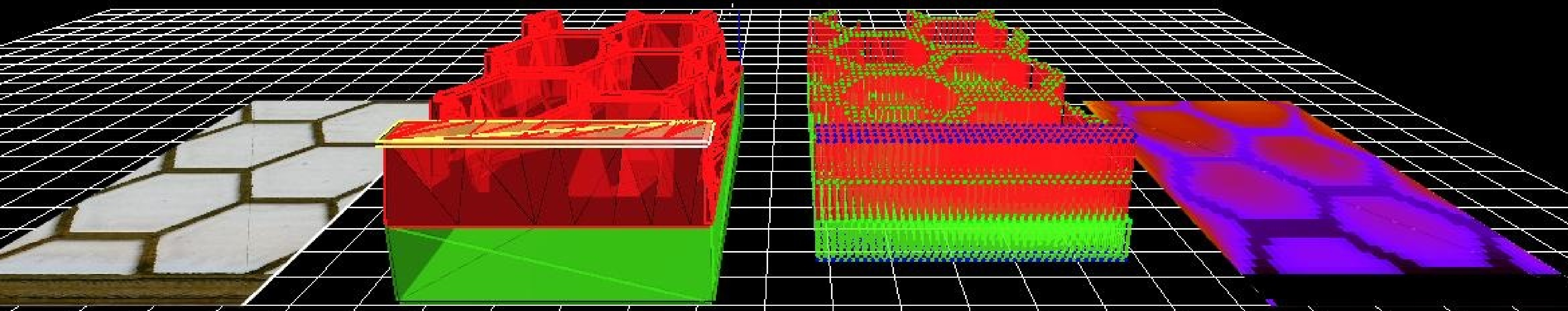
What is *OghmaNano?*

A tool for simulating: Organic solar cells, perovskites solar cells, OFETs and OLEDs. In time domain, steady state and frequency domain.



Dr. Roderick MacKenzie
roderick.mackenzie@oghma-nano.com
Autumn 2022

https://www.oghma-nano.com

Talk overview

- **History of OghmaNano**
- Overview of model
  - Electrical models
    - Drift diffusion
    - Circuit model
  - Optical models.
  - Exciton models
  - Simulation modes
  - Thermal models
  - Example simulation

History of OghmaNano

•The development of OghmaNano was started at **Imperial college in 2011** to simulate organic solar cells, since then it has been rewritten many times.

•**27/01/2012:** The model was named the Organic Photovoltaic Device Model or **opvdm** and released to the web.

• **17/01/2016:** Due to the rising popularity of perovskites the model was renamed the (general purpose photovoltaic device model) or **gpvdm**.

14/10/2022: The model was renamed **OghmaNano** to reflect the fact that the model can now simulate many classes of devices including transistors. (**Org**anic and **h**ybrid **Ma**terial **Nano** Simulation tool)

•Today the model can simulate **solar cells**, **sensors**, **OFETs**, **OLEDs**, and **many more** classes of devices.

Talk overview

- History
- **Overview of model**
    - Electrical models
        - Drift diffusion
        - Circuit model
    - Optical models.
    - Exciton models
    - Simulation modes
    - Thermal models
    - Example simulation

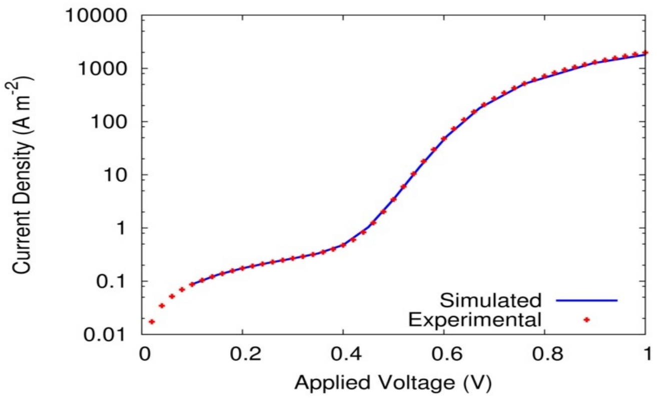
What is OghmaNano?

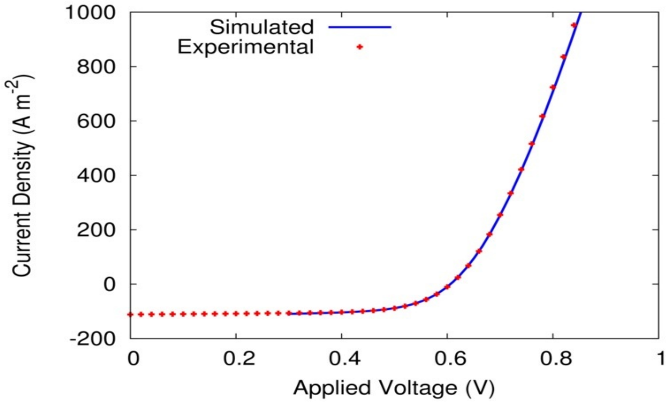
- OghmaNano is a 1D/2D/3D opto-electronic device model, which can be used to simulate ***solar cells***, ***OLEDs***, ***diodes***, ***FETs*** etc..
  - **Electrical models:** 1D/2D drift diffusion models and 1D/2D/3D equivalent circuit models
  - **Optical models:** Transfer matrix models in 1D/2D/3D, 3D ray tracing models, FDTD (beta).
  - **Exciton models:** Excitons, singlets, tripplets etc..
  - **PL/EL** models for emission
  - **Simulation modes:** Steady state, transient and FX-domain electrical models
  - **Thermal models:** Self heating

Talk overview

- History
- **Overview of model**
  - **Electrical models**
    - **Drift diffusion**
    - Circuit model
  - Optical models.
  - Exciton models
  - Simulation modes
  - Thermal models
  - Example simulation

Electrical simulation





- The most basic thing you can simulate when doing device simulation is the current voltage curves.

- Do simulate these you need to solve the drift diffusion equations.

Electrical simulations: Drift diffusion: Simulating charge transport

Gauss's Law

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

Electron driving terms

$$J_n = q \mu_e n \nabla E_c + q D_n \nabla n$$

Electron continuity

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

Hole driving terms

$$J_p = q \mu_h p \nabla E_v - q D_p \nabla p$$

Hole continuity

$$\nabla \cdot \boldsymbol{J}_p = -q \left(R_p + T_p + \frac{\partial p_{free}}{\partial t} \right)$$

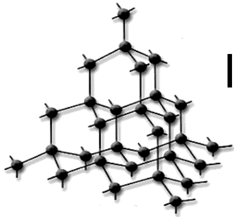
•Fermi-dirac and and Maxwell-Boltzmann statistics

•Solved in 1D/2D

•In this respect OgmaNano is similar to many other device models, where it differs is in the inclusion of trap states..

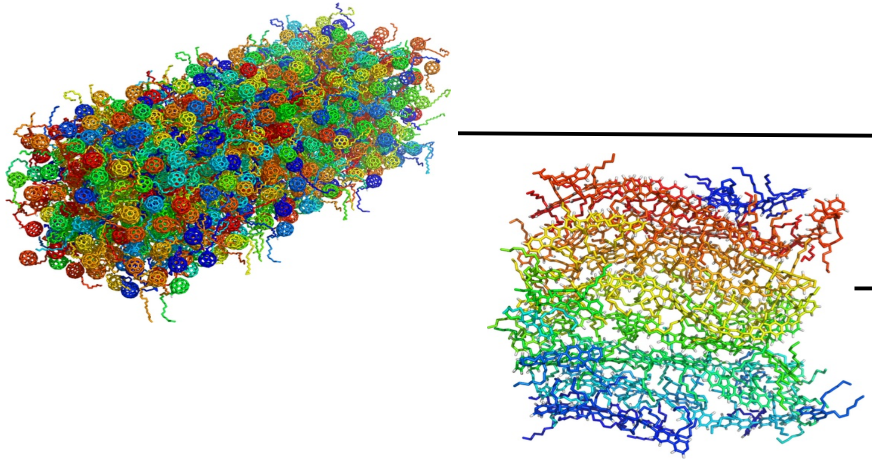
MacKenzie , Shuttle, Adv. Energy Mater. 2012, 2 (6), 662-669

