FLUXiM

Optoelectronic Simulation of Light-emitting and Light-harvesting Thin Film Devices

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SSOM Engelberg Lectures

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Motivation


Unser Planet bei Nacht
Der Anteil der Beleuchtung am
weltweiten Stromverbrauch
beträgt 19%
(und 14% in Europa)

Looking for innovation

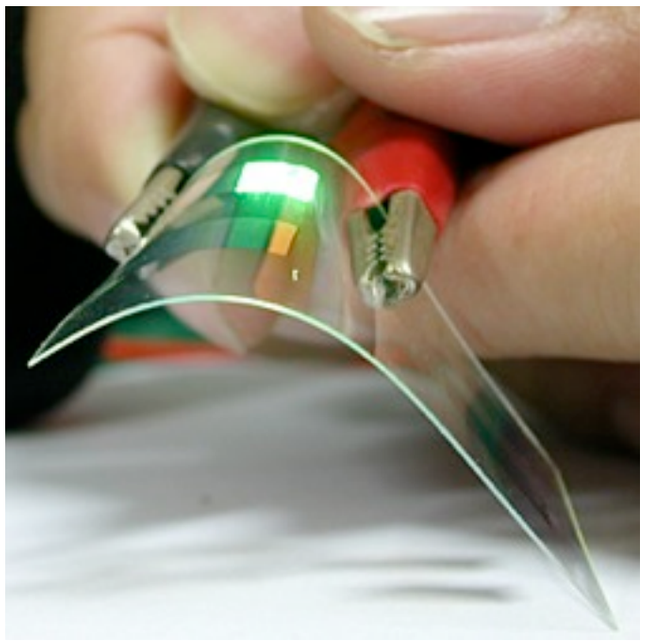
Exploit multitude of novel synthetic materials!

OLEDs for general lighting and displays

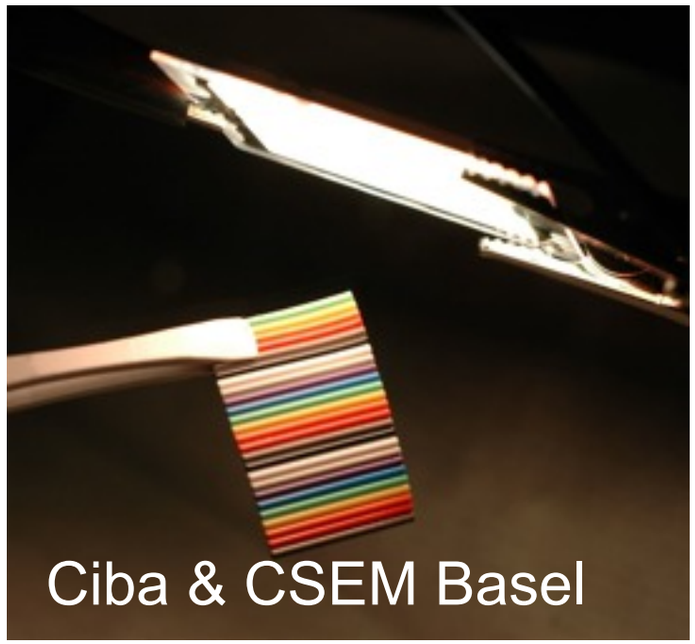
› low power consumption
› ultra-thin
› efficient wide-area light sources (up to 100 lm/W)
› high contrast ratio
› wide viewing angle, ...

