

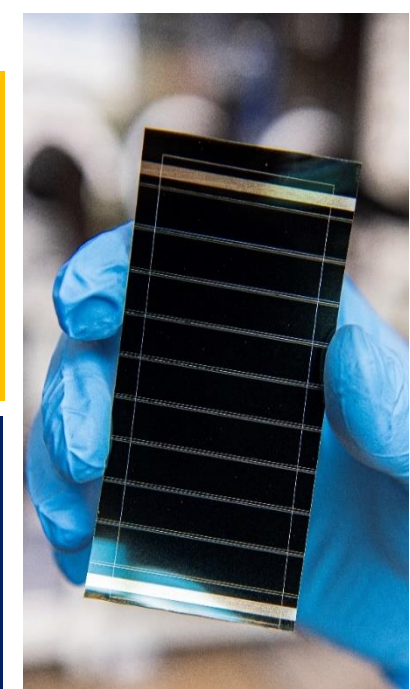
Motivation



- Cheap
- Lightweight
- Flexible
- Scalable with good efficiency
- Sun is free source of energy

THEORETICAL EXPLANATION OF ORGANIC AND PEROVSKITE SEMICONDUCTORS ARE NEEDED!

- Need for understanding of physical processes inside of solar cells, with the idea of reaching their full potential.
- Especially it is important to understand the influence of recombination as it is fundamental mechanism of losses.



Parameters

PARAMETERS

- q is the elementary charge,
- ϵ is the permittivity
- D_n, D_p are the diffusion coefficients of the electrons and the holes
- N_C, N_V are the effective densities of states for electrons and holes
- E_g is the energy gap of material
- n_i is intrinsic carrier concentration
- n_1, p_1 are electron and hole concentration
- τ_n, τ_p are electron and hole lifetimes
- γ_L is Langevin coefficient of recombination
- μ_n, μ_p are the electrons and holes mobilities

VARIABLES

- ϕ is electrostatic potential
- n, p are the electrons and holes concentration

GENERATION, RECOMBINATION, TRANSPORT

- G is the generation rate described by an optical model using optical transfer matrix method [2]
- R_n, R_p are recombination rates of electrons and holes
- We assume constant values for electron and hole mobility

SPECIAL VARIABLE COEFFICIENTS

- K_L coefficient corresponds to change in reduction coefficient of Langevin recombination (γ_L).
- K_{SRH} coefficient corresponds to change in concentration of trap states (N_t) of the material.

The drift-diffusion model

Poisson's equation: $\frac{\partial^2 \phi}{\partial x^2} = \frac{q}{\epsilon} [n(x) - p(x)]$

Continuity equations for electrons and holes:

$$\frac{\partial n(x)}{\partial t} = G - R_n + \frac{1}{q} \frac{\partial J_n(x)}{\partial x}, \quad \frac{\partial p(x)}{\partial t} = G - R_p - \frac{1}{q} \frac{\partial J_p(x)}{\partial x}$$

Current density equations for electrons and holes:

$$J_n(x) = -q\mu_n n(x) \frac{\partial \phi(x)}{\partial x} + qD_n \frac{\partial n(x)}{\partial x}$$

$$J_p(x) = -q\mu_p p(x) \frac{\partial \phi(x)}{\partial x} - qD_p \frac{\partial p(x)}{\partial x}$$

The boundary conditions:

Anode

$$\phi(x=0) = 0$$

$$n(x=0) = N_C \exp(-E_g/k_B T)$$

$$p(x=0) = N_V$$

Cathode

$$\phi(x=d) = V_{bi} - V$$

$$n(x=d) = N_C$$

$$p(x=d) = N_V \exp(-E_g/k_B T)$$

Important formulas

- Langevin recombination:

$$R_L = \gamma_L (np - n_i^2)$$

- Shockley-Reed-Hall recombination:

$$R_{SRH} = \frac{np - n_i^2}{(n - n_1)/\tau_p + (p - p_1)/\tau_n}$$

Numerical method

- The discretization of equations is performed by the finite-difference method with Scharfetter-Gummel approach obtaining a system of difference equations solved numerically using Newton's algorithm.

