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SILVACO'S ORGANIC SOLAR CELLS SIMULATION PACKAGE

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OUTLINE

1. Description of the simulation
2. Experimental vs. simulated comparison of current-voltage characteristics
    2.1. P3HT:PCBM solar cells
    2.2. Definition of Eg
    2.2. Light-intensity dependence
    2.4. Germinate pair bounding energy
    2.5. Case study: reduced hole mobility
    2.6. MDMO-PPV:PCBM solar cells : introduction of adapted Langevin recombination model
3. Novel models and tools for further optimization

Results in this presentation were simulated with the Silvaco's atlas 5.17.5.C version.

I. SIMULATED STRUCTURE

ANODE

WF=4.8 →ohmic contact and no exciton quenching at the interfaces

CATHODE

WF=3.8 →ohmic contact and no exciton quenching at the interfaces

Effective organic medium

(P3HT:PCBM or MDMO-PPV:PCBM)

Eg=1eV*

EA=3.8eV

ε_r=3.4*

μ_p =3 10^{-3} cm^2/Vs μ_n= 0.9 10^{-3}cm2/Vs

Exciton diffusion length: l=0nm

h^+-e^- distance in geminate pair:

a=1.8nm*

Exciton binding energy:

b=0.28eV

Maximum photogeneration rate:

Gmax=2.2 10^{21} $cm^{-3}s^{-1}$

Geminate decay rate:

k_f^{-1}=100µs

Exciton radiative recombination:

k_{rad}=1s

*Source: V. Mihailetchi and L.J.A. Koster thesis

I. PHOTON/EXCITON GENERATION RATE CALCULATION

constant photon generation profile (steady-state)

from experimental results:

$J_{ph}@2V = J_{sat} = q.G_{max}.L = 105 A/m^2$

$G_{max} = 2.2.10^{21} cm^{-3} s^{-1}$

all photons create an exciton

every exciton creates a geminate pair (GP)

solve the geminate pair continuity equation:

$$\frac{dS(x,y,t)}{dt} = \mathrm{RST.EXCITON}\, R_{Ln,p} - \mathrm{KNRS.EXCITON}\; S(x,y) - R_{Dn,p} S(x,y,t) + G_{ph} \mathrm{QE.EXCITON} - \frac{\mathrm{PHEFF.EXCITON}}{\mathrm{TAUS.EXCITON}} S(x,y,t) + \nabla D_S \nabla S(x,y,t)$$