Sony „XEL-11“ 2008

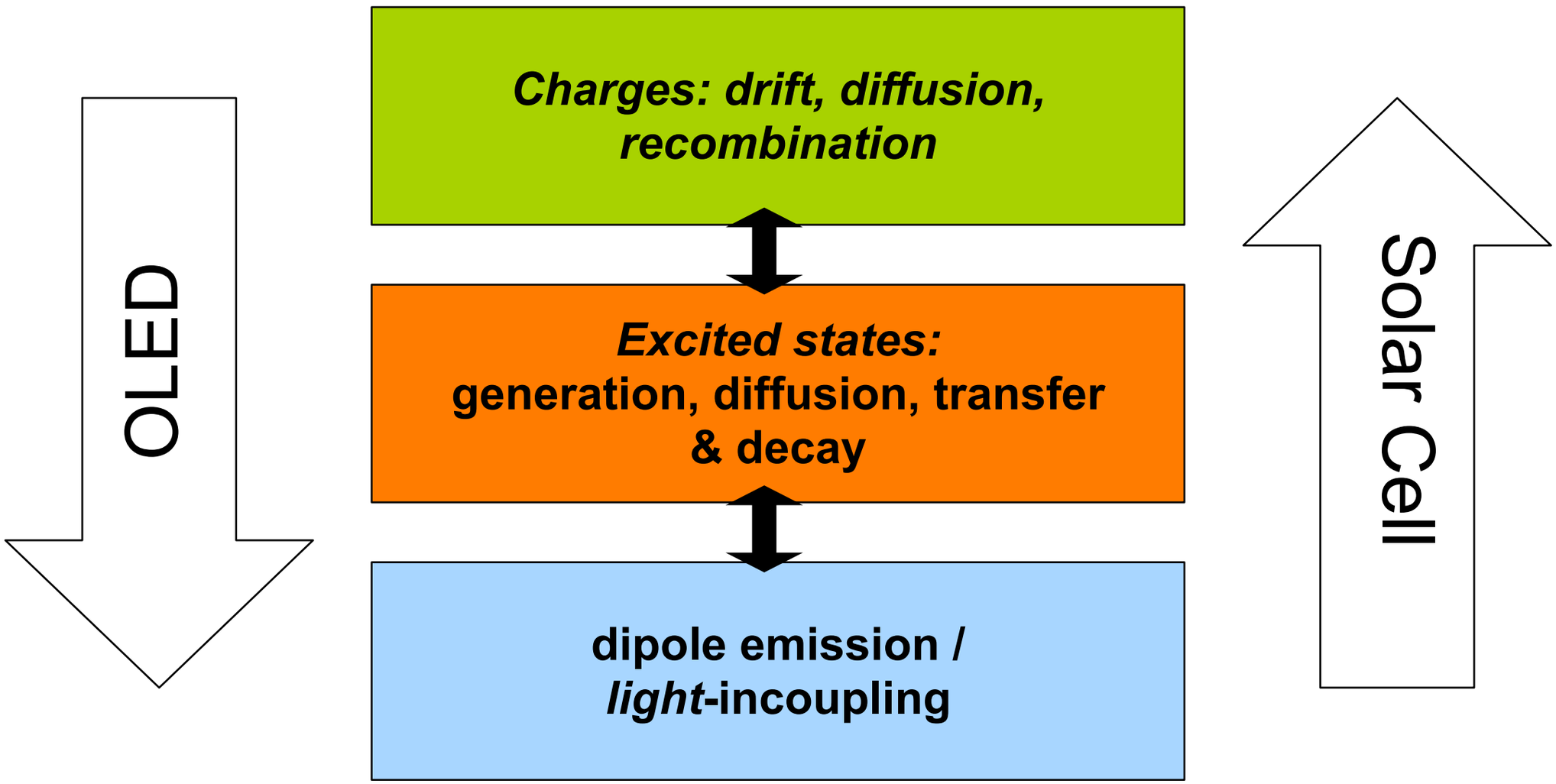
Flexible OLEDs



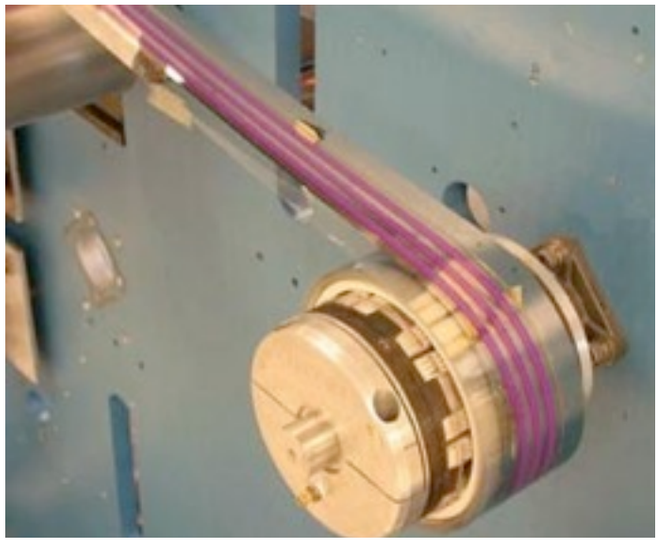
White OLED

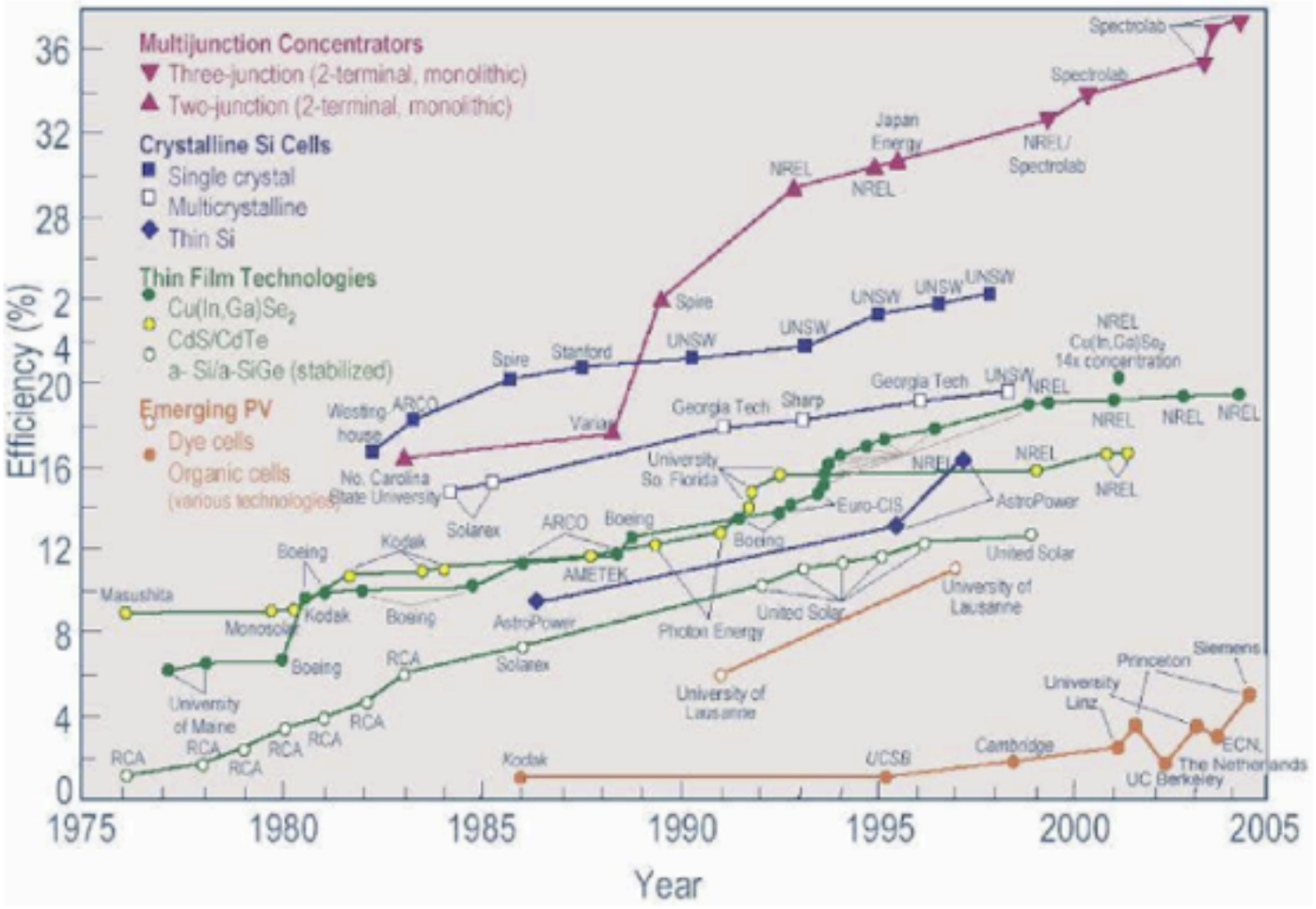


Same physics, time-inverted