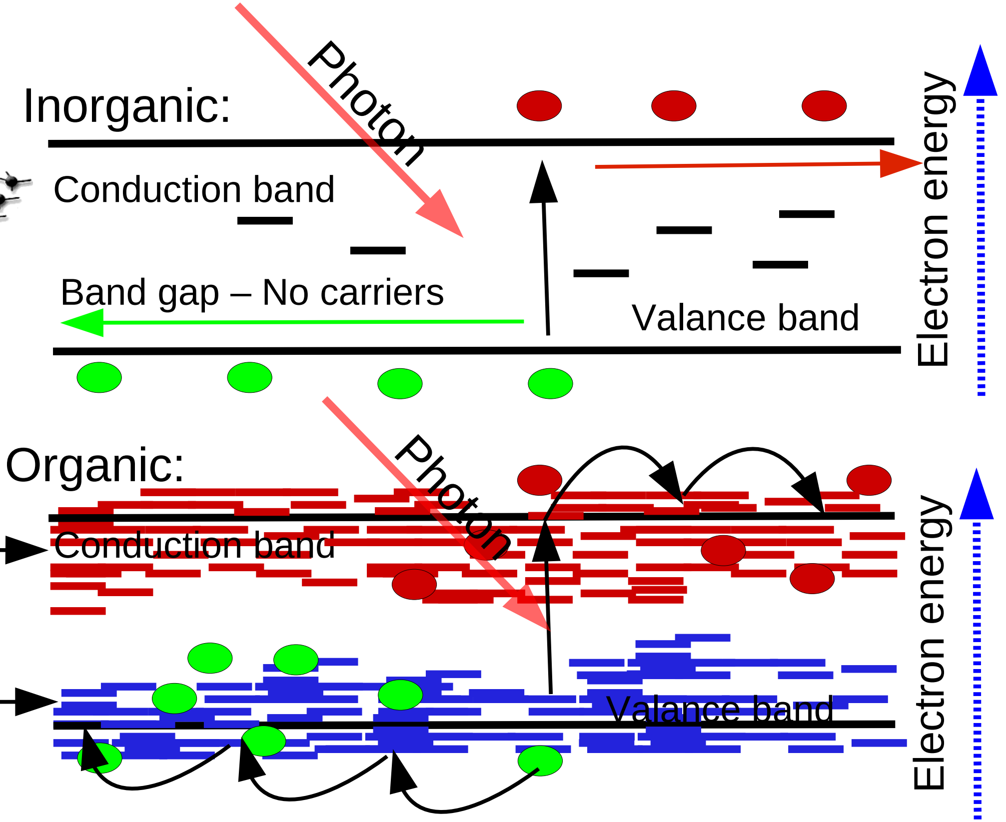
Trap states are needed to simulate disordered/organic materials



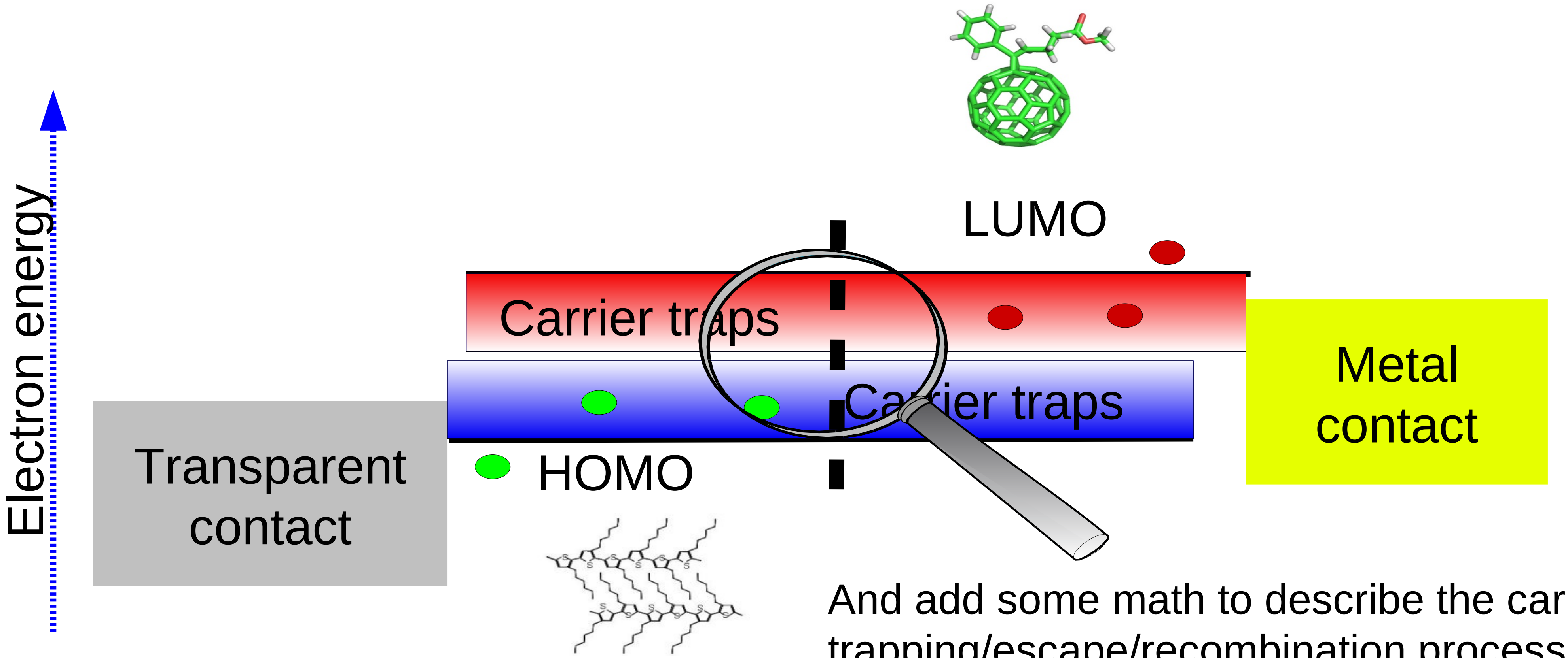
•Inorganic semiconductors are crystalline and have a well defined bandgap and few traps.

•Inorganic semiconductors are very disordered and have a distribution of trap states.





Take a slice down the device in energy space



And add some math to describe the carrier trapping/escape/recombination processes.

Trapping: To do time domain simulations you need to assume carriers can more dynamically in and out of traps.

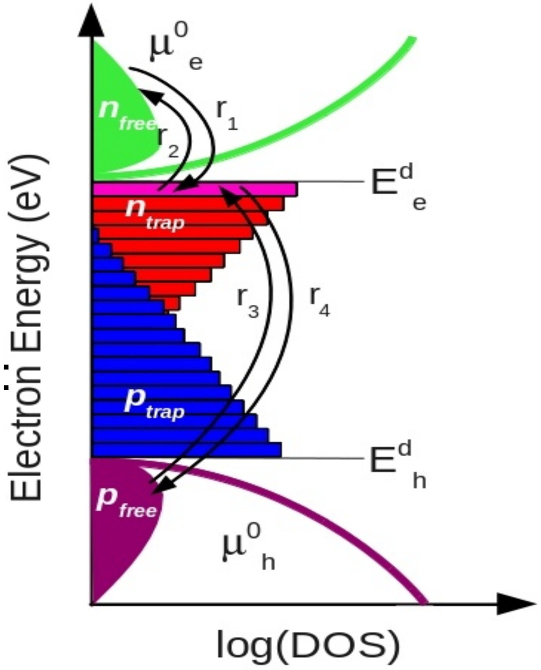
•We split energy space up into energy slices.

•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 equation:

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

Process	
electron capture	r_1
electron emission	r_2
hole capture	r_3
hole emission	r_4



