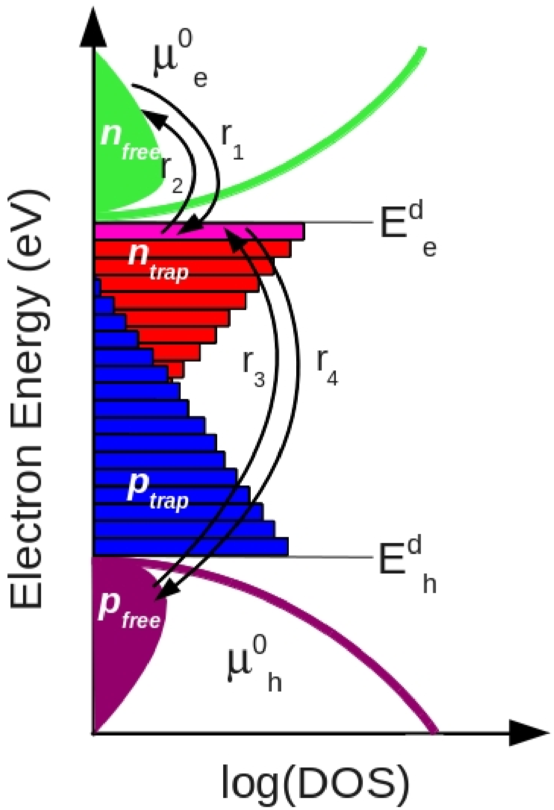
Continuum of trapping levels



Electron density of each trap:

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

Total electron recombination

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

Total hole recombination

$$R_n = \sum_{0}^{n_{band}} \left(r_4^e - r_3^e \right)$$

Modeling carrier transport across the device.

Inputs

- Applied Voltage
- Light intensity

Inputs

Poisson's equation

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

Current driving terms

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

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

Current continuity equations

Electron continuity

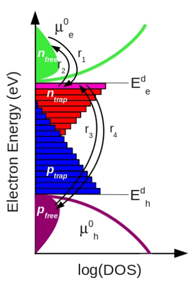
$$\nabla \cdot \boldsymbol{J}_n = q \cdot \left(\sum_0^{n_{band}} (r_1^e - r_2^e) + \sum_0^{p_{band}} (r_4^h - r_3^h) + \frac{\partial n_{free}}{\partial t} \right)$$

