

### An introduction to simulating optoelectronic devices with *gpvdm*.

# Covering: Organic solar cells, perovskites solar cells, OFETs and OLEDs. Both time domain and steady state.

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#### **Overview**



•What is gpvdm/theoretical overview?

#### Installing gpvdm

- •Running simple simulations
  - •Your first gpvdm simulation
  - Changing electrical parameters
- •Optical simulations and the materials database
- •Perovskite solar cells and time domain simulations
- •OFET simulations and finite difference meshing.
- •Editing the device structure using the layer editor
- Meshing and dumping
- •OLEDs
- •Closing remarks



•gpvdm is a 1D/2D opto-electronic device model, which can be used to simulate *solar cells*, *LEDs*, *diodes*, *FETs* etc..

•Solves the **drift diffusion** equations using the **finite difference** method.

•Solves the optical equations, using **ray tracing** or **the transfer matrix method**.

•Cross platform/open source

Very quick theoretical overview.....

Gauss's Law

$$\nabla \epsilon_o \epsilon_r \cdot \nabla \phi = q \cdot (n-p)$$

Electron driving terms  $J_n = q \mu_e n \nabla E_c + q D_n \nabla n$  Hole driving terms  $J_p = q \mu_h p \nabla E_v - q D_p \nabla p$ 

Electron continuity  $\nabla \cdot \boldsymbol{J}_n = q \left( R_n + T_n + \frac{\partial n_{free}}{\partial t} \right)$ 

```
Hole continuity

\nabla \cdot \boldsymbol{J}_{p} = -q \left( \boldsymbol{R}_{p} + \boldsymbol{T}_{p} + \frac{\partial p_{free}}{\partial t} \right)
```

•In this respect gpvdm is similar to many other device models.

However to simulate disordered materials you need to include trapping/recombination via trap sates...



 This is often done using the following SRH equation, which assumes a *steady* state distribution of trapped charge carries in the trap states.

•This form of the SRH equation is therefore *not suitable for time domain* simulations where trapping/recombination via trap states dominate charge dynamics. As the charge carriers can not go out of equilibrium

# We therefore need to solve for the charge density of each trap state explicitly.



•We split energy space up into energy slices.

•And use the SRH equations but don't assume steady state, so solve the SRH equations explicitly in time domain.

•Each trap state gets its own rate <sup>L</sup> equation:

 $r_1$ 

$$\boxed{\frac{\partial n}{\partial t} = r_1 - r_2 - r_3 + r_4}$$

Process
electron capture
alactron amissia

electron emission	$r_2$
hole capture	$r_3$
hole emission	$r_4$



•Recombination can be calculated as:

Free carrier recombination



Detailed balance is maintained.

•Other models do not do this....  $_{6}$ 

This enables us to know where the charge carriers are in position/energy space.





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•The easiest way (*and recommended way*) to use gpvdm is to download gpvdm for Windows (https://www.gpvdm.com/ download.php), double click on the installer, and follow the instructions. I keep this version up-to-date.

•Alternatively If you are on Linux, you can compile from source. You can find instructions on how to do this here:

•https://www.gpvdm.com/code.php

•On Linux, I highly recommend using the *./build* as it will take care of a lot of the hard work for you.

gpvdm bu	ild system:		
(pa (in (ab (ex	Ickages) Instal stall) Instal pout) About tit) Exit	<b>ll deb/rpm depende</b> ll/Remove gpvdm	ncies

If you don't get a nice 3D interface it means your graphics drivers for you computer are not configured.



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### Your first gpvdm simulation