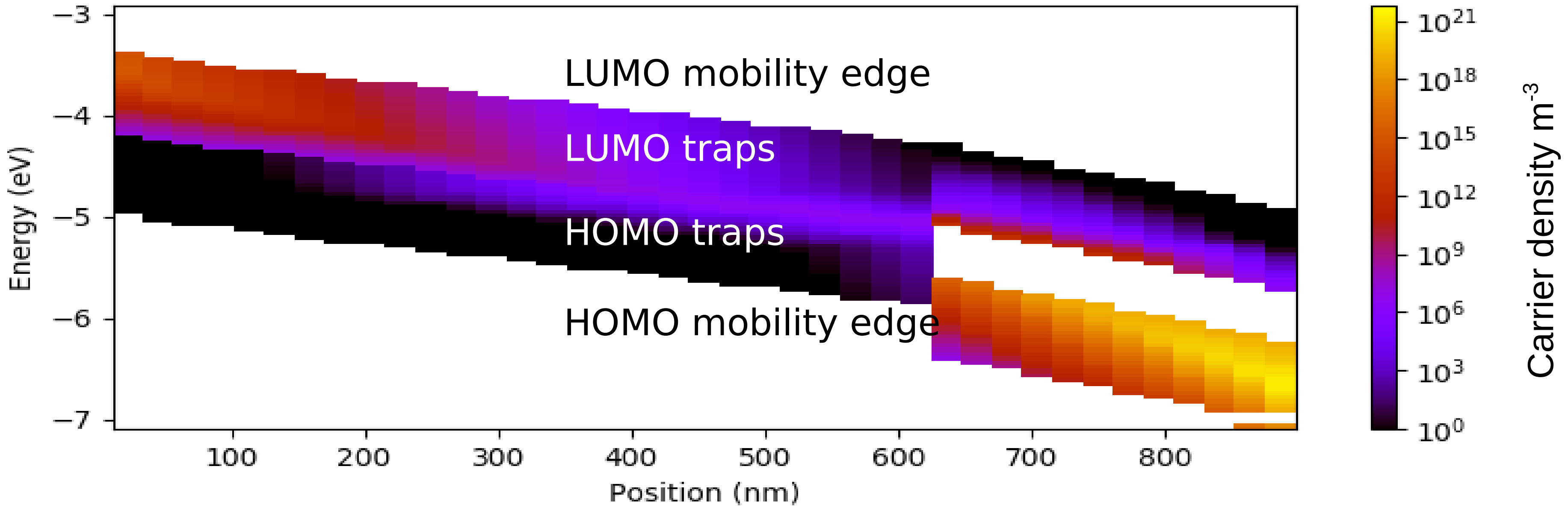
•Recombination can be calculated as:

Free carrier recombination

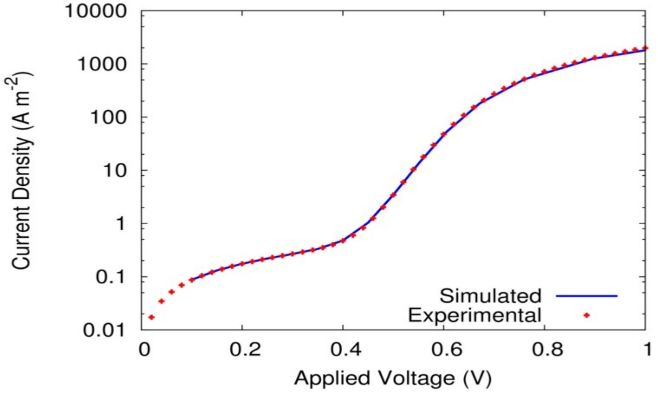
$$\boxed{R_n = \sum_{0}^{n_{band}} \left(r_1^e - r_2^e \right)}$$

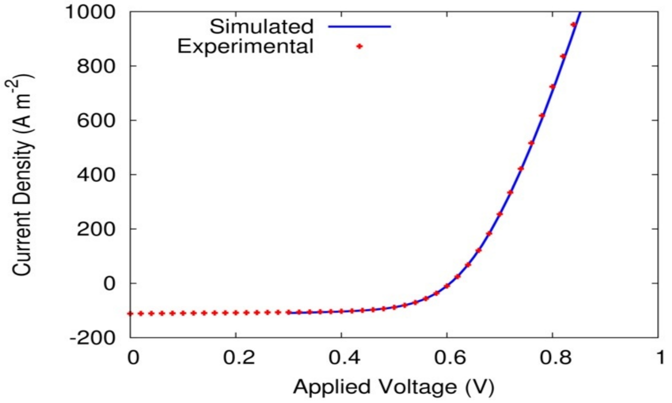
Detailed balance is maintained.

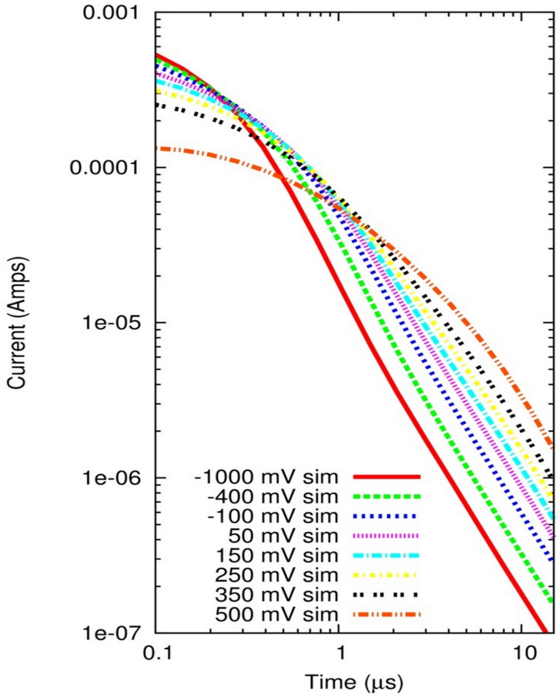
Drift diffusion: This enables us to know where the charge carriers are in position/energy space.

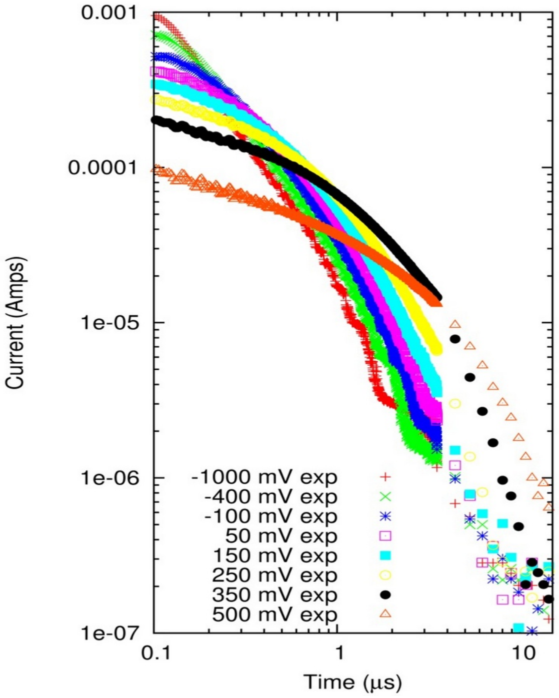


The allows accurate simulation of steady state and transient measuements.

