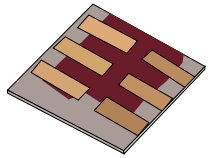

An introduction to simulating optoelectronic devices with *gpvdm*.

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

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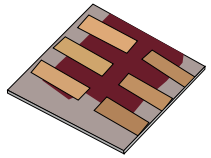
Autumn 2019

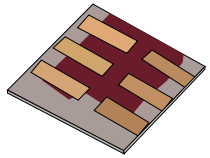
https://www.gpvdm.com

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

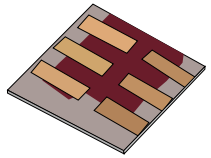
What is gpvdm?



- 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…..

Simulating charge transport:



Gauss's Law

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

Electron driving terms

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

Hole driving terms

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

Electron continuity

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

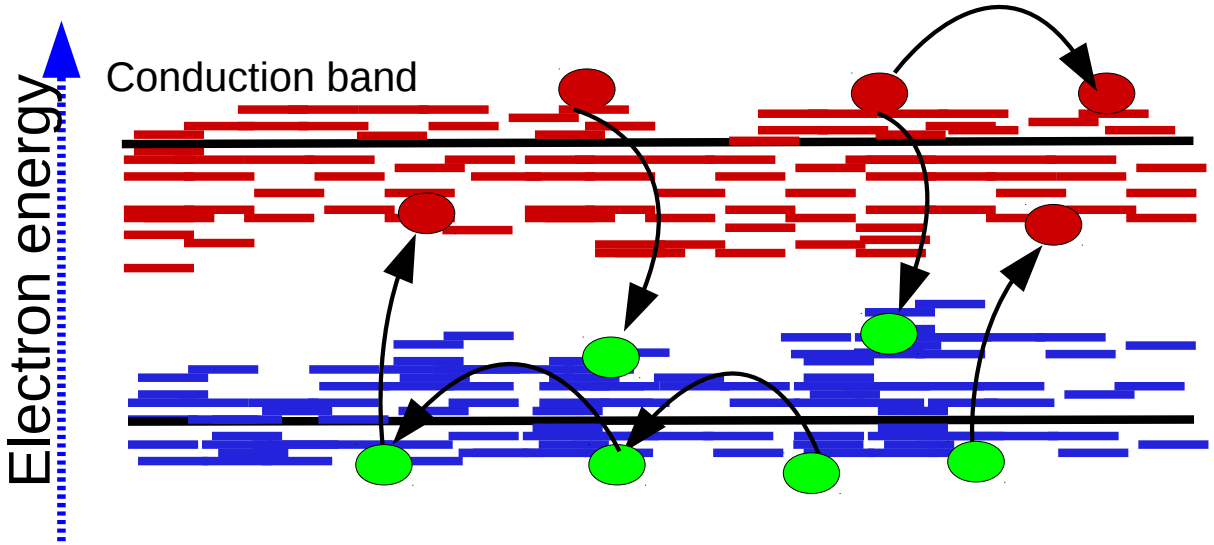
Hole continuity

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

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

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

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

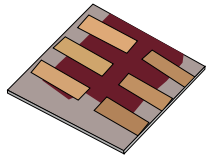


•This is often done using the following ***SRH*** equation, which assumes a ***steady state distribution*** of trapped charge carries in the trap states.

$$R_T = \frac{np - n_i^2}{\tau_{p0}\left[n + n_i \exp\left(\frac{E_t - E_i}{kT}\right)\right] + \tau_{n0}\left[p + n_i \exp\left(\frac{E_i - E_t}{kT}\right)\right]}$$

•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.



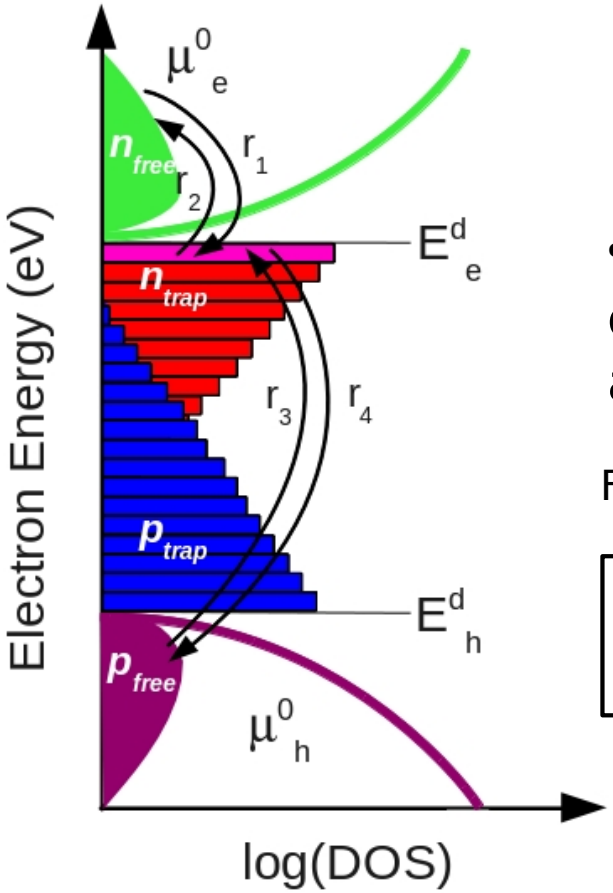
- We split energy space up into energy slices.

- 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 equation:

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

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

$$R_n = \sum_0^{n_{band}} \left(r_1^e - r_2^e \right)$$

Detailed balance is maintained.

- **Other models do not do this….**

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