mobility.
- The higher the number the faster charge carriers move. μ_e , μ_h

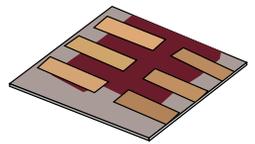


The electrical properties of the materials can be set here..



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

Setting the mobilities.



Electrical parameter editor (<https://www.gpvd.com>)

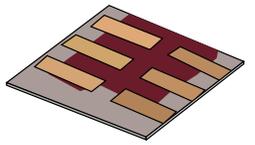
Electrical parameters | Luminescence

DoS of P3HT:PCBM

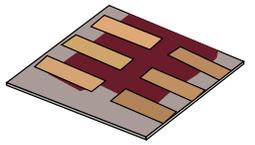
DoS distribution	exponential	au
Electron trap density	3.8e26	$\text{m}^{-3} \text{eV}^{-1}$
Hole trap density	1.45e25	$\text{m}^{-3} \text{eV}^{-1}$
Electron tail slope	40e-3	eV
Hole tail slope	60e-3	eV
Electron mobility	2.48e-7	$\text{m}^2 \text{V}^{-1} \text{s}^{-1}$
Hole mobility	2.48e-7	$\text{m}^2 \text{V}^{-1} \text{s}^{-1}$
Relative permittivity	3.8	au
Number of traps	20	bands
Free electron to Trapped electron	2.5e-20	m^{-2}
Trapped electron to Free hole	1.32e-22	m^{-2}
Trapped hole to Free electron	4.67e-26	m^{-2}
Free hole to Trapped hole	4.86e-22	m^{-2}

- k is at the bottom of the window...

Question 9:

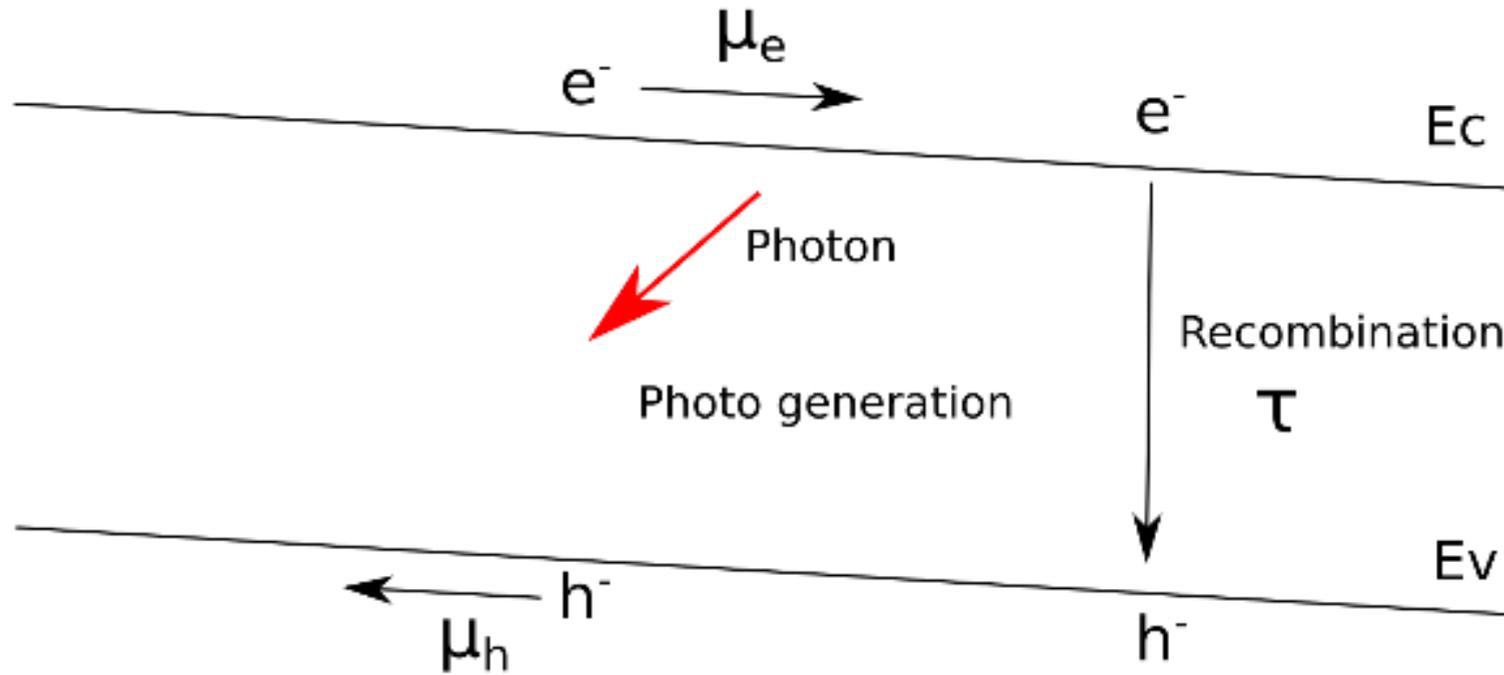
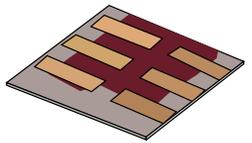


What is the optimum active layer thickness with the lower mobility value? If you wanted a really efficient solar cell what values of mobility and recombination rate would you use?