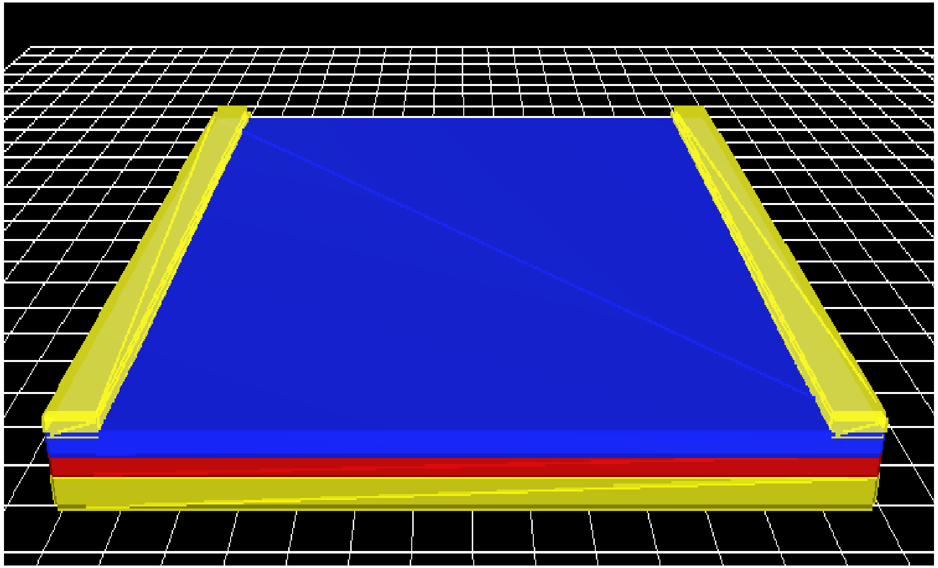


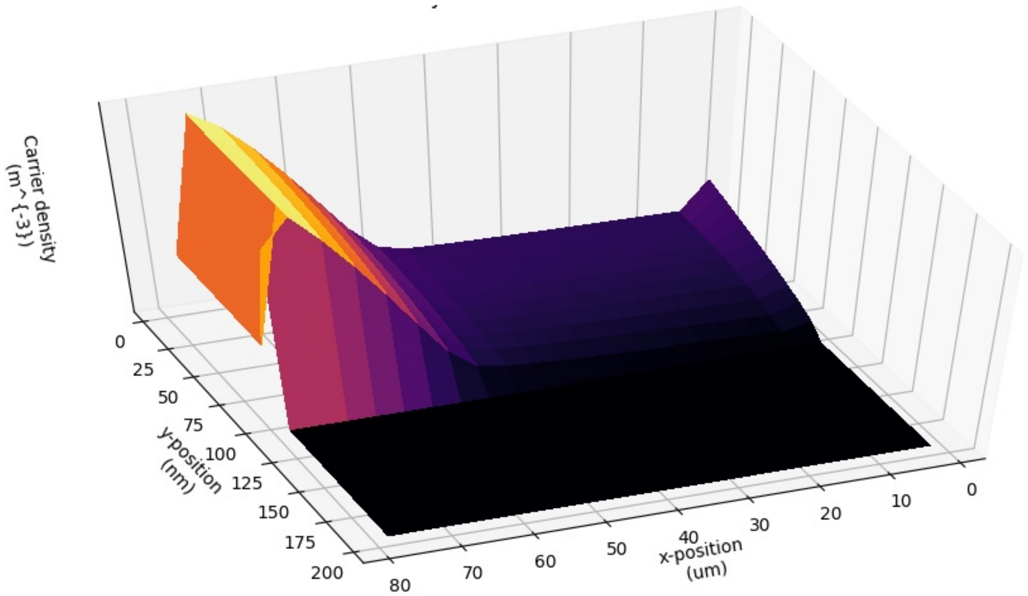






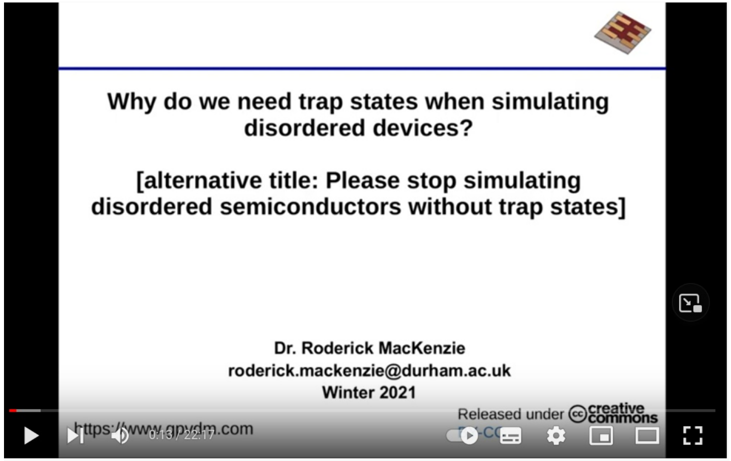
Drift diffusion: OghmaNano can also do 2D simulations including trap states





OghmaNano's party trick is that it can: Do traps really really well.

- To **simulate disordered materials you need to include**:
  - Carrier trapping
  - Recombination via trap states through a mechanism such as SRH.
- **OghmaNano does is specifically written to do this very well:**
  - If the device model you are using does not include trap states it is very likely you can not reliably simulate organic/disordered devices with it.
  - If you want to understand more watch this linked video.

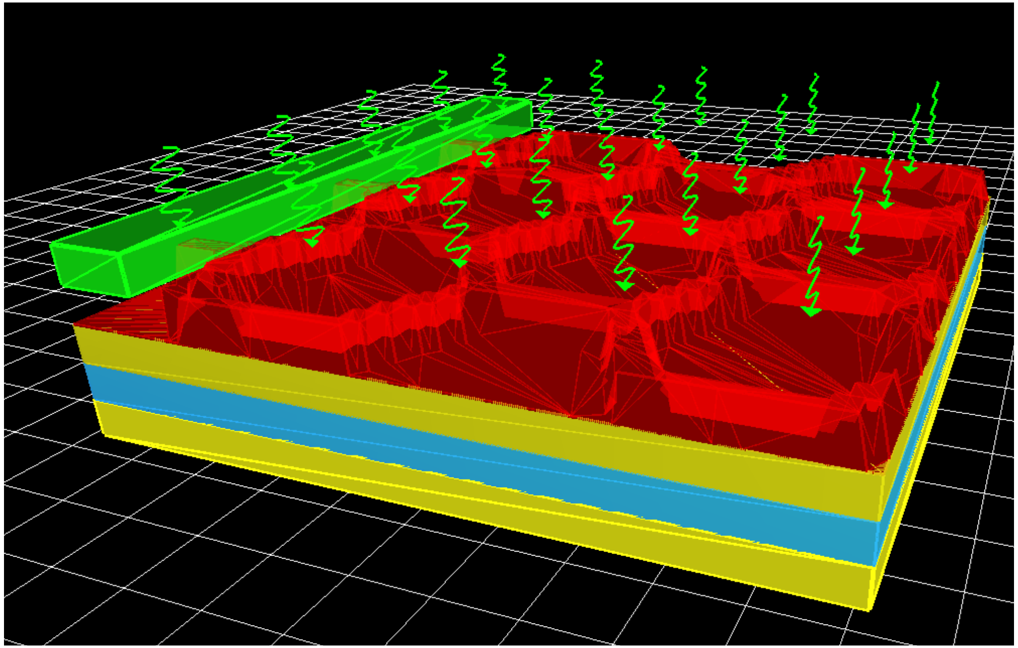


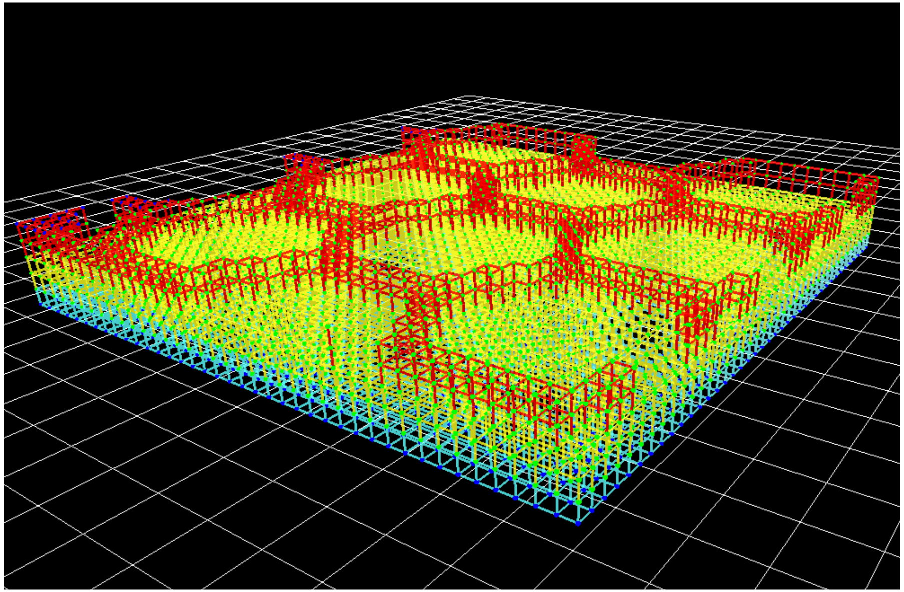
https://www.youtube.com/watch?v=2EHfulz7UDU