Langevin recombination

Non-radiative GP decay

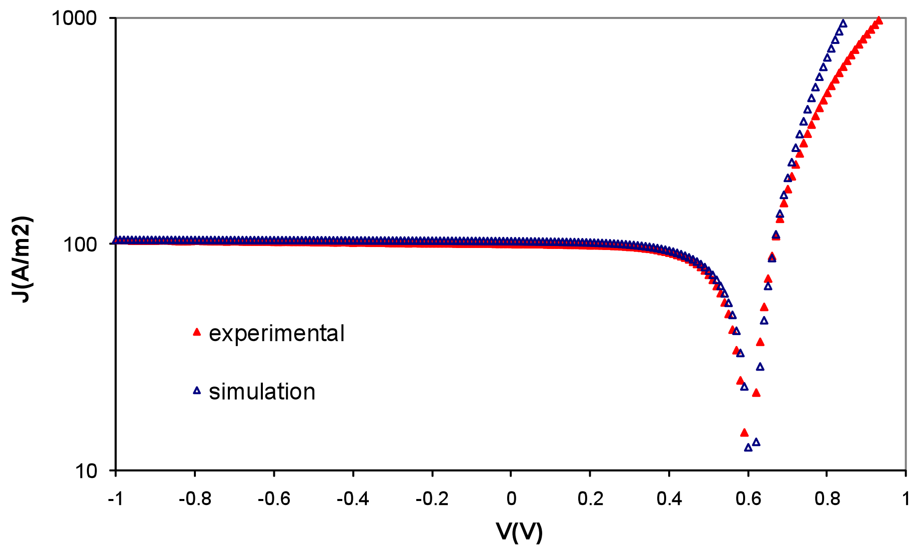
GP dissociation

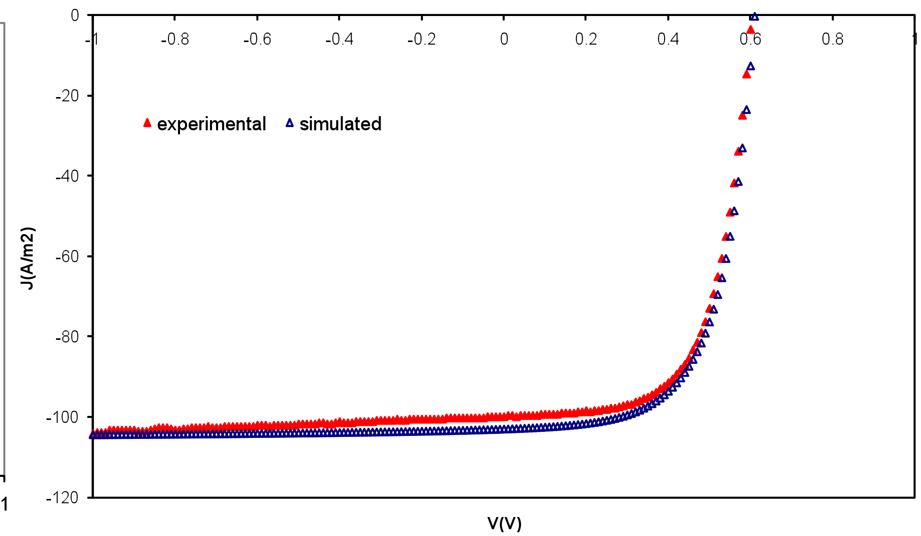
Photogeneration and efficiency of photon to GP transitions

Radiative GP decay and GP diffusion

2. 1. EXPERIMENTAL VS. SIMULATION

ITO/PEDOT:PSS/P3HT:PCBM/Yb/Al



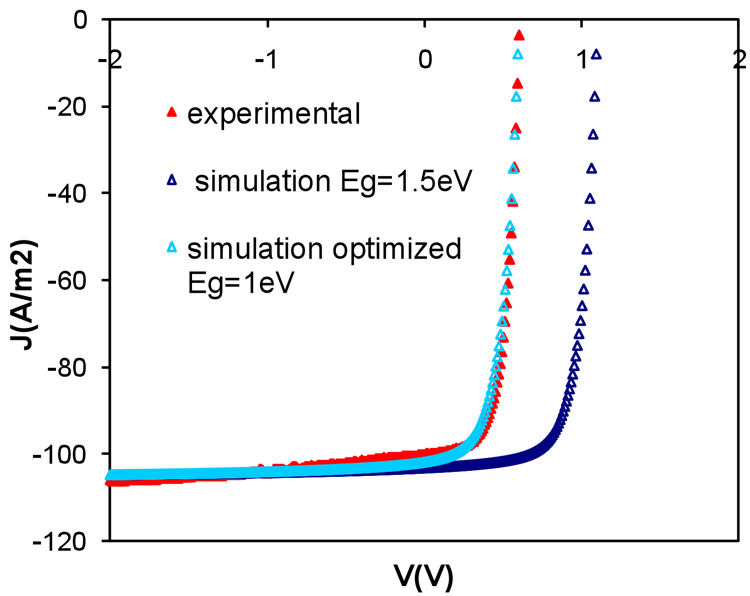


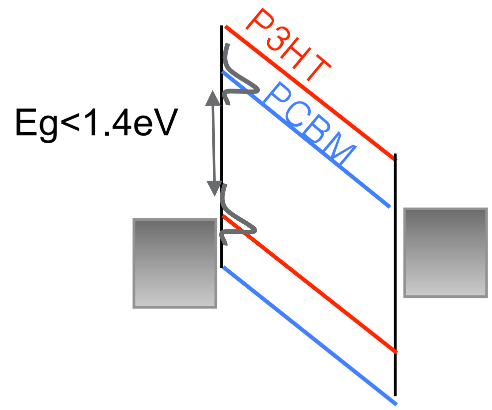
	Voc(V)	Jsc(mA/m2)	FF(%)	Eff(%)
simulation	0.595	103.0	64.3	3.94
experimental	0.603	100.0	63.7	3.85

Exact fitting parameters are available from Silvaco or from the authors.

