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

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•Download all the software used in this talk from:

http://www.gpvdm.com/download.php

•Please report bugs to:

roderick.mackenzie@durham.ac.uk



•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)
    - The materials database
    - Importing n/k data into the model.
- Setting up device structures
- Running optical simulations using gpvdm.
- Light sources
- Output



•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?

https://www.Oghma-Nano.com

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



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

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

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.







#### https://www.Oghma-Nano.com

### Why perform optical simulations? Designing optical systems





Why perform optical simulations? Optical filter example:







•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





https://www.Oghma-Nano.com

### 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.





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Help



•We now need some data to fill it.



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)

Optical spectrum editor (https://www.gpvdm.com) new_spectra	_ = ×	Import data (https://www.gpvdm.com)
File From Lisert reference File information Absorption Basic	With the second	Load/Import         Import         Open data         Import         Title:         Wavelength - Intensity         x-label:         Wavelength         x-column:         0 \$\$ x units:         Wavelength (um)
Once opened the import window will appear with the data in it.		y-label:       Intensity       y-column: <ul> <li>y units:</li> <li>Intensity (um^{-{-1}}.Wm^{-{-2}})</li> <li>invert</li> </ul> The file to import:       The imported file. the numbers should now be in SI units:         280.0       2.5361E-26         280.1       0.0917Fe-24         281.0       6.1253E-24         281.5       2.7479E-22         282.0       2.8346E-21         283.0       6.7646E-20         283.0       6.7646E-20         283.5       1.4614E-19         284.0       4.9838E-18         284.0       4.9838E-18         285.5       6.4424E-16         285.5       6.4424E-16         285.6       1.8458E-14         286.0       2.85000e-04         287.0       2.845000e-04         287.0       2.84511         288.0       2.86500e-04         288.0       2.86500e-04         288.0       2.8651E-12         288.0       2.8061E-12         288.0       2.8061E-12         288.0       2.8061E-12         288.0       2.8061E-12         288.0       2.8061E-12         288.0       2.8061E-12

### 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

#### https://www.Oghma-Nano.com



•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 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.











•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 also governs how much light is reflected/transmitted at an interface:

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

T=1-R



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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.





•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<sup>-1</sup>, in this case as the model works only in SI, m<sup>-1</sup>.





### 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  $\overline{n} = n + j \kappa = n + j \frac{\lambda \alpha}{4 \pi}$

•The relationship between alpha and k is given as  $\alpha = \frac{4 \pi \kappa}{\lambda}$ 

•The model takes **alpha** (m<sup>-1</sup>) 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





# The materials database: n/alpha





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

### The materials database: Other parameters



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Absorption Ref	ractive index	Basic	Electrical parameters	Thermal parameters	Life cycle		
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Absorption Refractive in	dex Basic Electrical parameters	Thermal parameters	Life cycle	
Thermal conductivity	1.0			W m <sup>-1</sup> C <sup>-1</sup>
Electron relaxation time	1e-8			s
Hole relaxation time	1e-9			s
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Material editor (https://www.gpvdm.com) PMMA

•Other tabs show other basic material parameters



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### Importing n/k data into the model.

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### Making a new material





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....

n.csv (~/.ca	che/.fr-1	MXDBi) - Pluma		^ _ O X
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k.csv × n.csv ×				
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2 305.79 1.9154				
<b>3</b> 316.66 1.90433				
4 323.66 1.88767				
<b>5</b> 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				
<b>13</b> 377.23 1.81841				
14 395.86 1.81574				
<b>15</b> 398.18 1.81593				
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https://www.Oghma-Nano.com

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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					
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### Let's import k.csv



,	М	aterial editor (https://www.gpv	dm.com) new_material		^ _ U X
File	f(x) From Refere	) \$/W •3. (	Click		
from file Absorption	Equation information	Basic Electrical parameters	Thermal parameters	Life cycle	нер

•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.



P Import data (http	s://www.gpvdm.com)	*
Load/Import Plot		
Open data Import file data Title: Wavelength - Wavelength x-label: Wavelength	x-column: 0 – + x units Wavelength (nm)	•Set these to the units use
y-label: Wavelength The file to import:	y-column: 1 - + y units Wavelength (nm) The imported file, the numbers should now be in SI units	in the RAW
<pre>#opvdm #title Refractive index #type xy #x_mul 1e9 #y_mul 1.000000 #x_label Wavelength #y_label Refractive index #x_units nm #y_units au #logscale_x 0 #logscale_y 0 #section_one Materials #section_two Refractive index 3e=07 1.37356 3.02e=07 1.36947 3.04e=07 1.36536 3.06e=07 1.36122</pre>	<ul> <li>#gpvdm</li> <li>#title Wavelength - Wavelength</li> <li>#type xy</li> <li>#x_mul 100000000.0</li> <li>#y_mul 100000000.0</li> <li>#z_mul 1.0</li> <li>#data_mul 1.0</li> <li>#x_label Wavelength</li> <li>#y_label</li> <li>#z_tabel Wavelength</li> <li>#x_units nm</li> <li>#y_units</li> <li>#z_units</li> <li>#data_units nm</li> <li>#logy False</li> <li>#logy False</li> </ul>	to SI, ported

•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..