Model validation

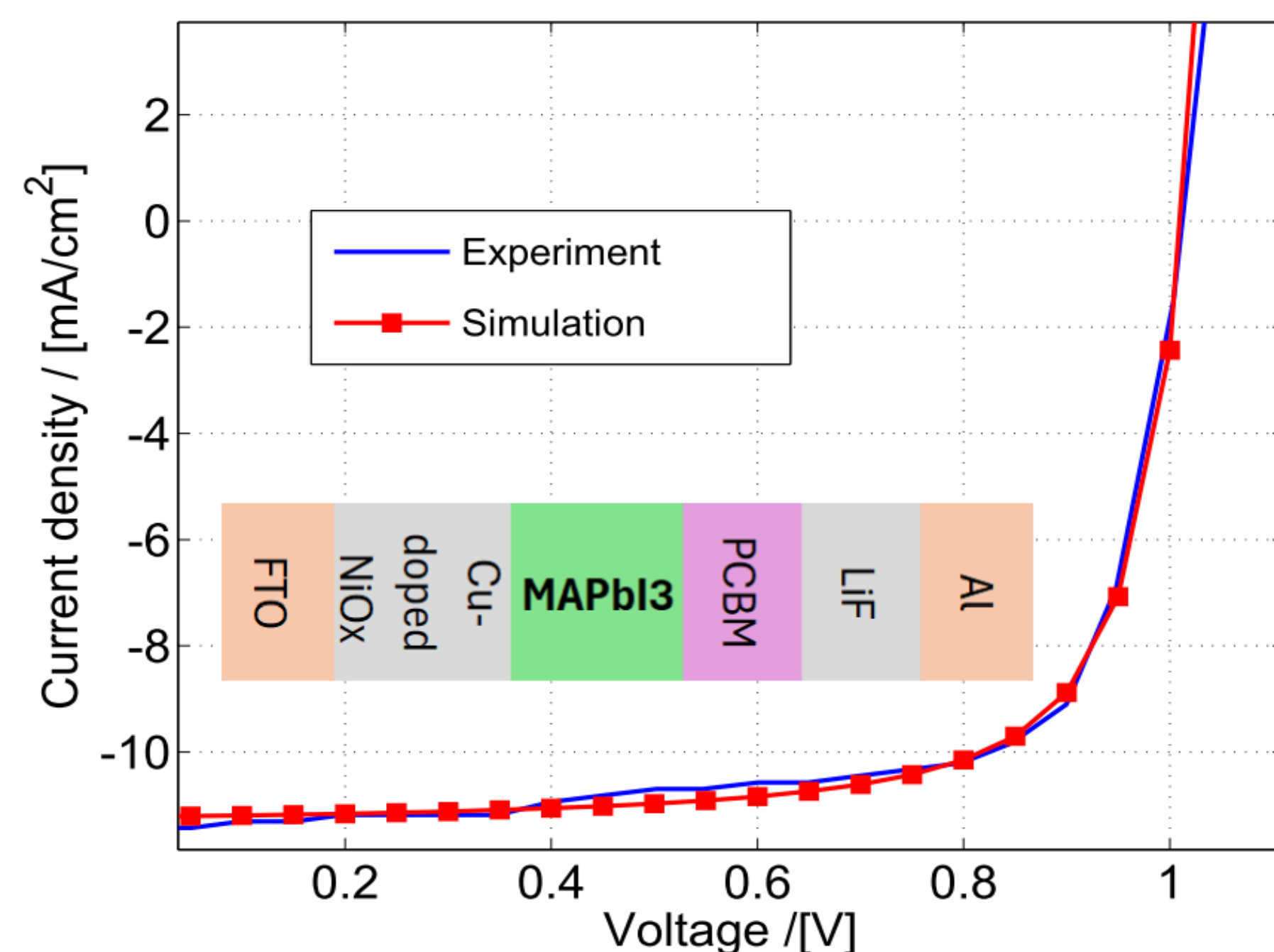


Fig.1 Validation of applied model based on the example of planar FTO/Cu-doped NiOx/MAPbI3/PCBM/LiF/Al perovskite solar cells. Inset on the figure shows the structure of solar cell from ref [1].