2. 2. DEFINITION OF Eg

ITO/PEDOT:PSS/P3HT:PCBM/Yb/Al



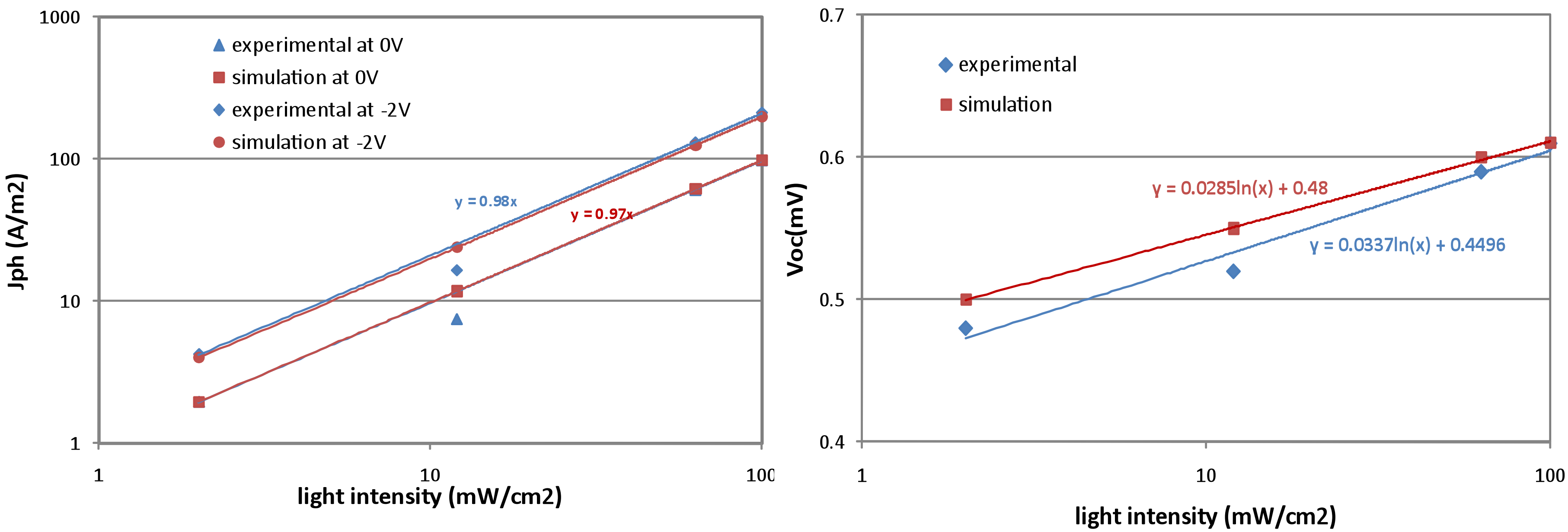


The energetic disorder characteristic of organic semiconductors (DOS), leads to at least 2x0.1eV lowering of the effective bandgap (Eg):