#### • Click on New simulation, in the file menu.



#### •Save it somewhere but *not* in the install directory.

### You should get this window.





#### **Click the play button**

#### The core solver will be run on CPU 0



*			Gen	eral-purpose I	photovolta	aic Device Model (	https://www	.gpvdm.com)				↑ _ □ ×
File	Home	Simulations	Configure	Databases	Informat	tion					llh.	About
<b>\$</b>	•		<b>A</b>	× Line	I mail	du	Light inten	sity (Suns):				
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evice s	tructur	Terminal	Output									
CPU 0		Voc = Voltag	6.022378e-0 e=0.620000	01 0.624972	) Curre	ent = 2.51698	0e-01 mA	(4.249316e+	01 A/m^2)	1.025101e-13		
CPU 1		Voltag Voltag	e=0.640000 e=0.660000	(0.653038	) Curre ) Curre	ent = 6.65244 ent = 1.25100	6e-01 mA 0e+00 mA	(1.114346e+ (2.090772e+	·02 A/m^2) ·02 A/m^2)	7.776147e-14 5.572298e-14		
CPU 2		Voltag	e=0.700000 e=0.720000	(0.720333) (0.761928) (0.810684)	) Curre ) Curre ) Curre	ent = 2.06479 ent = 3.17210 ent = 4.64669	3e+00 mA 7e+00 mA	(3.44/25/e+ (5.292941e+ (7.750745e+	·02 Α/m·2) ·02 Α/m^2) ·02 Δ/m^2)	2.599258e-14 1.683624e-14		
CPU 3		Voltag Voltag	e=0.740000 e=0.760000	(0.868162	) Curre ) Curre ) Curre	ent = 6.56851 ent = 9.02125	8e+00 mA 4e+00 mA	(1.095393e+ (1.504196e+	·03 A/m^2) ·03 A/m^2)	1.091178e-14 7.069920e-15		
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/home/rod	l/Desktop/nev	w_simulation										

•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.





#### The snapshots window, this is used to show changes in the device as a function of voltage and time.





### Using the snapshots window





•Click play and the simulation will iterate through each voltage step. If you were doing a time domain simulation it would do the same.

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# Editing the electrical parameters of a material





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

### This is the electrical parameter window



?	Electrical parameter	editor (https://www.gpvd	im.com) 🕆 _ 🗆
			<b>(</b>
	Electrical parameters		Luminescence
ĺ	DoS distribution	exponential	▼ au
	Hole trap density	3.8e26 1.45e25	m <sup>-3</sup> eV <sup>-1</sup>
	Electron tail slope Hole tail slope	40e-3 60e-3	eV eV
DoS of P3HT:PCBM	Electron mobility Hole mobility	2.48e-7 2.48e-7	m <sup>2</sup> V <sup>-1</sup> s <sup>-1</sup> m <sup>2</sup> V <sup>-1</sup> s <sup>-1</sup>
	Relative permittivity	3.8	au
	Free electron to Trapped electron	2.5e-20	m <sup>-2</sup>
	Trapped electron to Free hole Trapped hole to Free electron	1.32e-22 4.67e-26	m <sup>-2</sup>
	Free hole to Trapped hole	4.86e-22	m <sup>-2</sup>

•Here you can edit the electrical parameters of the electrically active layers. Each *electrically active* layer will get a new tab here. 20

### Types of layers in gpvdm:



Layer type	Description	Electrical Equations solved	Optical Equations solved.
active	The electrical model is solved over these layers, each layer gets it's own set of electrical parameters.	Yes	Yes
other	No electrical equations are solved in these layers.	No	Yes
contact	These layers are used to define the electrical contacts, no electrical equations are solved in the layers.	No	Yes

•The layer type can be changed using the layer editor.... more on this later.

# Editing an electrical parameter...the trap density....

9	Electrical parameter editor (https://www.gpvdm.com)						
				1			
	Electrical parameters		Luminescence				
	DoS distribution	exponential	▼ au				
	Electron trap density	3.8e26	m <sup>-3</sup> eV <sup>-1</sup>				
	Hole trap density	1.45e25	m <sup>-3</sup> eV <sup>-1</sup>				
	Electron tail slope	40e-3	eV				
	Hole tail slope	60e-3	eV				
	Electron mobility	2.48e-7	m <sup>2</sup> V <sup>-1</sup> s <sup>-1</sup>				
DoS of P3HT:PCBM	Hole mobility	2.48e-7	m <sup>2</sup> V <sup>-1</sup> s <sup>-1</sup>				
	Relative permittivity	3.8	au				
	Number of traps	20	bands				
	Free electron to Trapped electron	2.5e-20	m <sup>-2</sup>				
	Trapped electron to Free hole	1.32e-22	m <sup>-2</sup>				
	Trapped hole to Free electron	4.67e-26	m <sup>-2</sup>				
	Free hole to Trapped hole	4.86e-22	m <sup>-2</sup>				
		1 20 27					

a) Make the density of trap state symetric at  $1 \times 10^{24}$  m<sup>-3,</sup> and rerun the simulation.

b) Now re-plot the JV curve (**jv.dat**), also find the (**sim\_info.dat)** file, double click on it and find the power conversion efficiency.