Talk overview

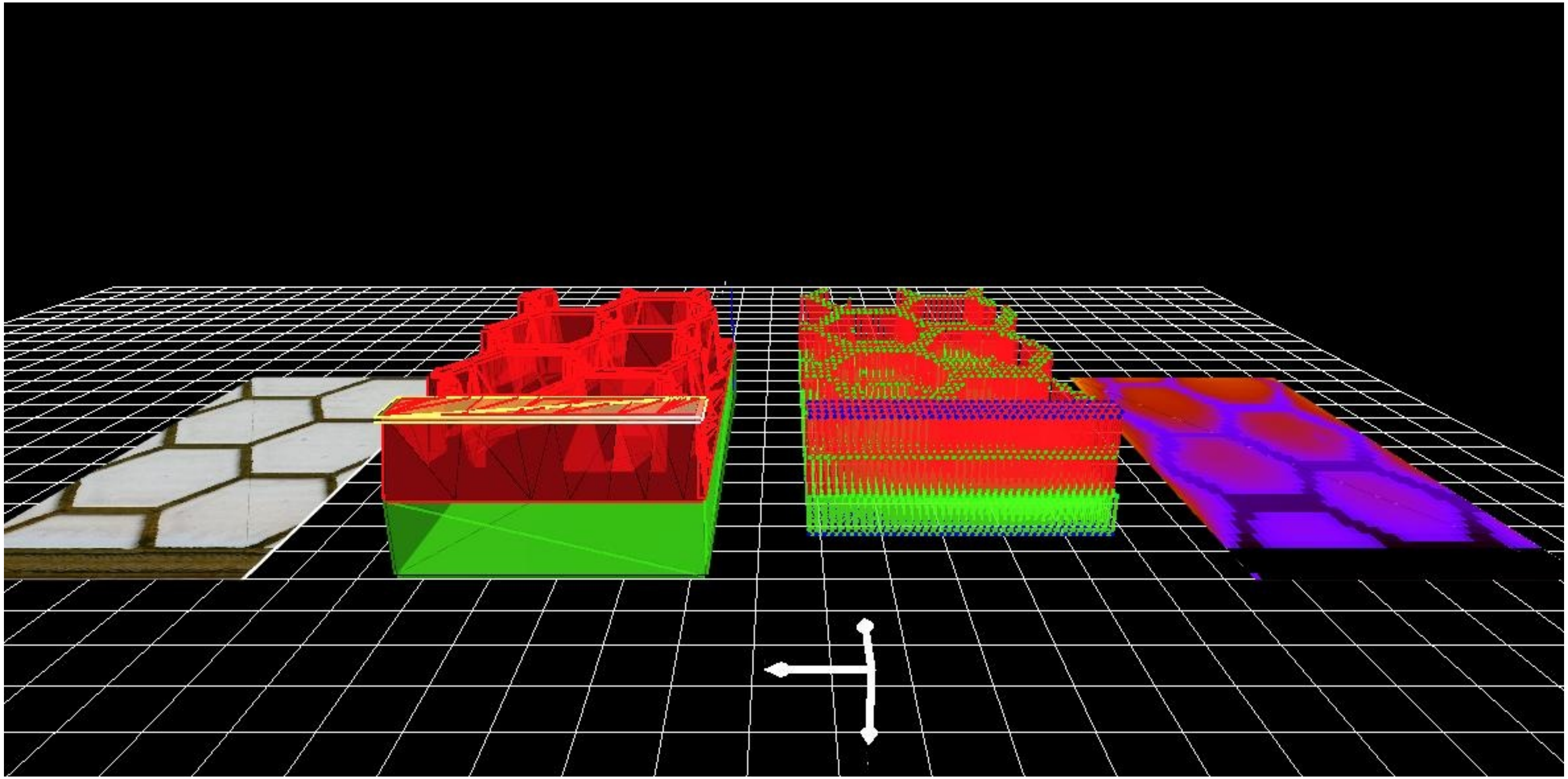
- History
- **Overview of model**
    - **Electrical models**
        - Drift diffusion
        - **Circuit model**
    - Optical models.
    - Exciton models
    - Simulation modes
    - Thermal models
    - Example simulation

Electrical circuit simulation for large area devices:
3D electrical circuit simulations

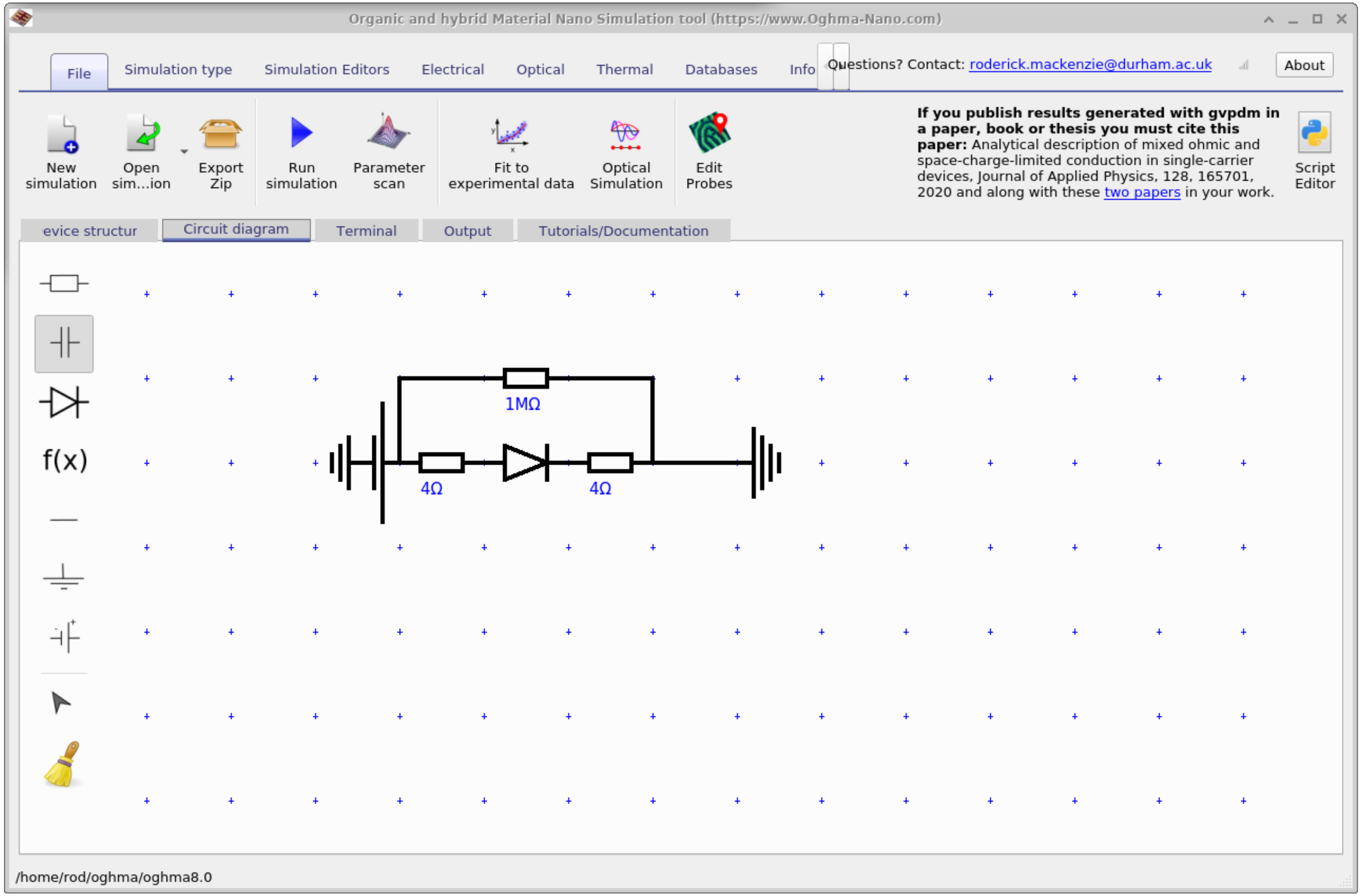




Electrical circuit simulation for large area devices: 3D electrical circuit simulations



Really simple electrical circuit simulations:

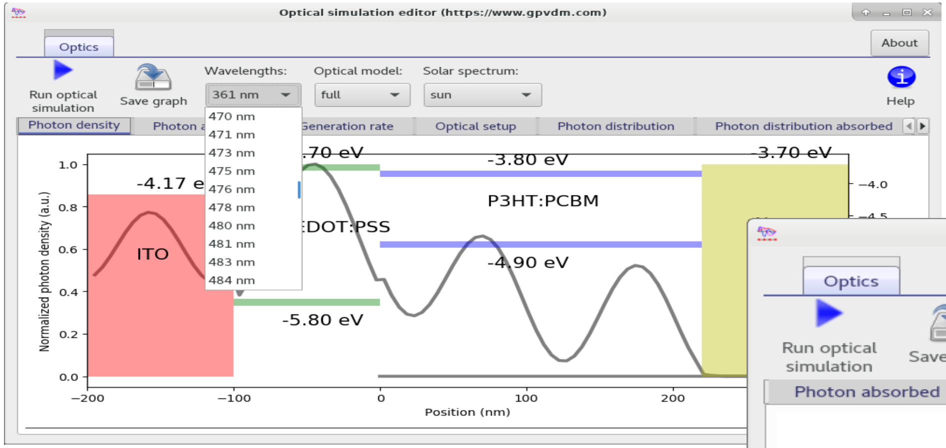


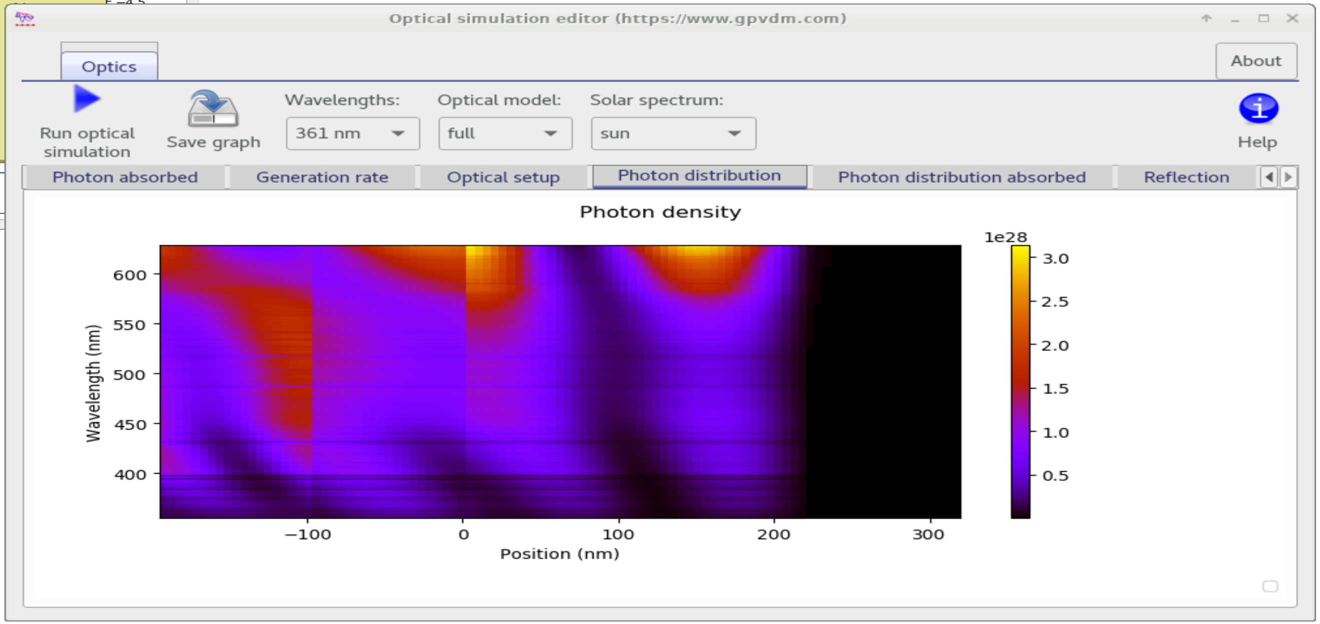
Talk overview

- History
- Overview of model
  - Electrical models
    - Drift diffusion
    - Circuit model
  - **Optical models**
  - Exciton models
  - Simulation modes
  - Thermal models
  - Example simulation

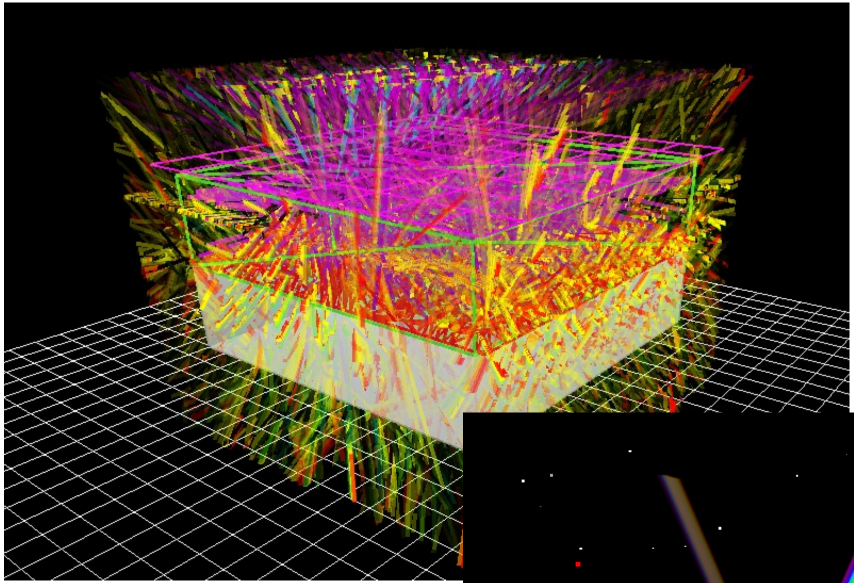
Overview…...

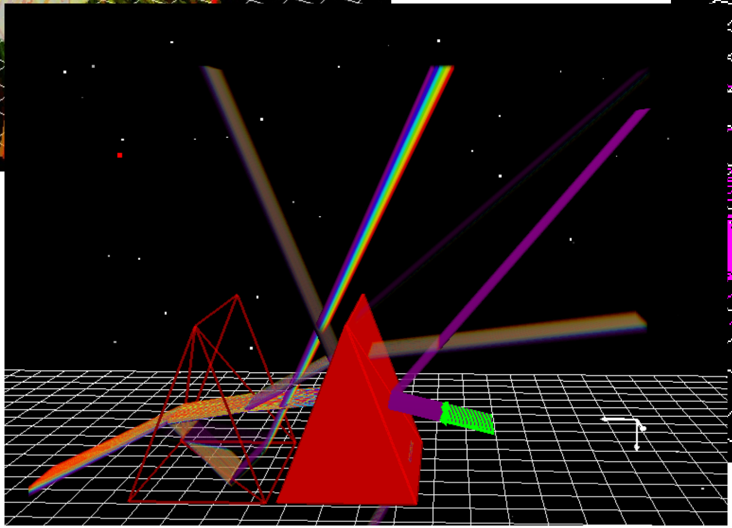
Optical simulations: Transfer matrix method

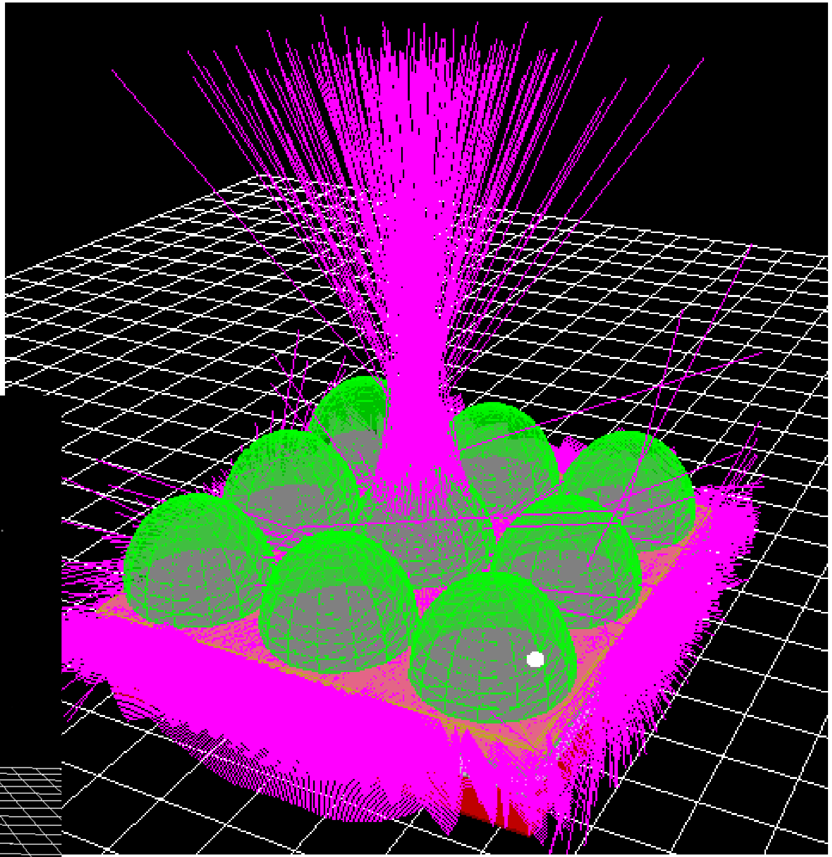




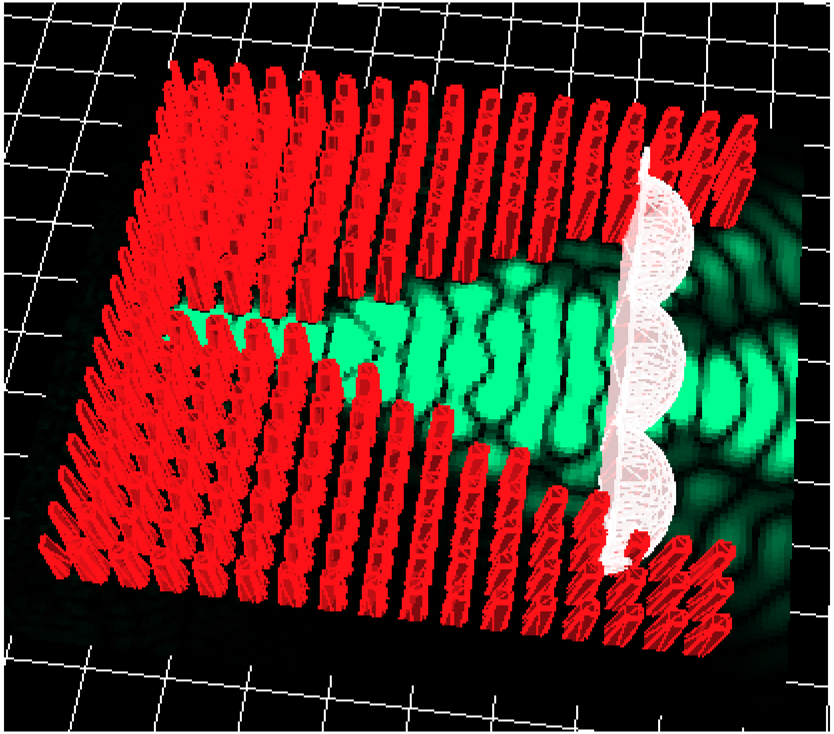
Optical simulations:
General ray tracing solver