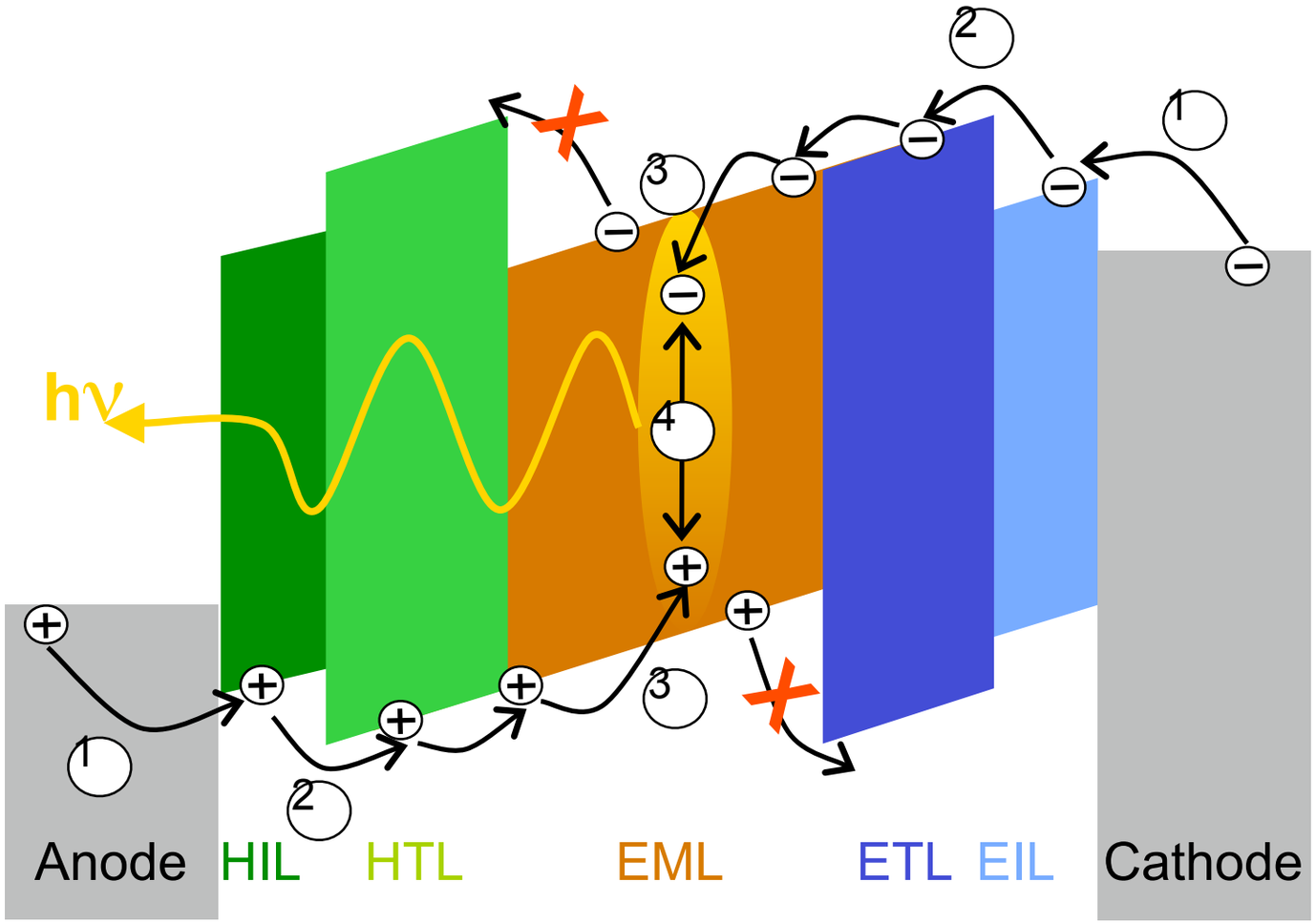
Organic solar cells





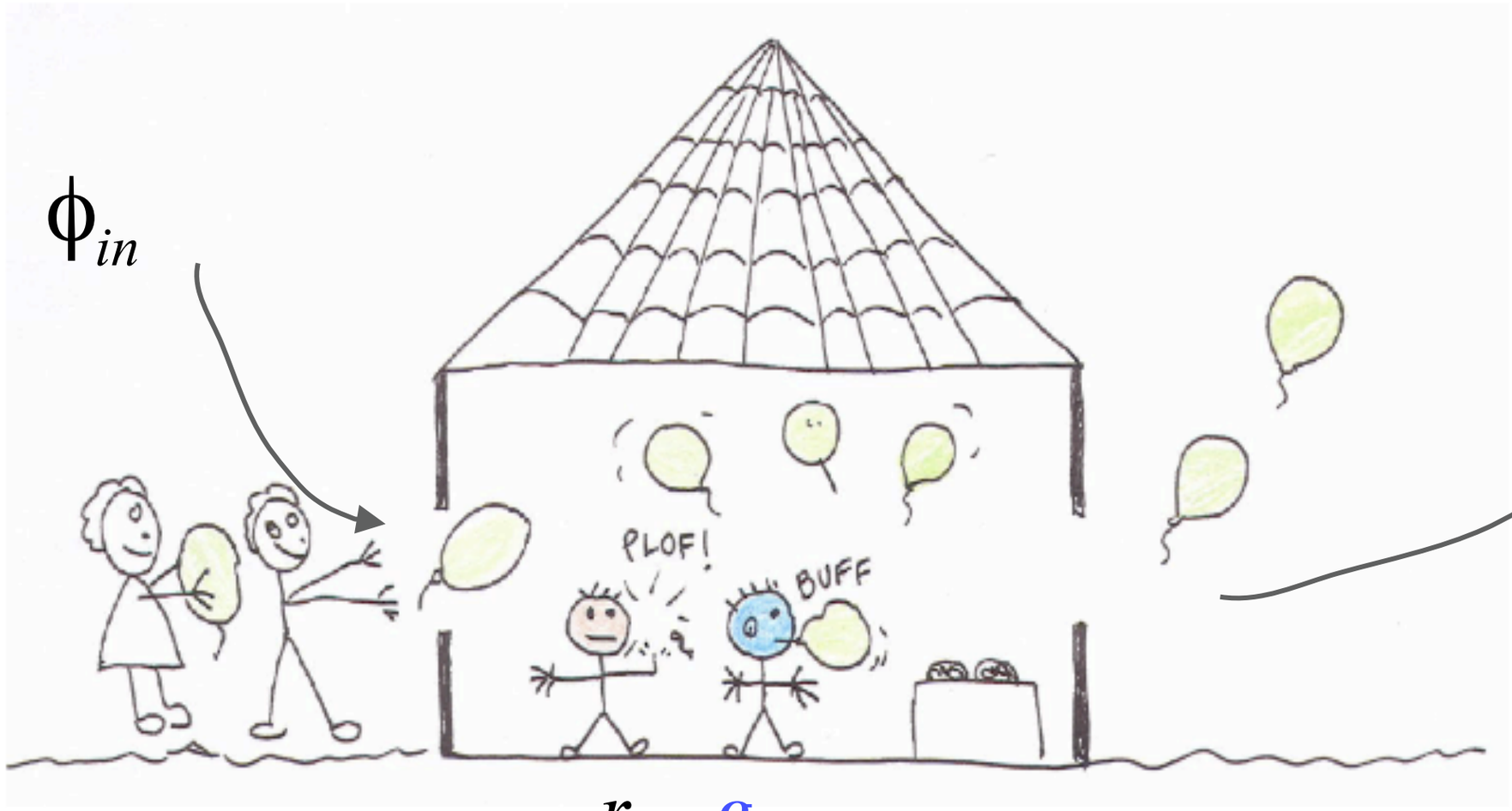
› thinness
› flexibility
› printability (roll-to-roll)

Optoelectronic device physics



- Processes:
  - › Charge injection (1)
  - › Charge transport (2)
  - › Exciton formation, transfer & diffusion (3)
  - › Light outcoupling (4)
- Multilayer design:
  - › facilitates injection
  - › improves confinement
  - › reduces leakage