# You should have results which look a bit like this:



## Varying a parameter many times using the Parameter Scan, window.





•Often we want to change a simulation parameter several times to understand how a parameter affects a device.

•To do this, use the *Parameter Scan* tool

/home/rod/Desktop/new\_simulation

#### •Click on the parameter scan tool

#### The parameter scan window



Scan Simulations		Param	neter scan - gpvdm		↑ _ □ × About	•Click on the +
Run scan Stop Plot	et view of the second s	Notes	▶ 👚 ▶			to add a new line to the
scanl	+ -	🛃 🏠 🖻				scan.
	File	Token	Parameter to change	Values	Opperatio	

### A new line should appear...



À		Parameter scan - gpvdm		↑ _ □ ×
Scan Simulations				About
	a k	¢ 🕨 🚍		Select simulation parameter (https://www.gpvdm.com) + = • ×
Run Stop Plot	Time domain Notes	🤹 🗭		<ul> <li>Simulation parameters</li> </ul>
scan1	<b>_</b> 🎍 🛦			light
	<b>T – X –</b>			math
	File Token	Parameter to change Select parameter	Value	• fit
				- dump
				parasitic
				- epitaxy
				start
				-P3HT:PCBM
				✓ dos
				-DoS distribution
				Electron trap density
	<u>.</u>			Hole trap density
			++	Electron tail slope
CIICK ON T	ie icor	i, expand the	tree as	SNOWN, Hole tail slope
elect 'Hole	e trap den	sity' and click	KOK.	
	•			OK ZQncel

### The parameter scan window...



4			Parameter scan - gpvdm		↑ _ □ X			
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Run Stop Plot	Time domain plot	Notes	✿ ▶ 😑 ∡ ▶					
scanl	+ -	*						
	File	Token	Parameter to change	Values	Opperation			
	dos0.inp	#Ntraph	pitaxy/P3HT:PCBM/dos/Hole trap density	0.0 0.0	scan 🔻			
This shows	the			Enter the	ese (1e24	1e25		
file/section	of the	file		1e26) va	1e26) values in here.			
which will be edited			They are the trap					
(generated			densities we are goin					
(generated	11. A							
automatica	lly).			to scan c	over (units	s are		
				m <sup>-3</sup> eV <sup>-1</sup> )				

# But we want to simulate a symmetric device (where Ntraph=Ntrape)...



<b>*</b>					Parameter scan - gpvdm	↑ _ □ X
S	Scan	Simulations	5			About
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scan1			+ -	*		
			File	Token	Parameter to change Values Opperation	
			dos0.inp	#Ntraph	epitaxy/P3HT:PCBM/dos/Hole trap density 1e24 1e25 1e26 scan 🗸	
			dos0.inp	#Ntrape	epitaxy/P3HT:PCBM/dos/Electron trap density 0.0 0.0 scan 💌	

So using the '+' button add another row and then using the '...' buttons make it look like the above..

# But we want to simulate a symmetric device (where Ntraph=Ntrape)...



4			Parameter scan - gpvdm			↑ - □ X
Scan Simulations						About
Run Stop Plot	e x Time domain plot	Notes	≱ ▶ 😑 { ▶			
scanl	+ -	۰	2			
	File	Token	Parameter to change	Values	Opperation	
	dos0.inp	#Ntraph	epitaxy/P3HT:PCBM/dos/Hole trap density	1e24 1e25 1e26	scan	•
	dos0.inp	#Ntrape	epitaxy/P3HT:PCBM/dos/Electron trap density	mirror	epitaxy/P3HT:PCBM/dos/Hole trap density	•

- •Then from this menu select, 'epitaxy/P3HT:PCBM/dos/Hole trap density'.
- •The words 'mirror' will appear in the values column. This means that the values for Electron trap density will follow that of the Hole trap density.
- •Now click 'Run scan'...., it will run the simulations in parallel across all cores of your CPU.