Optical simulations: FDTD solver

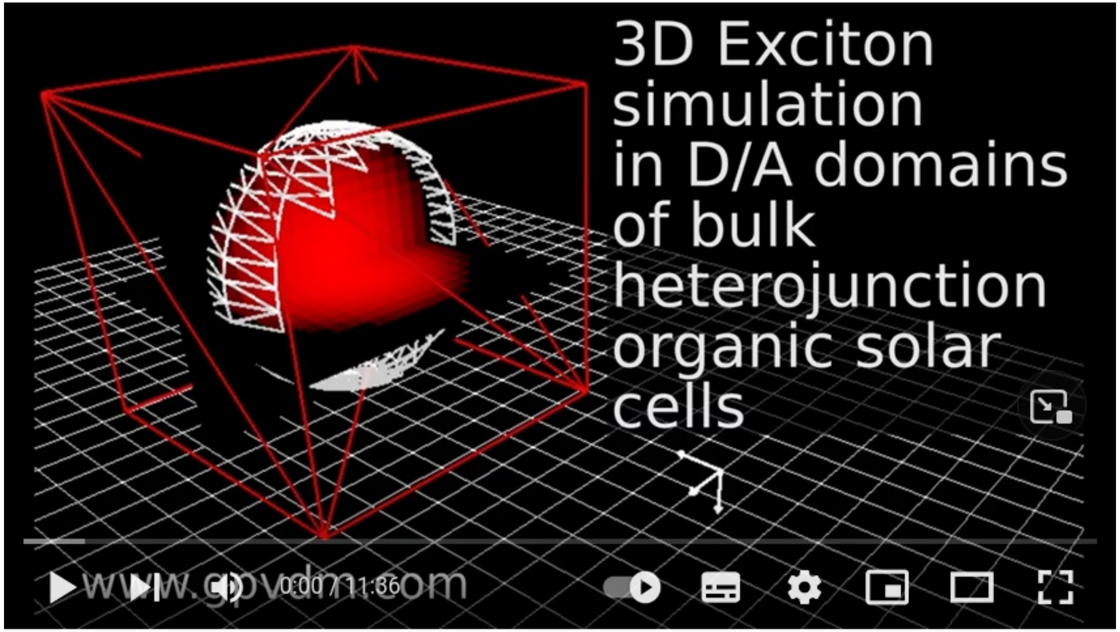


- The FDTD solver is currently fairly rudimentary

Talk overview

- History
- Overview of model
  - Electrical models
    - Drift diffusion
    - Circuit model
  - Optical models
  - **Exciton models**
  - Simulation modes
  - Thermal models
  - Example simulation

Exciton models

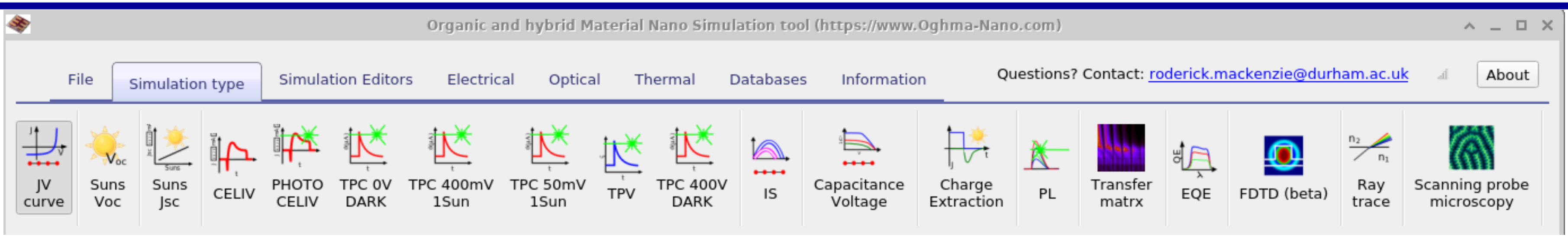


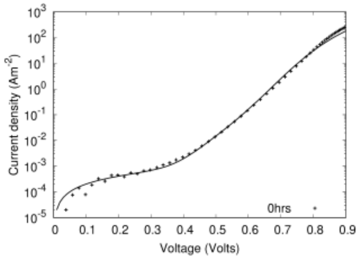
https://www.youtube.com/watch?v=Viu7WYcbqyw

Talk overview

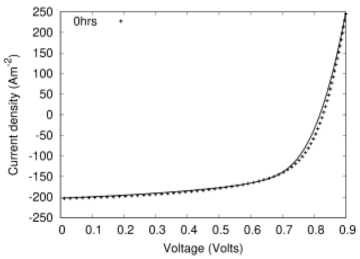
- History
- Overview of model
    - Electrical models
        - Drift diffusion
        - Circuit model
    - Optical models
    - Exciton models
    - **Simulation modes**
    - Thermal models
    - Example simulation

Simulation modes: Steady state, time domain and frequency domain.