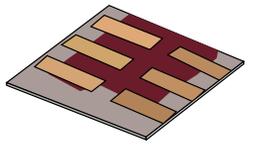


- Motivation – why learn this?
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- Charge carrier mobility
- The $\mu \cdot \tau$ product
- Parasitic resistances in a solar cell.
- Charge carrier traps.

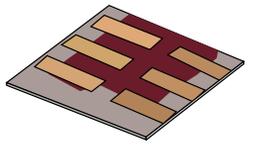
The $\mu \cdot \tau$ product



Question 10:

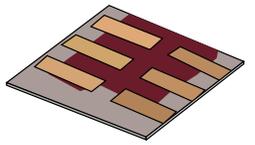


Make a fresh simulation. Set both the electron mobility to $1 \times 10^{-6} \text{ m}^2 / (\text{V s})$ and the hole mobility to $1 \times 10^{-5} \text{ m}^2 / (\text{V s})$. Then calculate the value of $\tau * \mu$, for your device. Show your working in your report.



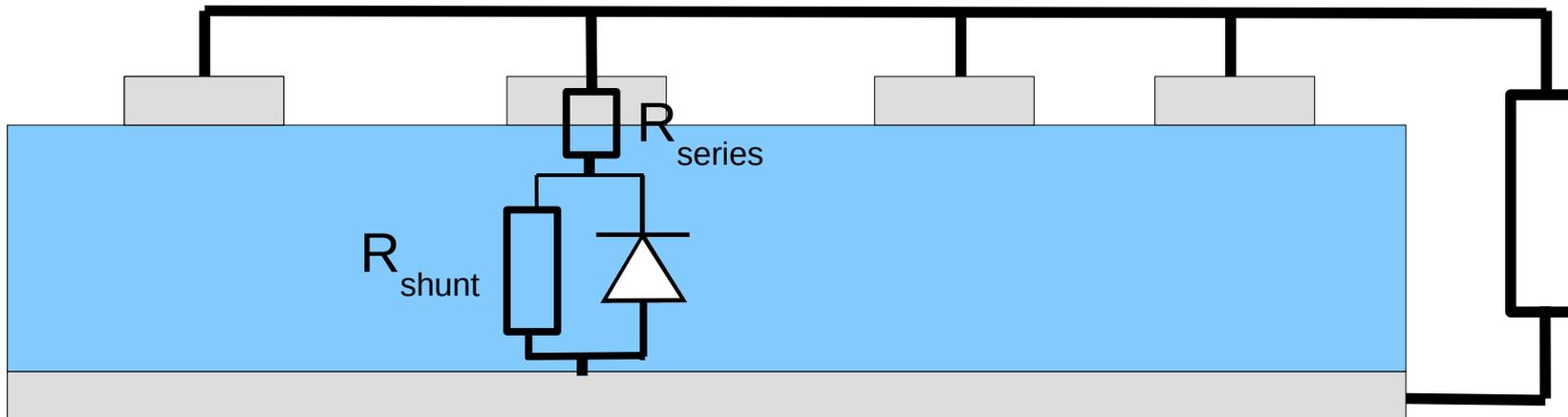
- Motivation – why learn this?
- The basic structure of 3rd generation solar cells.
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- The solar spectrum and material choice
- Performing optical simulaions
- Recombination
- Charge carrier mobility
- The $\mu \cdot \tau$ product
- **Parasitic resistances in a solar cell.**

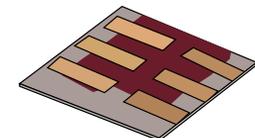
The ideal diode equation



• This equation is for an ideal diode with no resistance. However in a real solar cell there will be:

- Series resistance
- And shunt resistance





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

File Home Simulations Configure Databases Information About

Undo Run simulation Stop simulation Parameter scan Fit data Plot File Light intensity (Suns): 1.0 Help

Device structure Terminal Output

Layer editor
Contacts
Doping/Ions
Parasitic components
Electrical parameters
xz-size

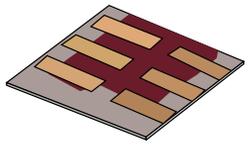
Edit parasitic components (<https://www.gpvdm.com>)