### Plotting the results.





•Click plot, and plot the file scan1/1e24/jv.dat.

•All jv.dat curves will be plotted from the simulation tree.

### A final note on the electrical parameter window...

1.0

Light intensity (Suns):

Ŧ

↑ \_ □ ×

About

Help

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

Examine results

in time domain

Information

Plot

File

•We can assign a photon generation efficiency to each ecombinatio n process, so we an get a oredicted PL/EL spectrum...

are in energy space across the device.

https://www.gpvdm.com

×

File

Undo

Home

Run simulation

Device structure Terminal

Simulations

Stop

simulation

Output

Configure

Paramete

scan

Databases

Fit

data

				•
Contacts	Electrical parameters		Luminescence	
Doping/ lons Parasitic components Electrical parameters	Luminescence of perovskite Luminescence of zno	Turn on luminescence n <sub>free</sub> to p <sub>free</sub> photon generation efficiency n <sub>free</sub> to n <sub>trap</sub> photon generation efficiency n <sub>trap</sub> to p <sub>free</sub> photon generation efficiency p <sub>trap</sub> to n <sub>free</sub> photon generation efficiency p <sub>free</sub> to p <sub>trap</sub> photon generation efficiency	OFF 1.0 0.0 0.0 0.0 0.0	True/False 0.0-1.0 0.0-1.0 0.0-1.0 0.0-1.0 0.0-1.0
e/rod/Desktop/new_si	Luminescence of pedotpss			



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•gpvdm will always perform an optical simulation if the light intensity is not set to zero, but it will not dump all the information it calculates to disk as this is too slow.

•Therefore there is an optical simulation window to explore the optical performance of the device in more detail.....

### Running the full optical simulation...





### Looking at the photon distribution.





•Normally the model shows the sum of all optical modes, but you can select which mode you would like to look at. Using the above menu.

## Plot the photon density as a function of wavelength/position




### And also reflected light from the cell





### You can also vary the light source.



•Try rerunning the simulation with the xenon lamp.

#### •How does the Photon distribution change?

https://www.gpvdm.com

## There is a database of light sources, you can edit it, it is far from exhaustive....





### There is also a materials database..





### The materials database







for my simulaions.

### Getting (lots) more materials



•There is also data from https://www.pvlighthouse.com.au (Keith McIntosh) and refractiveindex.info (Mikhail N. Polyanskiy).

•I've included this as an add on pack.

\$					Ge	eneral-	purpose Phot	tovoltaic De	evice Model (https://www.g		
	File	Home	Simulations	Configure	Datab	ases	Informatior	n			
Ma da	() aterials tabase	Optical database	Download ex materials	ttra							
J					Down	load up	odates (https	s://www.gp	/dm.com)		↑ _ □ ×
D	ownload	l updates									
		File		Description		5	Size	md5	status	Version	
pvl	ighthous	e.com.au.zi	p Material	ls database u	pdate	509.3	KiB 012	2f320a6b	update-avaliable	5.0	
ref	ractivein	dex.info.zip	Materia	ls database u	pdate	46.4M	liB c90	4bc2c37	update-avaliable	5.0	
Do	ne										

#### https://www.gpvdm.com



•If you want to add new material, just copy the a directory containing an old material to a new one i.e.:

cp c:\gpvdm\materials\polymers\p3ht c:\gpvdm\materials\polymers\new\_material -rf

•Each material contains about 10 files, the only ones you really need to care about are *alpha.omat*, and *n.omat* 