- **Special variable coefficients K_L and K_{SRH} are introduced with the idea of controlling Langevin and SRH recombination rate!**

SIMULATION AND RESULTS

ORGANIC SOLAR CELLS

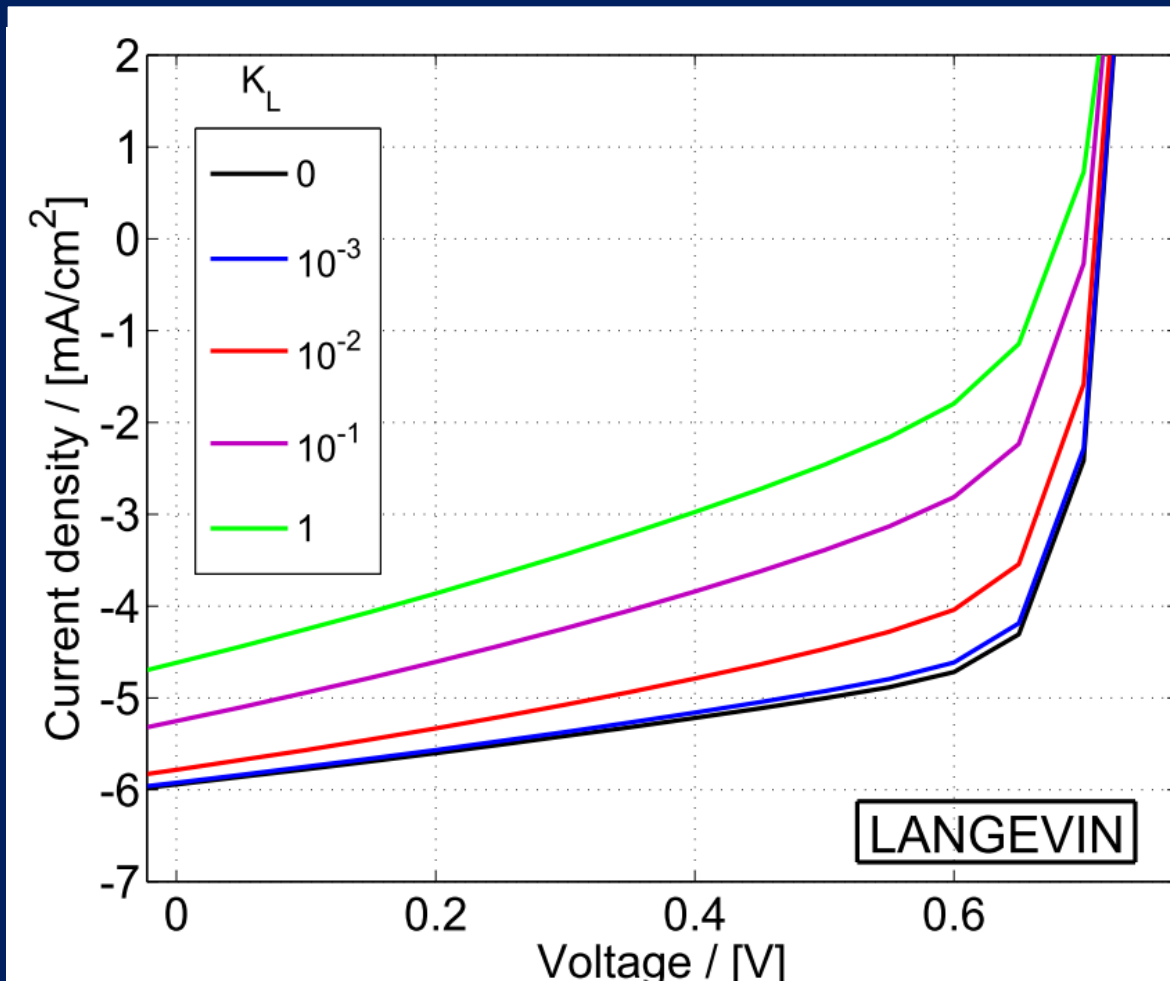


Fig.2 Current-voltage characteristics of OSC for different orders of magnitude of Langevin recombination (above) and important parameters of solar cell (below)