Hole continuity

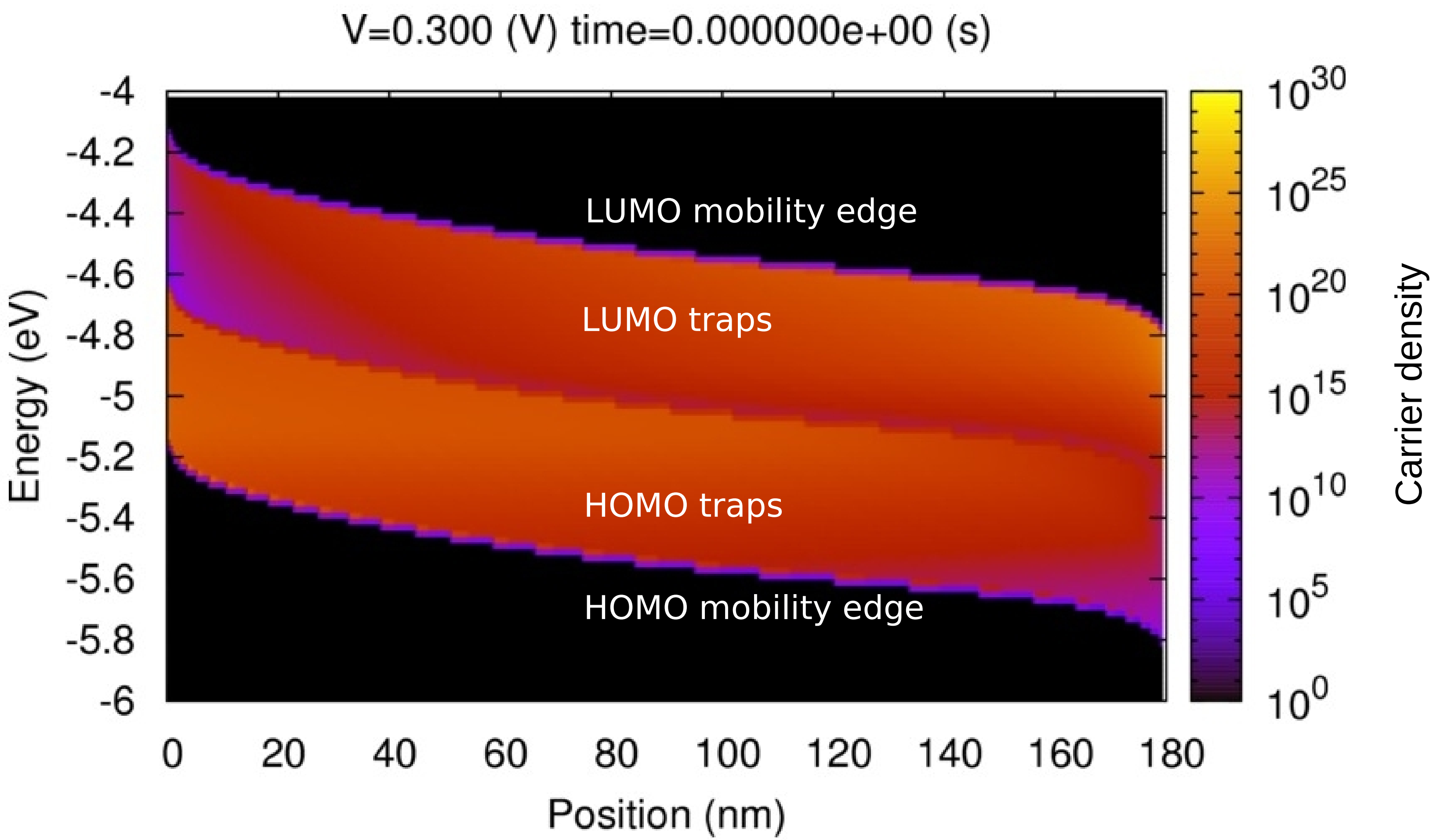
$$\nabla \cdot \boldsymbol{J}_p = -q \cdot \left(\sum_0^{n_{band}} (r_4^e - r_3^e) + \sum_0^{p_{band}} (r_1^h - r_2^h) + \frac{\partial p_{free}}{\partial t} \right)$$

Outputs

- Current density
- Recombination rates
- Average charge density

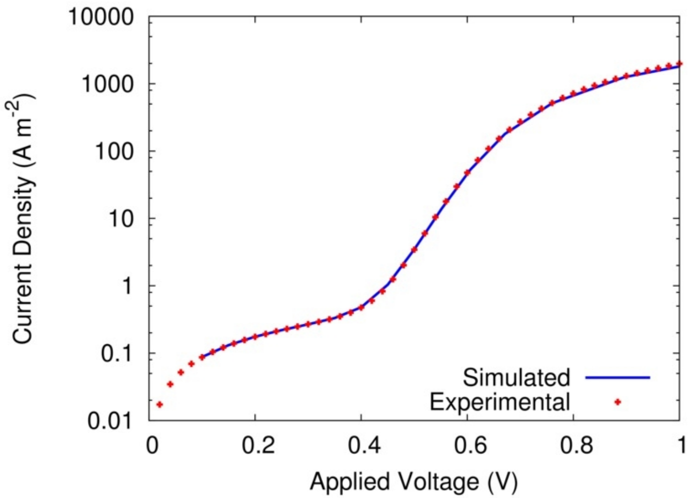


0D energy model + 1D device model

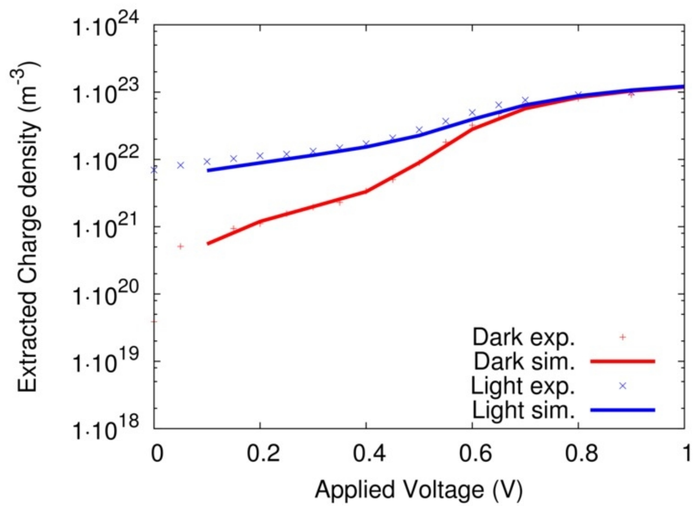


We have a device model, but can it reproduce experimental results?