[rod@rodlinu	uxbo	ox p3	3ht]\$	\$ls·	all			
total 60								
drwxr-xr-x.	2	rod	rod	4096	Feb	28	13:05	
drwxrwxr-x.	11	rod	rod	4096	0ct	16	21:37	
- rw-rr	1	rod	rod	6232	0ct	16	21:37	alpha.omat
- rw	1	rod	rod	308	0ct	16	21:37	alpha.ref
- rw- rw- r	1	rod	rod	4856	0ct	16	21:37	cost.xlsx
- rw	1	rod	rod	714	0ct	16	21:37	dos.inp
- rw-rr	1	rod	rod	144	0ct	16	21:37	fit.inp
-rw-rr	1	rod	rod	186	0ct	16	21:37	mat.inp
- rw-rr	1	rod	rod	6256	0ct	16	21:37	n.omat
- rw-rr	1	rod	rod	475	0ct	16	21:37	n.oplot
- rw	1	rod	rod	308	0ct	16	21:37	n.ref
- rw	1	rod	rod	100	0ct	16	21:37	pl.inp
[rod@rodlinu	nxpo	ox p3	3ht]s	5				

•\**.ref* files tell you where the data in the file came from

•*dos.inp/pl.inp* files contain the the default electrical parameters for, realistically you are going to have to tune these through fitting anyway... so ignore the files during materials creation.<sub>43</sub>

### 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<sup>-1</sup>) Replace the data with your new data.

### Making a new material the easy way...





https://www.gpvdm.com

Let's get hold of some data to import..., usually you would get this from experiment.

### •Download this zip archive https://gpvdm.com/demo/materials.zip and UNZIP it.

#### •You should have two files....

🕎 k.	dat (~	/t/gpvd	lm5.0/m	aterials	/blend	ls/ptb7p	c70bn	↑ _ □ ×
File	Edit	View	Search	Tools	Docu	uments	Help	
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3	25	2.94	ŀ 0.	615	23			
4	254	4.54	ŀ0.	619	51			
5	25	6.13	80.	617	9			
6	25	7.73	80.	613	11			
7	259	9.32	20.	608	45			
8	326	9.92	20.	604	82			
g	262	2.51	. 0.	597	22			
10	264	4.11	. 0.	593	48			
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13	268	8.89	) ().	585	19			
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🍄 🔄 Open	▼ 🛃 Save	8	•
🖹 k.dat 🗶	🗋 n.dat  🛛		
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2 252.94	1.73988		
3 254.54	1.74155		
4 256.13	1.74679		
5 257.73	1.76971		
6 259.32	1.77795		
7 260.92	1.79008		
8262.51	1.80517		
9264.11	1.80383		
10 265.7	1.81409		
11 267.3	1.83196		
12 268.89	1.84133		
13 270.49	1.84207		
Plain Text 👻	Tab Width: 4 🔻	Ln 1, Col 1	INS

### Let's import k.dat





•Note from the previous slide the data is not in SI, so we can't import is straight into gpvdm.

### •gpvdm can only deal with SI data.

•Select k.dat to import..., from where ever you extracted n/k.dat

### The import window used to convert data to SI

			1	
Minimport data (https://w	vww.gpvdm.com)	$\uparrow$ $\Box$ $\times$		
Load/Import Plot				
Open data Import file data		Help		
Title: Wavelength - Wavelength			,	•Set these to
5 5				
x-label: Wavelength	x-column: 0 - + x units Wavelength (nm)	-		the units of
				4   <b> </b>
y-label: Wavelength	y-column: 1 — + y units Wavelength (nm)	•		the <b>input file</b> .
				-
The file to import:	The imported file, the numbers should now be in SI units			
<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 1.36132</pre>	<ul> <li>#gpvdm</li> <li>#title Wavelength - Wavelength</li> <li>#type xy</li> <li>#x_mul 1000000000.0</li> <li>#y_mul 1000000000.0</li> <li>#z_mul 1.0</li> <li>#data_mul 1.0</li> <li>#data_mul 1.0</li> <li>#data_label Wavelength</li> <li>#y_Label</li> <li>#z_label</li> <li>#data_label Wavelength</li> <li>#x_units mn</li> <li>#y_units</li> <li>#z_units</li> <li>#data_units nm</li> <li>#logy False</li> <li>Home/rgd//(npvdm5 0/materials/polymers/my, new, material/alpha.omat</li> </ul>	i nto ie		