	Import data (https://www.	.gpvdm.com)						↑ □
Load/Import Plot								
Open data file								Hel
Title: Wavelength - Wavelength								
x-label: Wavelength		x-column:	0		+	x units:	Wavelength (nm)	~
y-label: Wavelength		y-column:	1		+	y units:	Wavelength (nm)	
The file to import:	Th	ne imported file, the r	numb	ers sh	ould	now be ir	n SI units	
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- •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.

https://www.Oghma-Nano.com

### 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



*	Ge	eneral-purpose Photovo	oltaic Device Model (https://www.	.gpvdm.	com)			^ _ D X				
File Simulation type	Simulation Editors Ele	ectrical Optical T	hermal Databases Inform	ation C	Questions? Contact: <u>roderic</u>	k.mackenzie@durham.a	<u>c.uk</u>	af About				
New Open Export simulation simion Zip	Run Parameter simulation scan	۲ Fit to ( experimental data Sir	Optical Machine Edit Hachine Learning Probes		If you publisl a paper, boo paper: Analyt space-charge- devices, Journ	h results generated w k or thesis you must of ical description of mixed limited conduction in sin al of Applied Physics, 120	ite ti ohmi gle-ca 3, 165	<b>/pdm in</b> <b>is</b> c and rrier Script 701, Editor				
Device structure Terminal	Output Tutorial	s/Documentation						Layer editor https://www.g	pvdm.com		^ _	
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Electrical					ZnO	3e-08		chemnitz/ZnO	other	• Yes •	Yes 👻	
parameters	_ 2	2.3368		(iling	PM6:Y6	2e-07		chemnitz/active_fresh	active layer	• Yes •	Yes 👻	
Emission	3.22	22.59.3		\$}{ <sup>2</sup>	MoOx	1e-08		chemnitz/MoOx	other	• Yes •	Yes 🔹	
×		4 2 2 2		<b>?•</b>	Ag	1e-07		chemnitz/Ag	contact	• Yes •	Yes 🔹	
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### The layer editor



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+	🛃 🏠 🚽							
Layer name	Thicknes (m)	Optical material	Layer type	Sol	ve optical roblem	Solve the proble	rmal m	ID
ІТО	1e-07	 chemnitz/ito	contact •	Yes	-	Yes	٣	
ZnO	3e-08	 chemnitz/ZnO	other	Yes	¥	Yes	÷	
PM6:Y6	2e-07	 chemnitz/active_fresh	active layer	Yes	٠	Yes	¥	
МоОх	1e-08	 chemnitz/MoOx	other	Yes	Ŧ	Yes	*	
Aa	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.

https://www.Oghma-Nano.com

### Homework task:



1		Layer editor https://www.gp	ovdm.com			^ _	
+	* *						
Layer name	Thicknes (m)	Optical material	Layer type		Solve optical problem	Solve thermal problem	10
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 🔹	
МоОх	1e-08	 chemnitz/MoOx	other	•	Yes 🔹	Yes 🔹	
Aa	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...





https://www.Oghma-Nano.com

### 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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	General-purpose Photovoltaic Device Model (https://www.gpvdm.com) 🔦 🗕 🗖
File Simu	lation type Simulation Editors Electrical Optical Thermal Databases Information Questions? Contact: roderick.mackenzie@durham.ac.uk al About
ght Lasers rces (fs)	Light intensity (Suns): 1.0 Ray tracing Optical FDTD detectors Simulation Boundary Conditions
vice structur	Terminal Output Tutorials/Documentation
PU 0	Max threads: 8
DI 1	Runing simulation
101	Isothermal heat model
PU 2	Power density of the optical spectra (no filter): 9.913312e+02 (9.913312e+02) Wm^{-2}
PU 3	Loading electrical dll load: materials
	Light: Building object pointer array
PU 4	Power density of the optical spectra (no filter): 9.913312e+02 (9.913312e+02) Wm^{-2}
PU 5	Solve optical slice at 476.150000 nm Solve optical slice at 482.800000 nm
DILE	Solve optical slice at 489.450000 nm
FU 0	Solve optical slice at 502.750000 nm
PU 7	Solve optical slice at 509.400000 nm Solve optical slice at 516.050000 nm
luster	Solve optical slice at 522.700000 nm
	Solve optical slice at 536.000000 nm
bs list	Solve optical slice at 542.650000 nm Solve optical slice at 549.300000 nm
	Solve optical slice at 555.950000 nm Solve optical slice at 562.600000 nm
	Solved 0 Equations
	Bytes, written 15447576 , read 430693
	Files, read 26 written 1919

#### •You will





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

https://www.Oghma-Nano.com

### Now go back and rerun the optical simulation





### Now go back and rerun the optical simulation







https://www.Oghma-Nano.com





•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)
    - The materials database
    - Importing n/k data into the model.
- Setting up device structures
- Running optical simulations using gpvdm
- Light sources
- Output

### Outputs: Optical snapshots







	Simulation information (www.gpvdm.com)	^ _ X
		$\bigcirc$
formation		
Photo current density	2.751856e+02	Am <sup>-2</sup>
Photo current	2.861925e-03	A

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

### Statistics: light\_stats.json



```
light stats.json (~/Desktop/asddasdasdadad) - Pluma
1
File Edit View Search Tools Documents Help
 🛃 🚞 Open 👻 🕹 Save 🛛 🔮 🛛 🥎 Undo 🎓
                                       🖌 🔄 🎁 🔍 😪
 light_stats.json
 1 {
       "layers" : 5,
 2
 3
       "laver0": {
 4
            "light frac photon generation": 1.103641e-01
 5
6
           },
       "layer1": {
 7
            "light frac photon generation": 8.650944e-03
 8
9
           },
       "layer2": {
10
            "light frac photon generation": 8.050166e-01
11
           },
12
       "layer3": {
13
            "light frac photon generation": 5.804029e-02
14
           },
15
16
       "layer4": {
            "light frac photon generation": 1.792815e-02
17
18
```

•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.