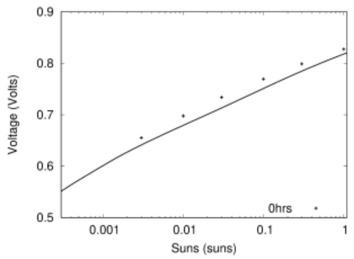




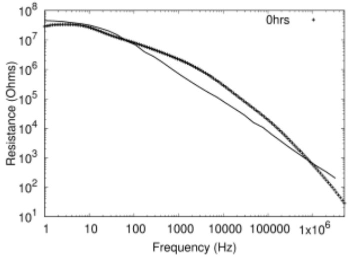
(a) JV dark



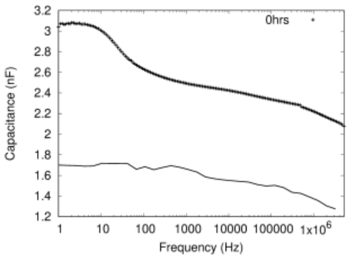
(b) JV light



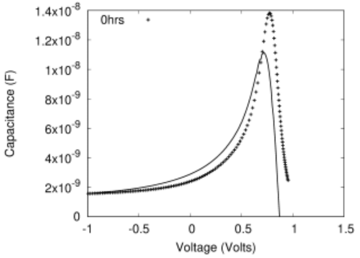
(c) Suns-Voc



(d) IS - dark



(e) IS - dark

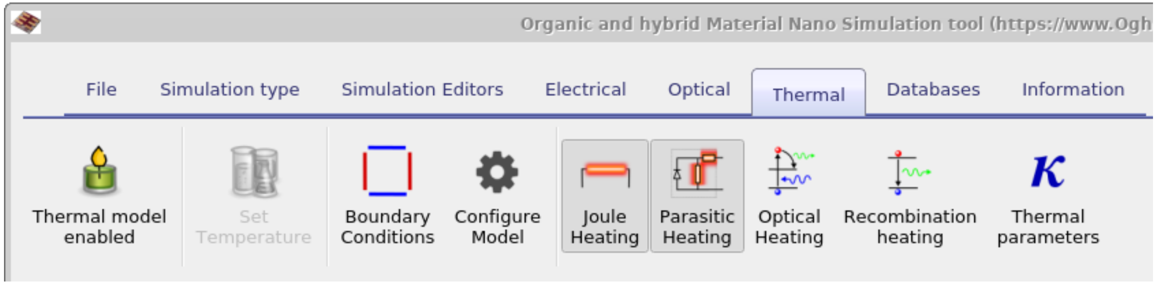


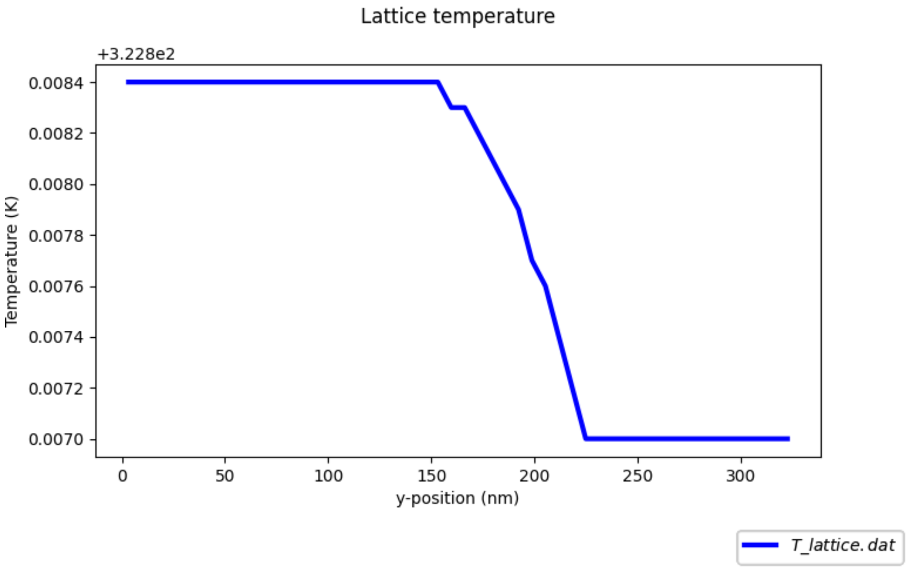
(f) CV - 1 Sun

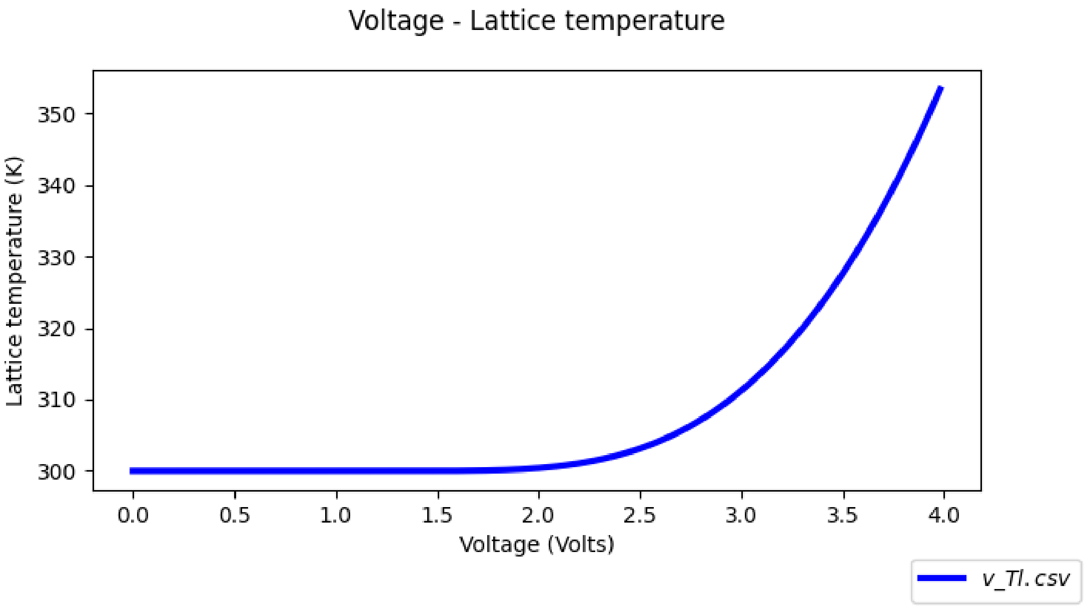
Talk overview

- History
- Overview of model
  - Electrical models
    - Drift diffusion
    - Circuit model
  - Optical models
  - Exciton models
  - Simulation modes
  - **Thermal models**
  - Example simulation

Thermal models/self heating



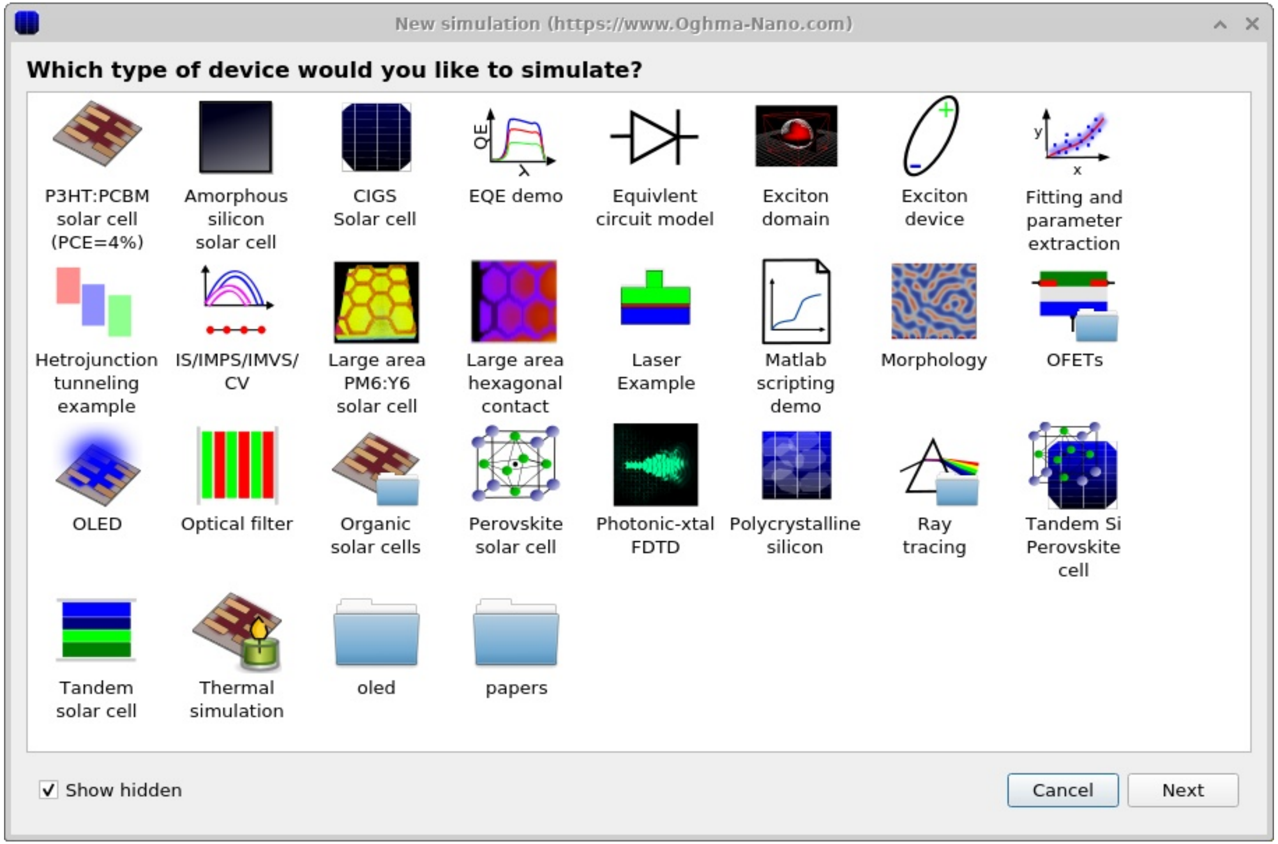




Talk overview

- History
- Overview of model
    - Electrical models
        - Drift diffusion
        - Circuit model
    - Optical models
    - Exciton models
    - Simulation modes
    - Thermal models
    - **Examples simulations**

Examples


New simulation (https://www.Oghma-Nano.com)
Which type of device would you like to simulate?
P3HT:PCBM solar cell (PCE=4%)
Amorphous silicon solar cell
CIGS Solar cell
EQE demo
Equivlent circuit model
Exciton domain
Exciton device
Fitting and parameter extraction
Hetrojunction tunneling example
IS/IMPS/IMVS/ CV
Large area PM6:Y6 solar cell
Large area hexagonal contact
Laser Example
Matlab scripting demo
Morphology
OFETs
OLED
Optical filter
Organic solar cells
Perovskite solar cell
Photonic-xtal FDTD
Polycrystalline silicon
Ray tracing
Tandem Si Perovskite cell
Tandem solar cell
Thermal simulation
oled
papers
Show hidden
Cancel
Next