Eg= LUMO (acceptor) - HOMO (donor) – 2xDDOS

2. 3. LIGHT-INTENSITY DEPENDENCE

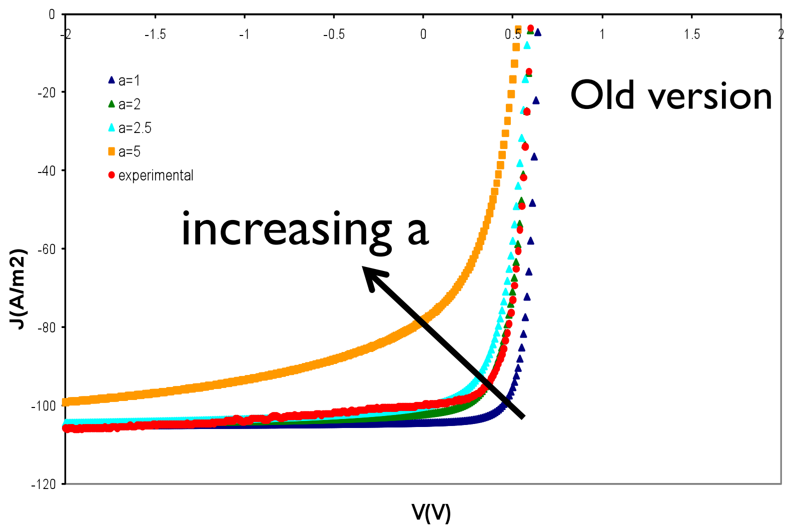
ITO/PEDOT:PSS/P3HT:PCBM/Yb/Al

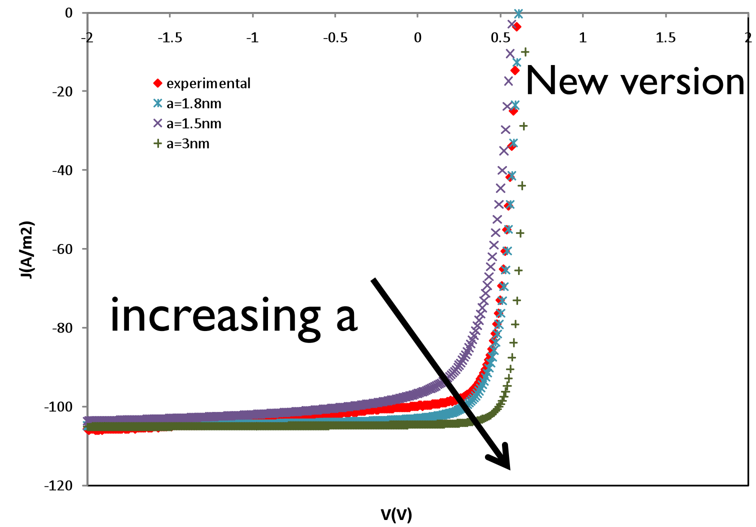


Light intensity dependence of the simulated results are in good agreement with the experimental results.

2. 4. GEMINATE PAIR BOUNDING ENERGY

ITO/PEDOT:PSS/P3HT:PCBM/Yb/Al



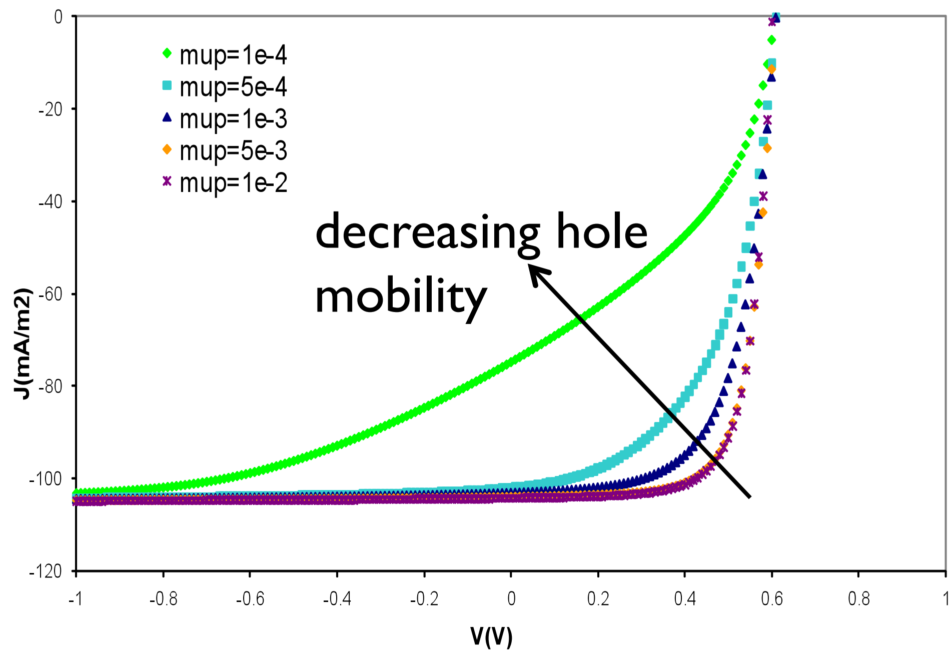


In the previous version of the simulator the geminate pair separation distance and binding energy were separate fitting parameters: producing non-physical results as this example. The new release links the two parameters with a Columbic relation where the user can still adjust the binding energy.*

* Arkhipov et al., APL, 2003, 82, 4605

2. 5. CASE STUDY: DECREASING MOBILITY

ITO/PEDOT:PSS/P3HT:PCBM/Yb/Al



Case of unbalanced charge carrier mobility leading to a space-charge limitation of the J_{ph} described by Mihailetchi et al.

The accumulation of the holes close to the anode leads to a large potential drop in this region as can be well observed with the simulation.