#### •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

https://www.gpvdm.com

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



Import of	data (https://www.gpvdm.com)	↑ □ >
Load/Import Plot		
Open data		(1) Help
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:	The imported file, the numbers should now be in SI units	
<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 1.36536 3.04e-07 1.36536 3.06e-07 1.36122</pre>	<pre>#gpvdm #title Wavelength - Wavelength #type xy #x_mul 100000000.0 #y_mul 100000000.0 #z_mul 1.0 #data_mul 1.0 #x_label Wavelength #y_label #z_label #data_label Wavelength #x_units nm #yy_units #z_units #data_units nm #logy False #logy False #logy False</pre>	

### **Overview**



•What is gpvdm/theoretical overview?

#### Installing gpvdm

- •Running simple simulations
  - •Your first gpvdm simulation
  - Changing electrical parameters
- •Optical simulations and the materials database

#### •Perovskite solar cells and time domain simulations

- •OFET simulations and finite difference meshing.
- •Editing the device structure using the layer editor
- Meshing and dumping
- •OLEDs

### Make a new perovskite simulation





# Perovskite solar cells/time domain simulations.



•A JV curve on a Perovskite device is really a time domain simulation due to the movement of ions.

•We will therefore use Perovskite simulations to learn about time domain simulation in gpvdm.

### The simulation mode menu



•This menu is used to select the simulation mode.

- •The simulations we have performed until now were in **jv** mode, this is a purely steady-state simulation.
- •Set the value to *jv\_perovskite*, this is a time domain simulation including perovskite ions.

https://www.gpvdm.com

# You can edit the density of ions using the ion/doping editor.







•Run the simulation (blue play button) then open the file *jv.dat* 



Notice it's a jv curve but it changes as a function of time
Plot *pulse\_v.dat* and *pulse\_j.dat*, these plot voltage and current against time.

### pulse\_v.dat, pulse\_j.dat Current/voltage against time.....





•Notice the saw wave of the time domain JV experiment and the resulting current transient.





### Editing time domain simulations





### Edit the applied voltage/light intensity





### Making new simulations



•Use these tools to create new transient simulations

•These new simulations will appear in the *simulation menu* in the main interface.



## You can change the external circuit conditions using the *Circuit* tab





•You could use this to do things like TPC/TPV, where you need short circuit/open circuit conditions.

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### Make a new OFET simulation





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

https://www.gpvdm.com

### This will create a new 2D simulation





•Notice the contacts which are 2D structures.

### Adding another electrically active layer



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





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

### Let's now look at the contacts





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

•		I	Edit contacts	(www.gpvdm	.com)		↑ _ □ >
-							8
Name	Top/Botto	m Ac	tive contact	Start	Width	Depth	Voltage
top	top	▼ fals	e 🔻	0.0	0.001	0.0	-1.0
top2	top	▼ fals	e 🔻	0.002	0.001	0.0	0.0
bottom	bottom	▼ tru∉	e 🔻	0.0	0.0034641	5e-08	0.0



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



Edit contacts (www.gpvdm.com)								
<b>-</b>	- ↓						훻 🚹	
Name	Top/Botto	om Active cor	ntact	Start	Width	Depth	Voltage	
	(		_	0.0	0.001	0.0	1.0	
top	top	<ul> <li>ralse</li> </ul>	•	0.0	0.001	0.0	-1.0	
top top2	top top	<ul> <li>▼ false</li> </ul>	•	0.002	0.001	0.0	0.0	





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



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



			Edit contacts	(www.govdm	.com)		↑ _
÷.							*
Name	Top/Bot	tom	Active contact	Start	Width	Depth	Voltage
top	top	•	false 🔻	0.0	0.001	0.0	-1.0
top2	top	-	false 🔻	0.002	0.001	0.0	0.0
bottom	bottom	-	true 🔻	0.0	0.0034641	5e-08	0.0





		Edit contacts	(www.gpvdm.	com)		↑ _ □
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Name	Top/Bottom	Active contact	Start	Width	Depth	Voltage
top	top 💌	false 💌	0.0	0.001	0.0	-1.0
			0.000	0.001	0.0	0.0
top2	top 🔻	false 🔻	0.002	0.001	0.0	0.0