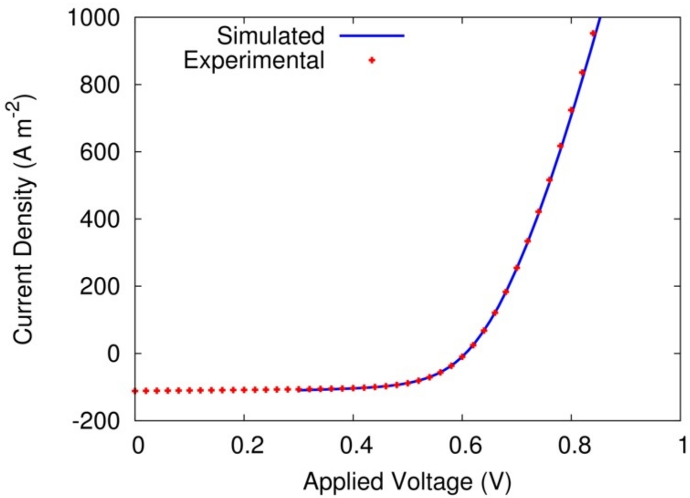
Reproducing steady state JV/CE curves



Dark simulated and experiment al JV curves



ight and dark harge xtraction urves.



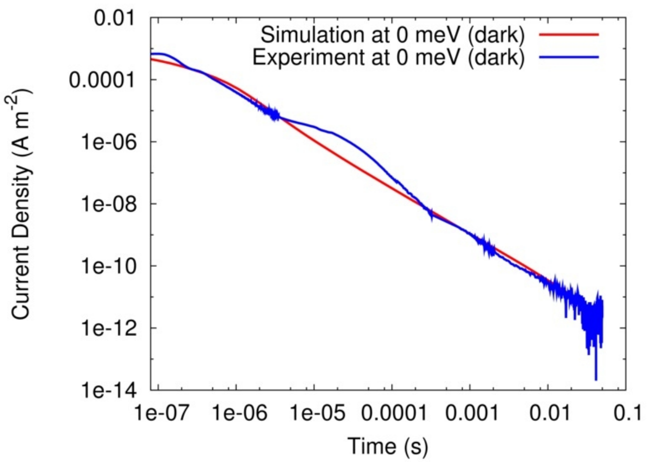
One sun simulated and experimental JV curves

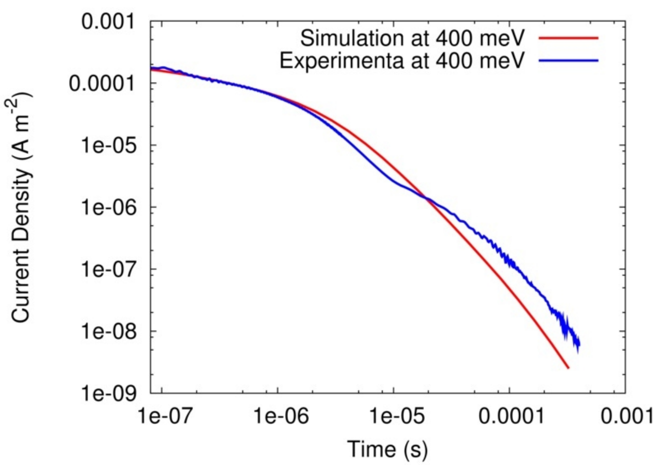
- The deep trap tail slope
- Absolute value of the DoS
- The carrier trapping times
- The recombination times
- Carrier mobilities
- Contact carrier densities