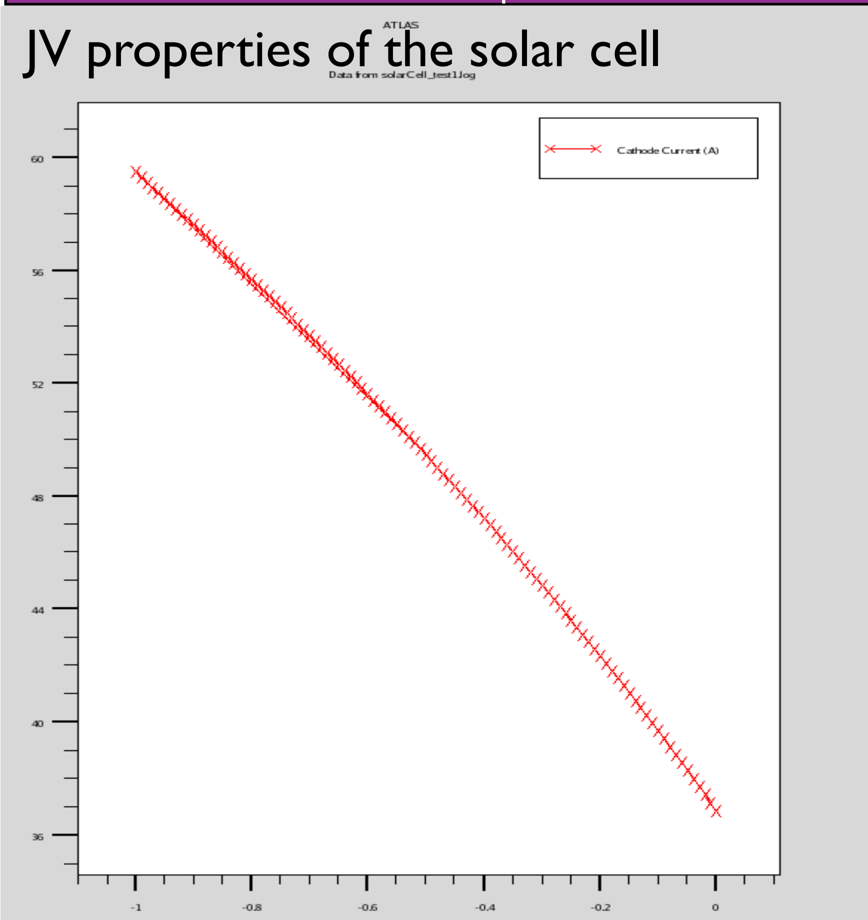
Mihailetchi et al., Phys. Rev. Lett., 2005, 94, 126602