Parasitic components

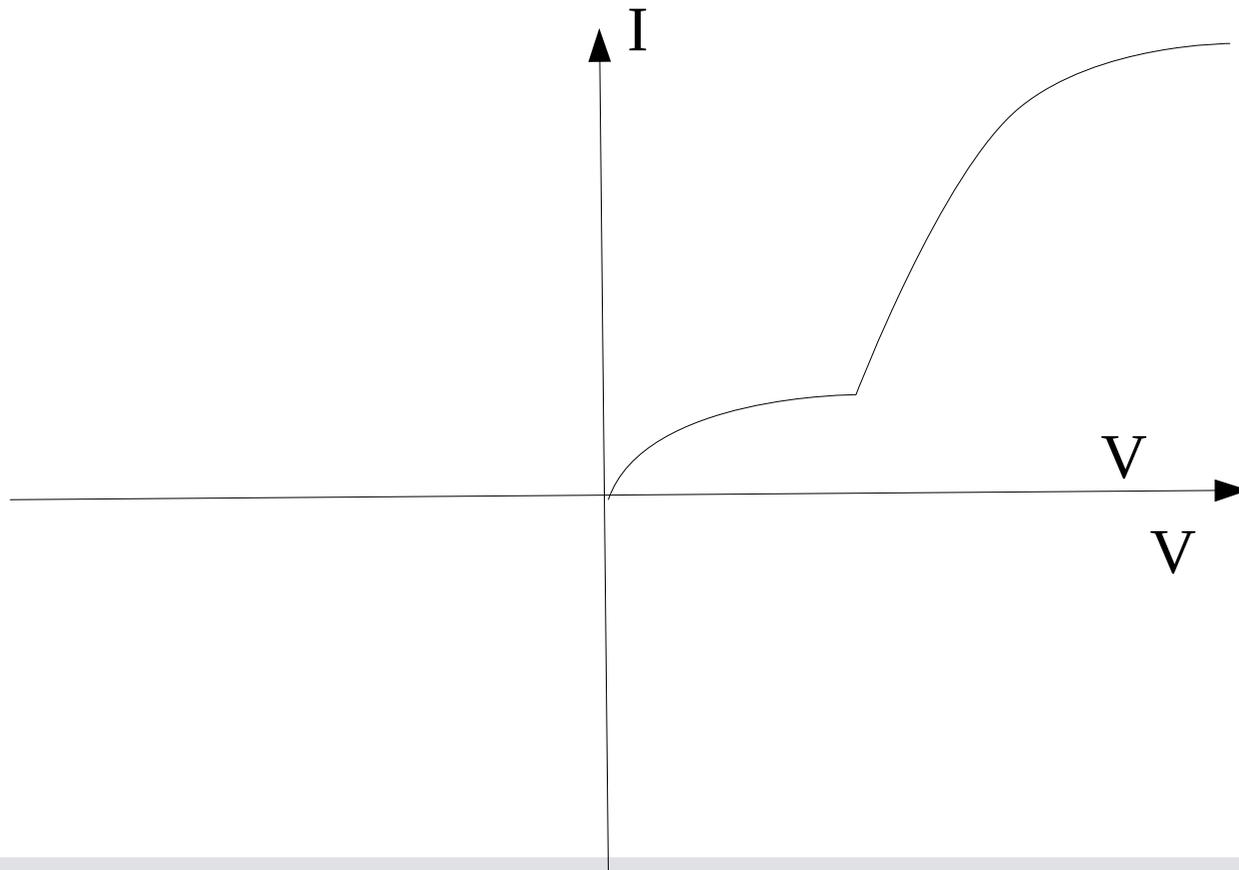
Series resistance	<input type="text" value="19.50"/>	Ohms
Shunt resistance	<input type="text" value="1.9e5"/>	Ohms
Other layers	<input type="text" value="0.0"/>	m

/home/rod/Desktop/hello

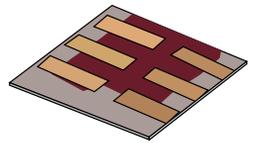
The dark JV curve



- Derive non-ideal diode equation

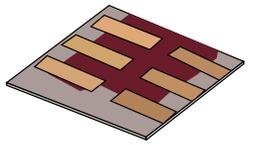


Question 11:

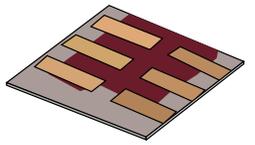


Make a fresh simulation, then run two JV curve simulations with a shunt resistance of $1 \times 10^6 \Omega$ (a very high value) one with a resistance of 100Ω . What happens to the solar cell efficiency as the shunt resistance is reduced? Plot a graph with shunt resistance on one axis, and device efficiency on the other (a minimum of four points) showing this effect. What is the reason for the trend on the graph?

Question 12:

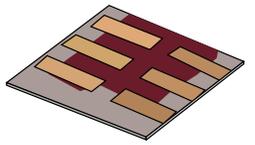


What values of series and shunt resistance, would produce the best possible solar cell? Enter these values into the device simulator and copy and paste the dark JV curve into your report.



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- Recombination
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- The $\mu \cdot \tau$ product
- Parasitic resistances in a solar cell.
- Charge carrier traps.

Question 13-14:



Only do these questions if you are interested. They are optional and you will get no marks for them.