Imperial College London

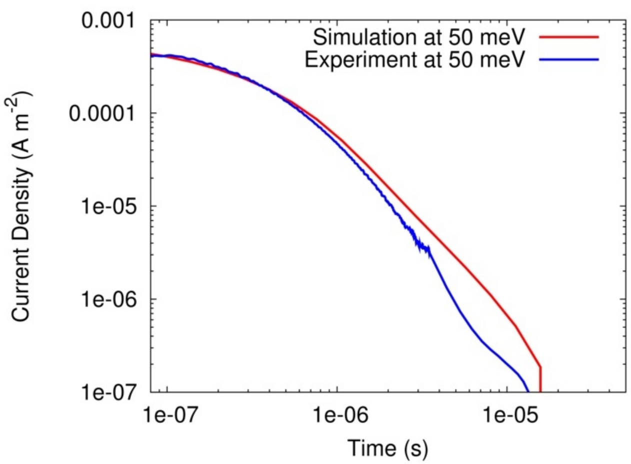
Reproducing transient photo current

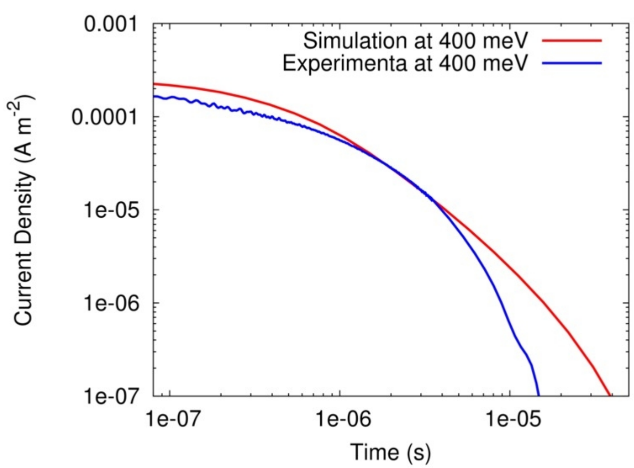
Dark





Light





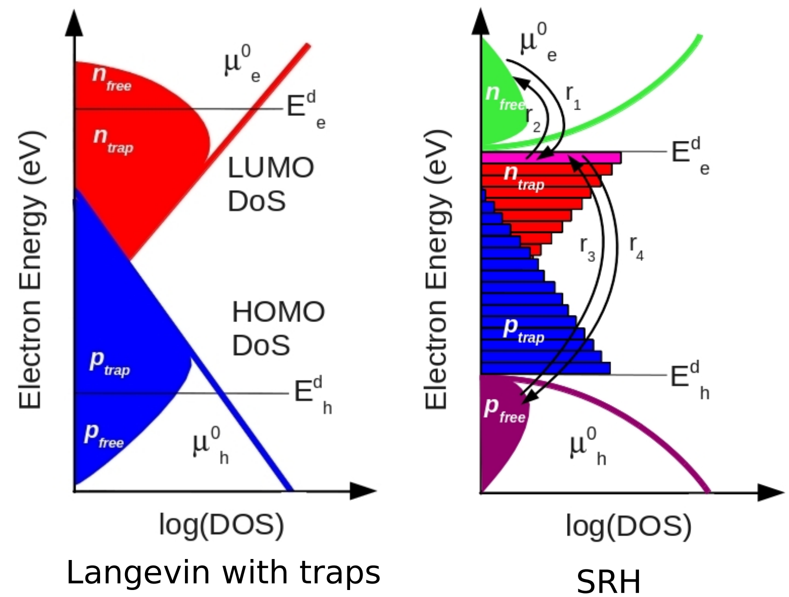
- We can also reproduce the TPC curves at two points on the JV in both the light and in the dark.

Are SRH and Langevin recombination comparable?

$$\mu_e(E_f) = \mu_e^0 \frac{n_{free}}{n_{total}} \qquad \mu_h(E_f) = \mu_h^0 \frac{p_{free}}{p_{total}}$$

$$R = \frac{q}{\epsilon_0 \epsilon_r}\left(\mu_e^0(n) + \mu_h^0(p)\right) n_{total} \, p_{total}$$

$$R = \frac{q}{\epsilon_0 \epsilon_r}\left(\mu_e^0 n_{free} \, p_{total} + \mu_h^0 p_{free} \, n_{total}\right)$$



The number of free carriers is much smaller than the number of trapped carriers therefore $n_{total} \approx n_{trap}$

$$R = \frac{q}{\epsilon_0 \epsilon_r}\left(\mu_e^0 n_{free} \, p_{trap} + \mu_h^0 p_{free} \, n_{trap}\right)$$

Therefore Langevin recombination with tails is equivalent to SRH recombination with an instantaneous carrier trapping time.

MacKenzie et al. J. Phys. Chem. C, 10.1021/jp200234m

Overview

1) Molecular level simulation of thin films

2) Electrical characterization of OPVs

3) Diffusion limited recombination in OPVs

4) The open circuit voltage

5) Conclusions