Coupled continuity equations

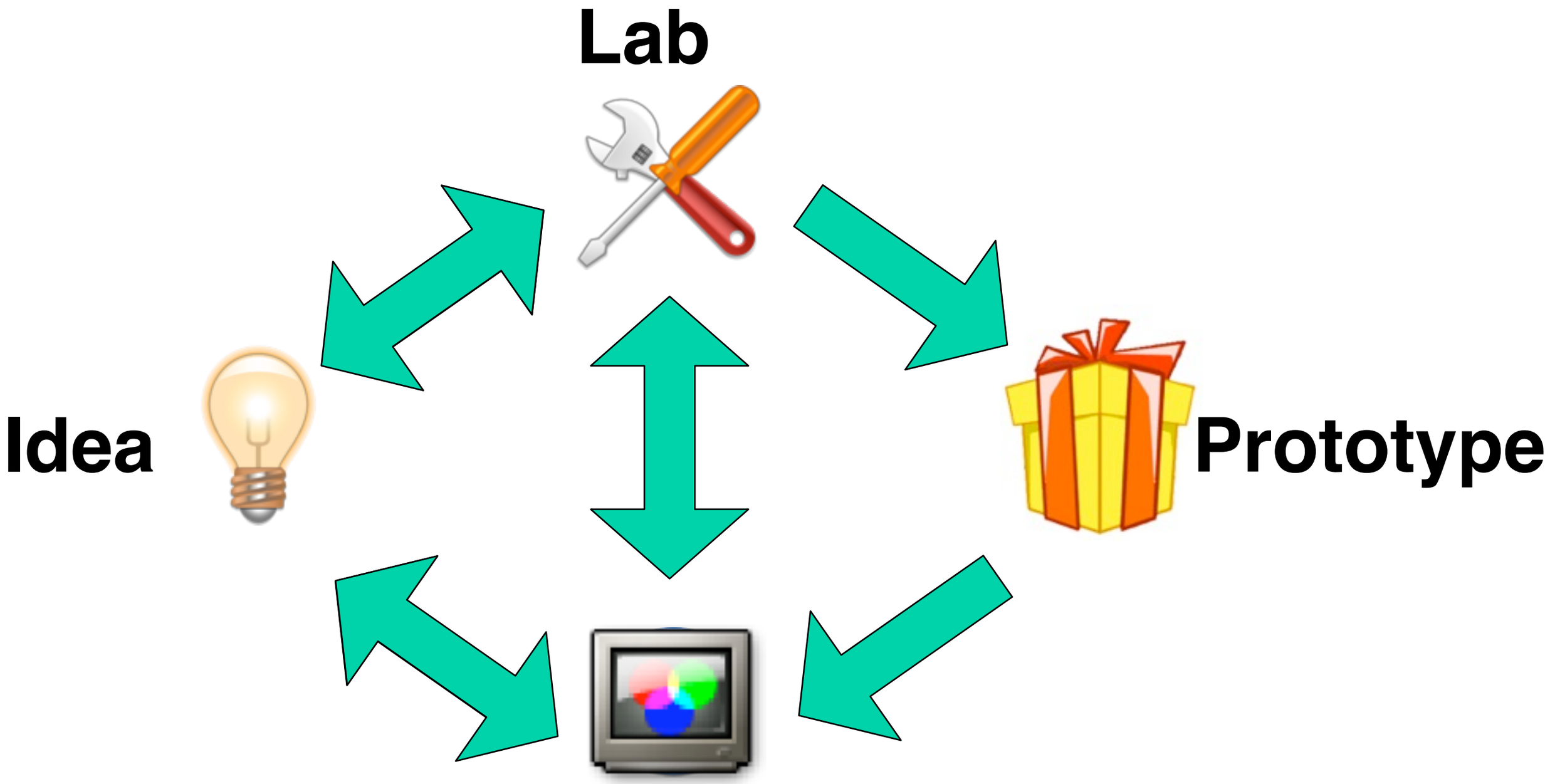


r g

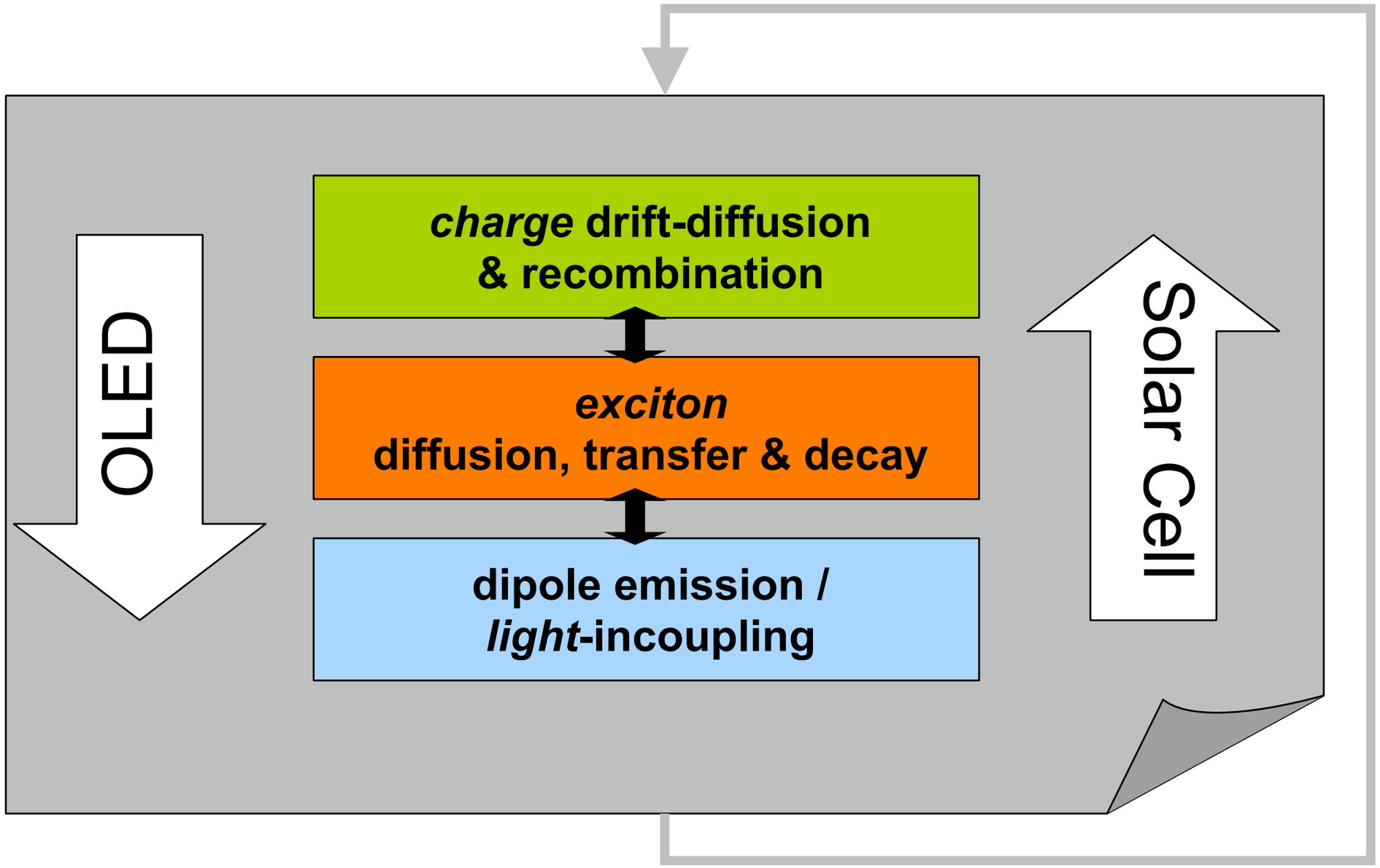
$$\boxed{\frac{\partial \psi}{\partial t} = q - \nabla \cdot \phi}$$