### The voltage applied to the contact.



	Top/Bot	tom	Active co	ntact	Start	Width	Depth	Voltage
top	top	•	false	•	0.0	0.001	0.0	-1.0
top2	top	•	false	•	0.002	0.001	0.0	0.0
bottom	bottom	-	true	-	0.0	0.0034641	5e-08	0.0

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


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



#### •Then let's look at the output.



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





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

Information

Plot





File

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Simulations

Stop

Databases

Fit

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# Meshing and dumping





# Now you should be able to see the electrical finite difference mesh





•*On* a mesh point click '*Set/Unset energy slice dump*' this will turn on dumping of the trap population at a given mesh point.

•Click '**Set/Unset verbose electrical solver dumping**', this will *turn off* the outputting files like Ec.dat, Ev.dat, Fn.dat etc...

•Click on another mesh point and select '**Set/Unset dumping 1D slice**', this will turn on the dumping of the trap population across the device.

# Your window should now look like this..





•We have turned off dumping of Ec.dat, Ev.dat etc...., and are going to be dumping the distribution of trap states along the blue line, and at the green point.





#### •From the *output tab* open the snapshot window.



•Then make sure npt\_map.dat is selected this is a slice through the device in position/energy space. Along the blue dots below.



# Select energy\_slice\_nt.dat, to show the trap population at a given point.





•You can step through the simulation as a function of time/voltage.



# You can turn on/off other output files through configure $\rightarrow$ configure $\rightarrow$ output files



9	Configure (https://www.gpvdm.com)	↑ _ □ >
Output files Detailed dump control		<b>I</b> Help
Plot bands etc	OFF	True/Fals
Dump from newton solver	OFF	True/Fals
Dump dynamic	OFF	True/Fals
Dump fx domain data	OFF	True/Fals
Time of pause	0.0	s
Dump optical information	OFF	True/Fals
Dump optics verbose	OFF	True/Fals
Print newton error	OFF	True/Fals
Print solver convergence		True/Fals
Write newton solver convergence to dis	Sk OFF	True/Fals
Print poisson solver convergence	OFF	True/Fals
Dump PL spectra	OFF	True/Fals
Dump zip files	OFF	True/Fal:

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- Simulation OLEDs with gpvdm

# **OLED** simulation





#### •This will setup an OLED simulation.

# You should get a window looking like this..

Senera Genera	al-purpose Photovoltaic Device Model (https://www.gpvdm.com)	↑ _ □ ×
File Home Simulations Configure Databases	Information	ما الآلي. About ال
Image: Stop simulation Image: Stop simulation Parameter scan Fit data   Device structure Terminal Output	Light intensity (Suns): Plot File	G Help
Layer editor		xy yz xz +
Contacts		ITO Contact
Doping/		HMTPD (HTL) (active) TAZ:Ir(ppv)3-BCP (EML) (active)
		Alq3 (ETL) (active)
Parasitic components		Al
Electrical parameters		
x xz-size		
/home/rod/Desktop/oled2		

### •Run the simulation...

# You will be able to see the rays emitted from the active layer.



### Hide the device





## In the output you will see two new files



•lj.dat and lv.dat.

•These are light intensity against voltage and current.

## Light emission.







### Where are the photons emitted?





### **Overview**



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- Closing remarks



•gpvdm can do quite a few other things like simulate PL/EL spectra, IS, IMPS, import FDTD data etc.. but I've either not had time to cover this in this tutorial or the features are not robust enough to release.

•gpvmd is a work in progress if you want a feature added it does not have let me know..... and please include me in your paper/collaboration ;). I am always after new experimental partners/collaborations



•Fitting complex data sets to experiment is a pain due to high CPU demand/number of parameters So I have built quite a lot of code to do the fitting on a cluster of 100 CPUs.

•I've released the code but it is a pain to use, SO: If you want to fit the model to data sets, I recommend you talk to me and see if I can do it for you.

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2	slave	node005	10.0.0.5	8	8	6 8	θ.	560000	Θ				4
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•Two immediate things I'm working on:

- •Ray tracing of complex surfaces
- •Better FDTD