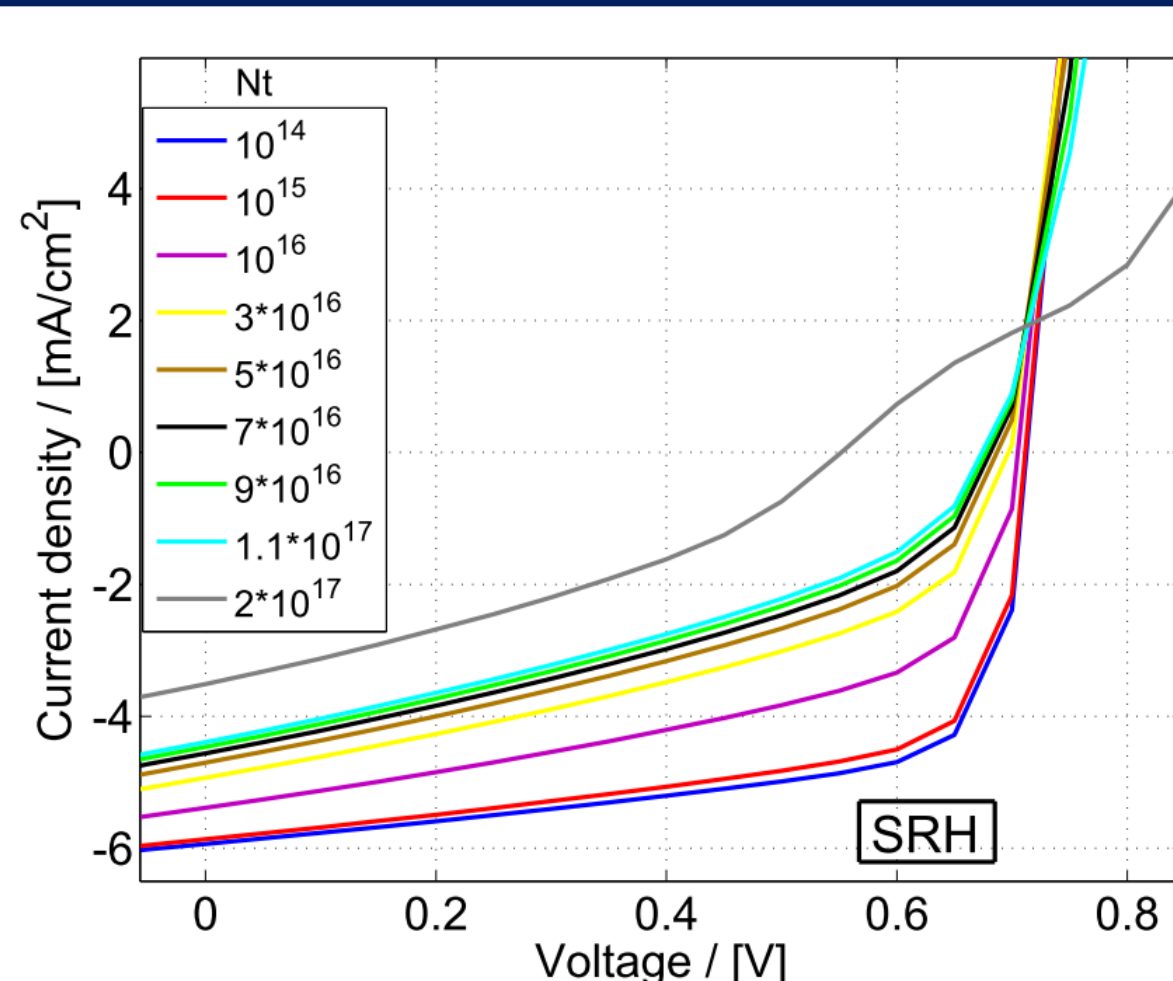


Fig.3 Current voltage characteristics of OSC for different orders of magnitude of SRH recombination (above) and important parameters of solar cell (below)