g - r $\quad \phi_{out} - \phi_{in}$

Research and development process

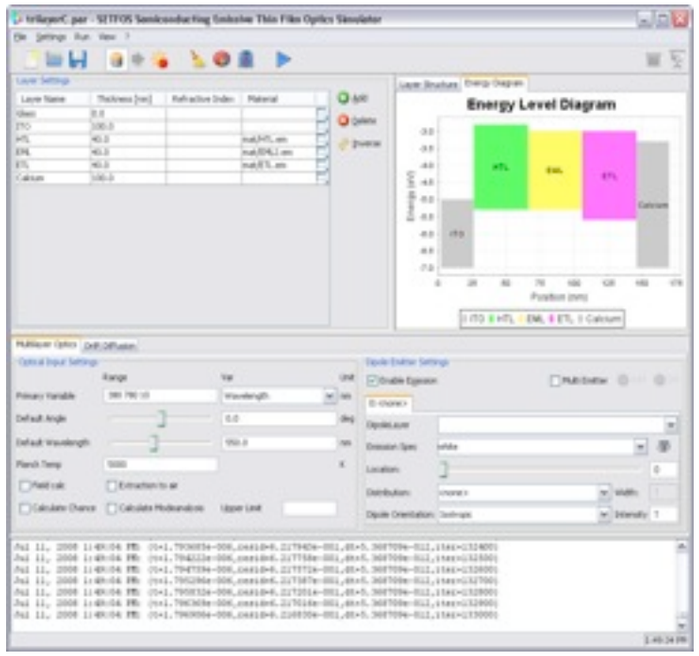


3 processes, one solver



setfos, semiconducting thin film optical simulator

Inputs




```
Structure

    Glass 0 nm
    ITO     100 nm
  Anode Thermionic WorkFunction 5.0 eV
    HTL     40  nm  Electrical "mat/HTL.em"
    EML     40  nm  Electrical "mat/EML1.em"
    ETL     40  nm  Electrical "mat/ETL.em"
  Cathode Thermionic WorkFunction 3.3 eV
    Calcium  100 nm

Define

  DriftDiffusion Gummel
    Temp 300 K
    Resid CurrentCont 1e-3 Check NIter 1000
    NoExcCalc
```