2. 5. CASE STUDY: DECREASING MOBILITY

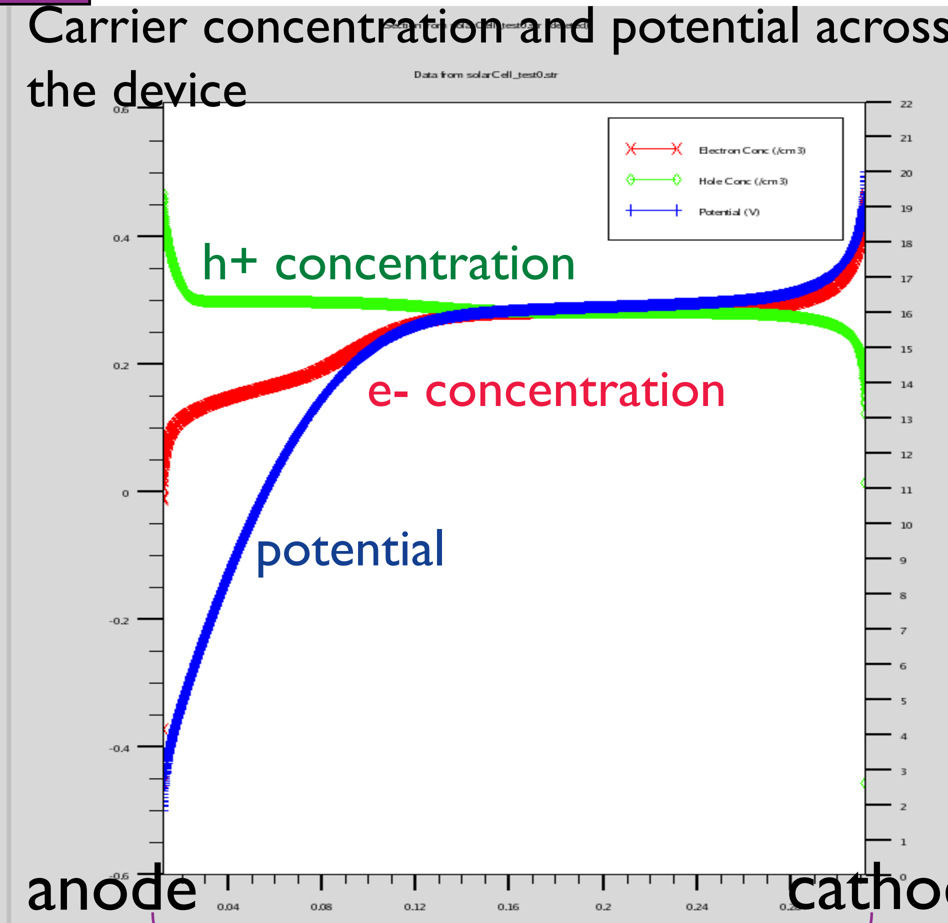
ITO/PEDOT:PSS/P3HT:PCBM/Yb/Al

μ_n =3 10^{-3} cm^2/Vs μ_p= 0.9 10^{-5} cm^2/Vs

JV properties of the solar cell



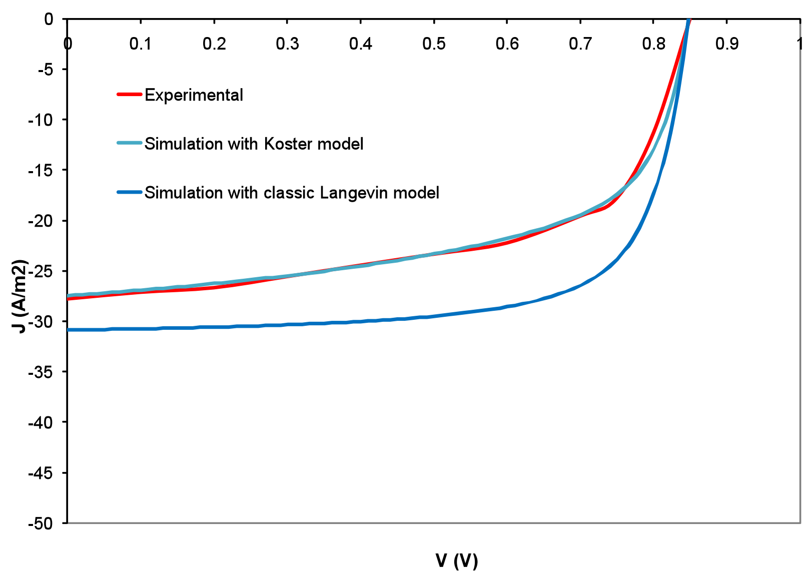
Carrier concentration and potential across the device



effective organic medium (~300nm)

2.6. LANGEVIN RECOMBINATION MODEL

ITO/PEDOT:PSS/MDMO-PPV:PCBM/Yb/Al



Langevin recombination in bulk heterojunction solar cells is described by the minimum of the charge carrier mobilities. Koster et al.

The modification of the classical Langevin model is crucial in case of MDMO-PPV:PCBM cells, for example.

Koster et al., APL, 2006, 88, 052104

3. NOVEL MODELS AND TOOLS

At the donor-acceptor interface, there are permanent dipoles, and energetic disorder.

Both affect the exciton dissociation, the geminate pair dissociation (cfr. Groves) or recombination, and the charge transport of the carriers (e.g.: dipoles create an electric field which influences carrier drift).

Groves et al., Nanoletters, 2010, 10, 1063

CONCLUSIONS

- Silvaco's Organic Solar Module simulation matches experimental results in the -1V<V<Voc region (provided exact material parameters)
- Access to physical parameters greatly helps in-depth understanding of the device physics (for examples, distribution of carrier concentration, potential across the device or the geminate pair dissociation efficiency in function of the voltage)
- Implementation of other available models such disorder, trapping and Poole-Frenkel mobility could further bring closer experimental and simulation results.