PEROVSKITE SOLAR CELLS

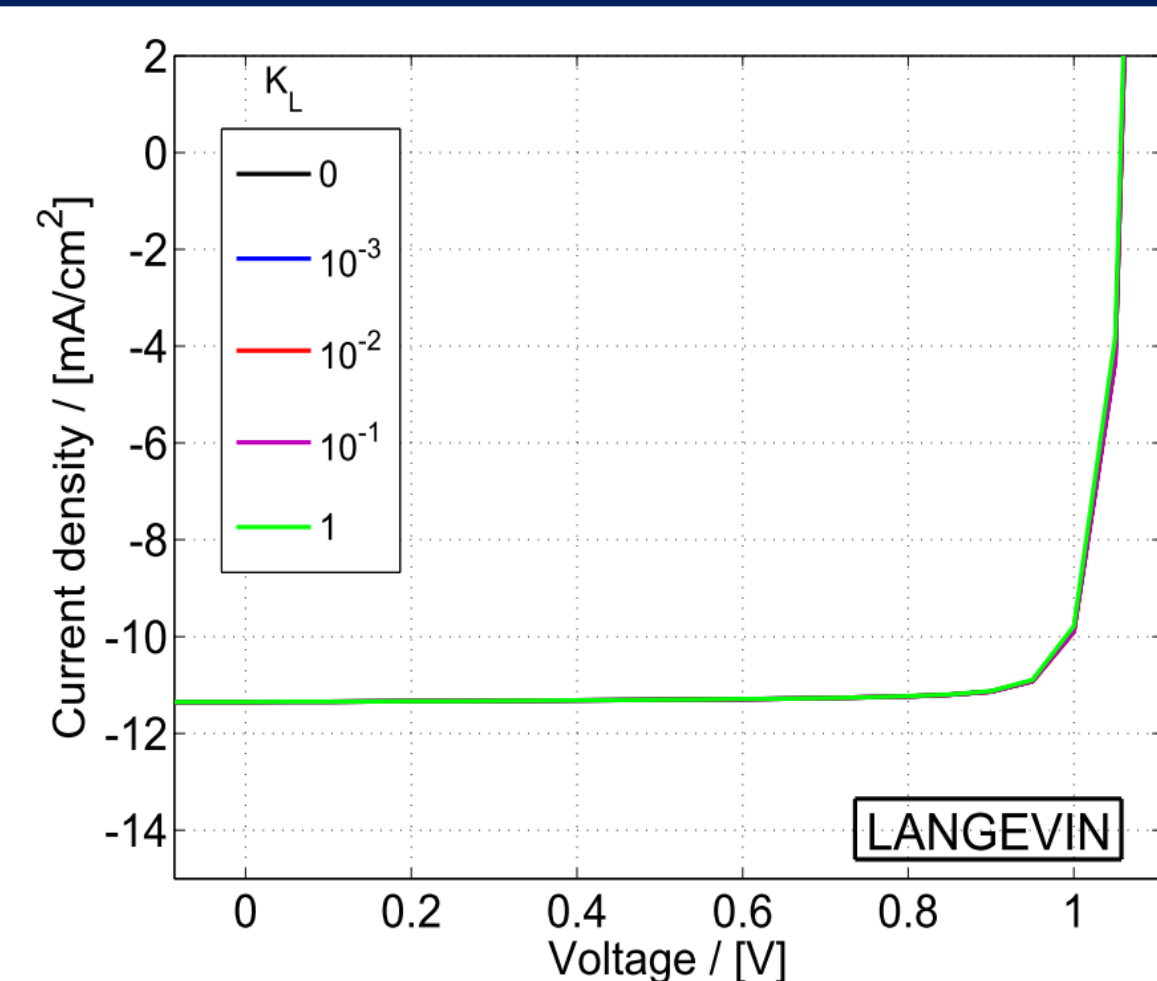


Fig.4 Current voltage characteristics of PSC for different orders of magnitude of Langevin recombination (above) and important parameters of solar cell (below)