Software Architecture

Graphical user interface

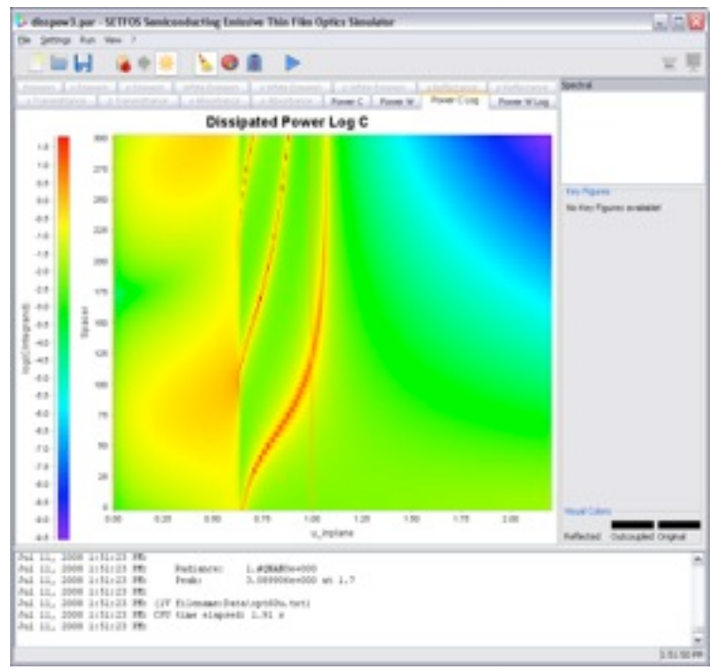
Simulation script

Simulation kernel

setfos

device simulation software

Outputs



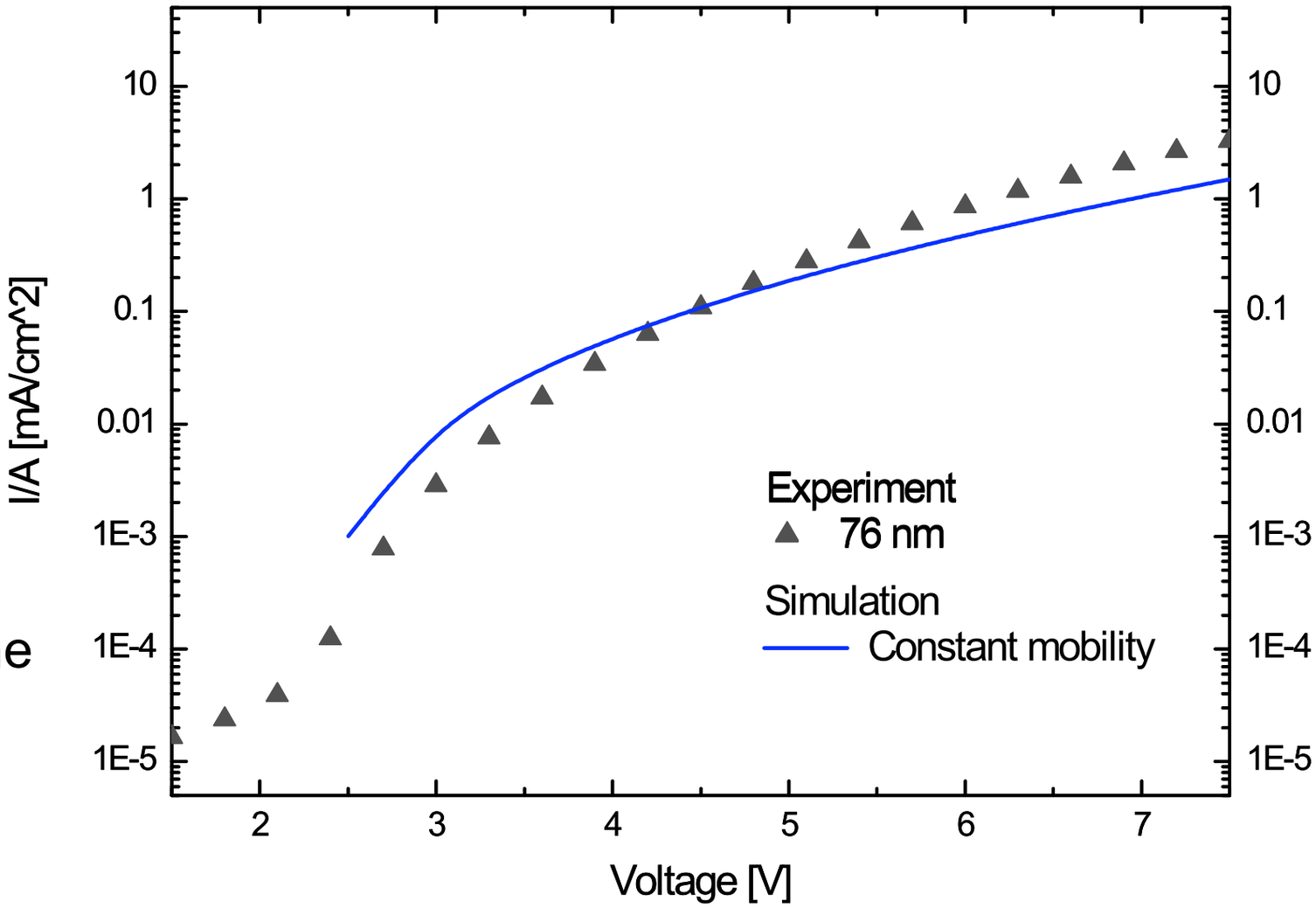

```
# Column format:
# Wavelength  C+  Cs+ Cp+ nCs+  W   Ws Wp Rs Ts As
380 2.176494e-004 1.088247e-004 1.088247e-004 7.25546
    1.360309e-002 1.360309e-002 3.351569e-001 ....
385 0.000000e+000 0.000000e+000 0.000000e+000 0.00000
    1.397787e-002 1.397787e-002 3.298139e-001 ....
390 0.000000e+000 0.000000e+000 0.000000e+000 0.00000
    1.441777e-002 1.441777e-002 3.244772e-001 ....
395 1.903083e-004 9.515415e-005 9.515415e-005 6.34403
    1.485623e-002 1.485623e-002 3.203269e-001 ....
400 0.000000e+000 0.000000e+000 0.000000e+000 0.00000
    1.520712e-002 1.520712e-002 3.186284e-001 ....
```

