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.gpv	rdm.com) \hat{T} –	• ×
	Electrical parameters		Luminescence	
Í	DoS distribution	exponential	▼ au	
	Electron trap density Hole trap density	3.8e26 1.45e25	m ⁻³ eV ⁻¹ m ⁻³ eV ⁻¹	
	Electron tail slope	40e-3	eV	
	Hole tail slope	60e-3	eV	
DoS of P3HT:PCBM	Hole mobility	2.48e-7 2.48e-7	m ² V ⁻¹ 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	
		1 20 27		

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

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.gpvd	m.com)	- ×
				D
	Electrical parameters		Luminescence	
	DoS distribution	exponential	▼ au	
	Electron trap density	3.8e26	m ⁻³ eV ⁻¹	
	Hole trap density	1.45e25	m ⁻³ eV ⁻¹	
	Electron tail slope	40e-3	eV	
	Hole tail slope	60e-3	eV	
	Electron mobility	2.48e-7	m ² V ⁻¹ s ⁻¹	
DoS of P3HT:PCBM	Hole mobility	2.48e-7	m ² V ⁻¹ 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	
		1 20 27		

a) Make the density of trap state symetric at $1 \times 10^{24} \, \text{m}^{-3}$, 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		Pa	rameter scan - gpvdm		↑ _ □ ×	•Click on the +
Run Stop Plot	Time domain plot	Notes	⊧ ▶ 🚔 [▶			line to the
scan1	÷ —	👱 🛧				scan.
	File	Token	Parameter to change	Values	Opperatio	

A new line should appear...





The parameter scan window...



A			Parameter scan - gpvdm		↑ _ □ >	<
Scan Simulations	5				About	
Run Stop Plot	ٹ <mark>و</mark> Time domain plot	Notes	✿ ▶ 😑 ∡ ▶			-
scan1	÷	* *				
	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	alues in he	ere.
which will b	e edite	ed		They are	e the trap	
(generated				densities	s we are o	ioina
outomotion	ILA					
automatica	пу <i>)</i> .			to scan (over (units	s are
				m ⁻³ eV ⁻¹)		

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



4							Parameter scan - gpvdm				↑ _ □ X
	Sca	in g	Simulatio	ns							About
R	un :an	Stop	Plot	Time domain	Notes	¢⊧ ► <mark>{</mark> ┣►	2				
sca	anl			÷	🛨 🏦		Devenation to change	Veluer	0		
				dos0.inp	#Ntraph	epitaxy/P3	HT:PCBM/dos/Hole trap density	1e24 1e25 1e26	scan		
				dos0.inp	#Ntrape	epitaxy/P3	BHT: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			÷ _	- ×
Scan Simulations	s					A	bout
Run Stop Plot	₽ Time domain plot	Notes	≿ ▶ ≘ [▶				
scan1	÷	* *	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.



4	Parameter scan - gpvdm							
Scan Simulatio	ns					About		
Run Stop Plot	Time domain	Notes	¢ ▶ 😑 <mark>ፈ</mark> ▶					
scanl	. - +	*						
	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	-		
				300	Current density - Applied voltage			
				- 200 - me (-2-) - 100 - - 0 -				
				+				
				-0.2	0.0 0.2 0.4 Applied Voltage (Volts)	0.6		

- •Click plot, and plot the file scan1/1e24/jv.dat.
- •All jv.dat curves will be plotted from the simulation tree.

1 × 10²⁶

A final note on the electrical parameter window...



*	General-purpose Photov	oltaic Device Model (https://www.gpvdm.com)	↑ _ □ X	
File Home Sir	mulations Configure Databases	Information	ail About	
Undo Run simulation	Stop Parameter Fit simulation	Plot File in time domain Light intensity (Suns):	() Help	
Device structure Term	ninal Output	Electrical parameter editor (https:	://www.gpvdm.com)	↑ _ □ 3
Layer editor				•
	Electr	ical parameters	Luminescence	2
Doping/ lons Parasitic components Lelectrical parameters	Luminescence of perovskite Luminescence of zno	Turn on luminescence Image: Comparison of the second s	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
/home/rod/Desktop/new_si	Luminescence of pedotpss			

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

•We can only do this because we know where the carriers are in energy space across the device.