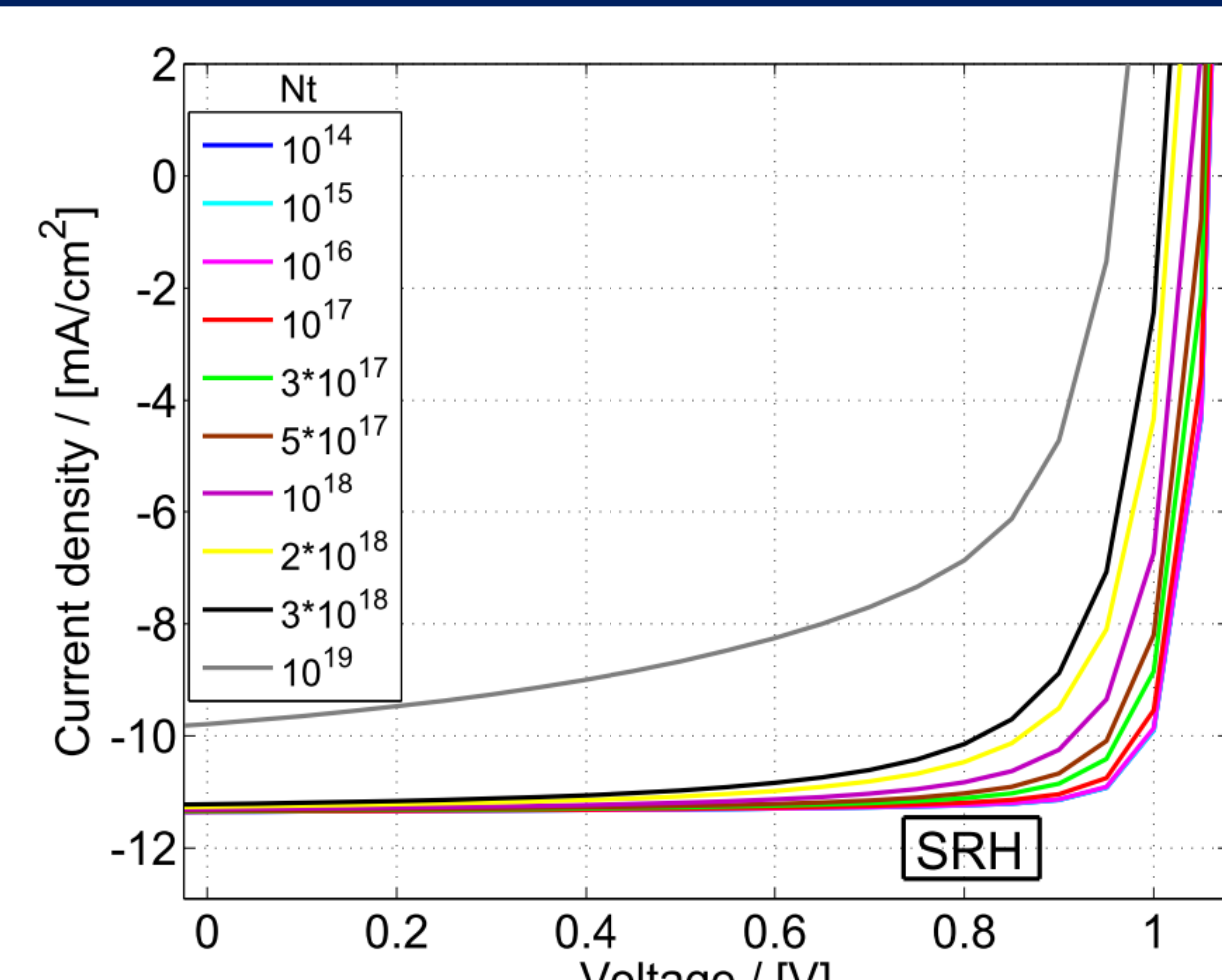


Fig.5 Current voltage characteristics of PSC for different orders of magnitude of SRH recombination (above) and important parameters of solar cell (below)

CONCLUSION

- Our analysis has concluded that Langevin recombination has strong influence on OSCs performance, while its influence on PSCs is negligible.
- Increase in SRH recombination rate has negative impact on both OSC and PSC, whereat in OSCs its dominant impact is on increasing J_{sc} , while in PSCs the V_{oc} is dominantly decreased.
- **In the case of OSCs stronger influence of SRH recombination begins with $N_t = 10^{15} \text{ cm}^{-3}$ and total degradation of the device starts at $N_t = 2 \cdot 10^{17} \text{ cm}^{-3}$**
- **In the case of PSCs stronger influence of SRH recombination begins at $N_t = 10^{17} \text{ cm}^{-3}$ and total degradation of the device starts at $N_t = 10^{19} \text{ cm}^{-3}$.**
- **THIS INDICATES DIFFERENT OPERATING MECHANISMS BETWEEN OSCs AND PSCs!**