Current-voltage modeling

Constant mobility

$$v_D = \mu E$$

$$\mu = const$$



►Constant mobility does not fit the experimental data

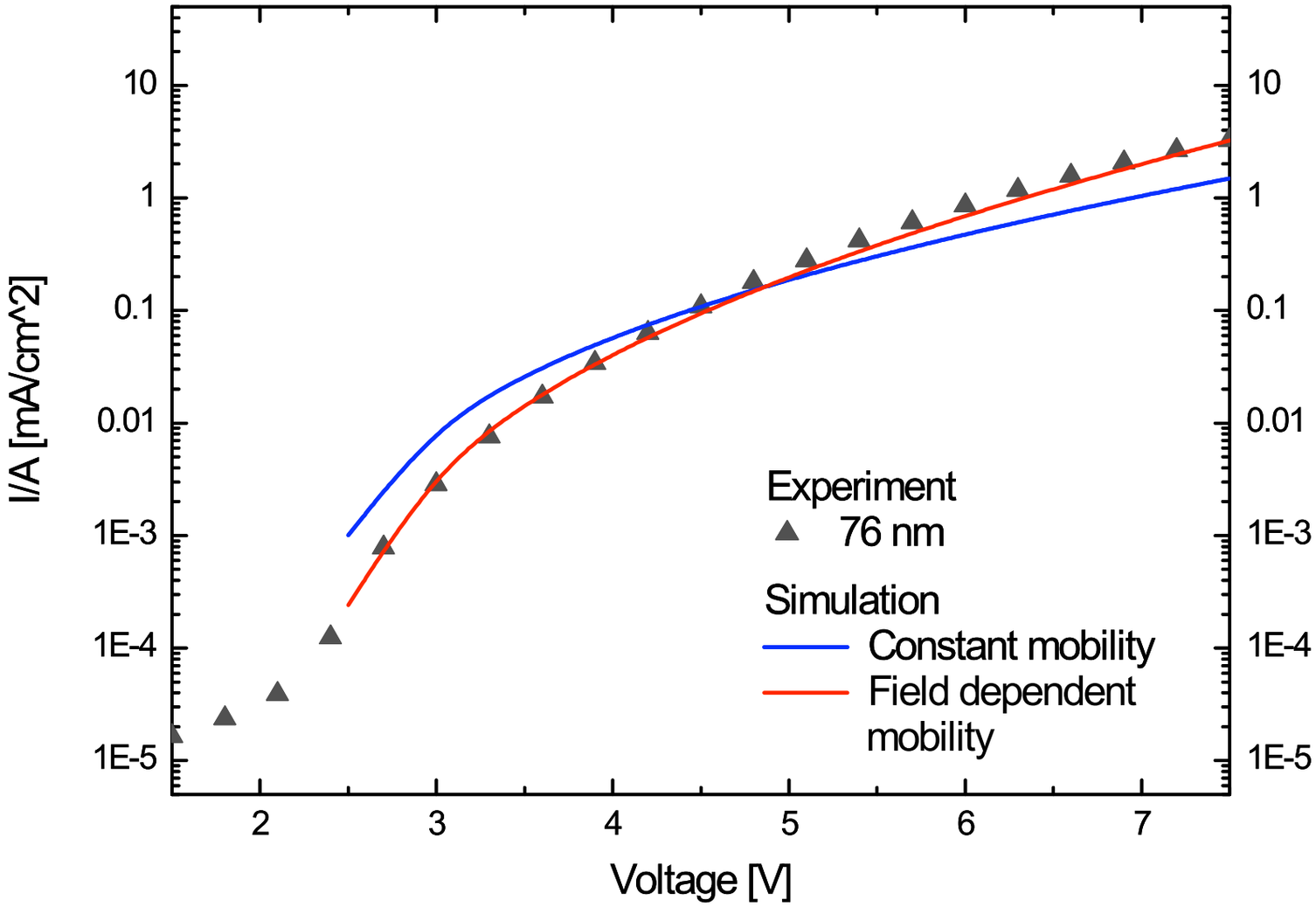
Current-voltage modeling

Field dependent mobility

$$v_D = \mu E$$

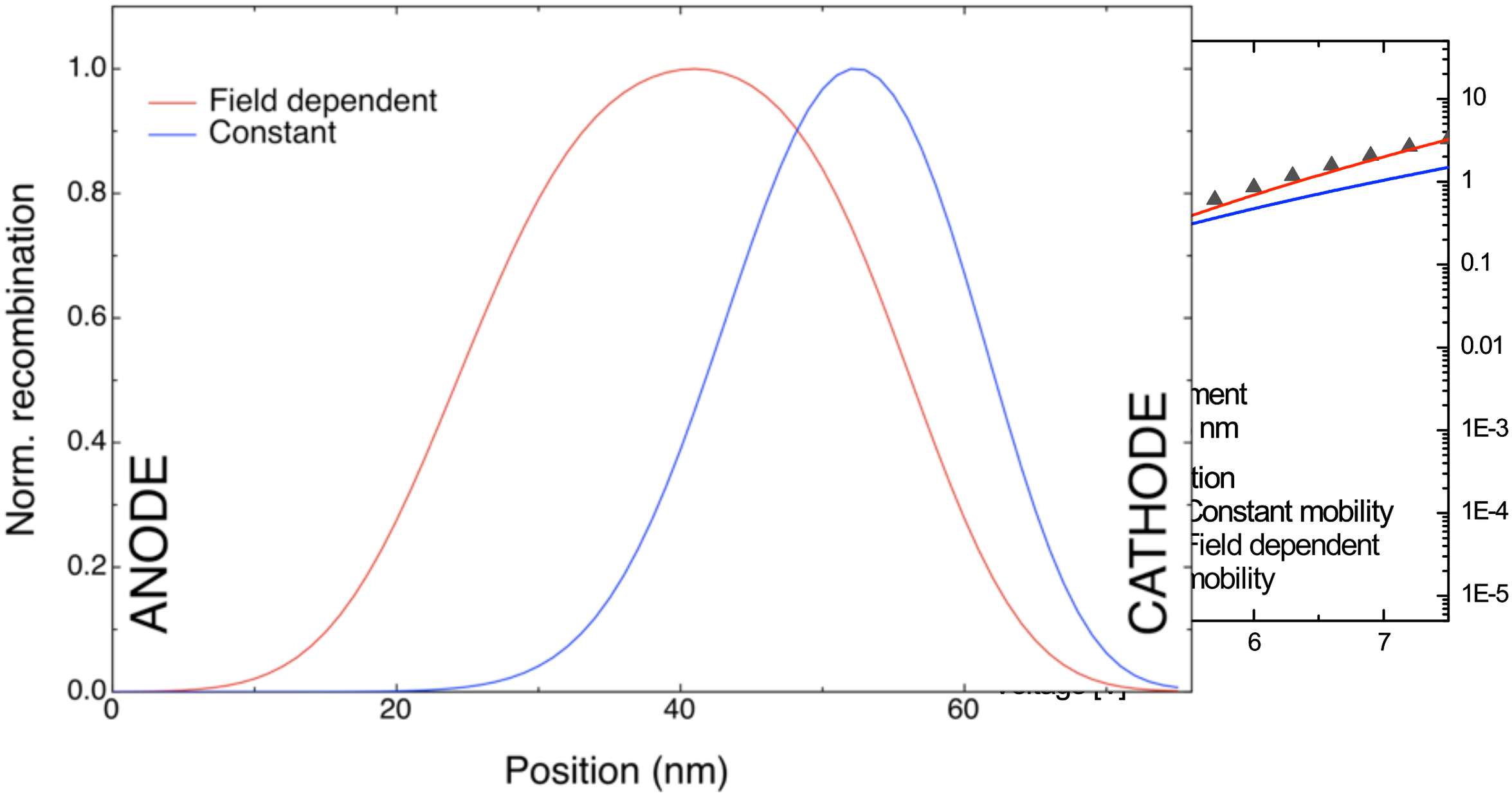
$$\mu = \mu_0 e^{\sqrt{\frac{E}{E_0}}}$$

► Field dependent mobility fits the experimental data



Current-voltage modeling

Field dependent mobility



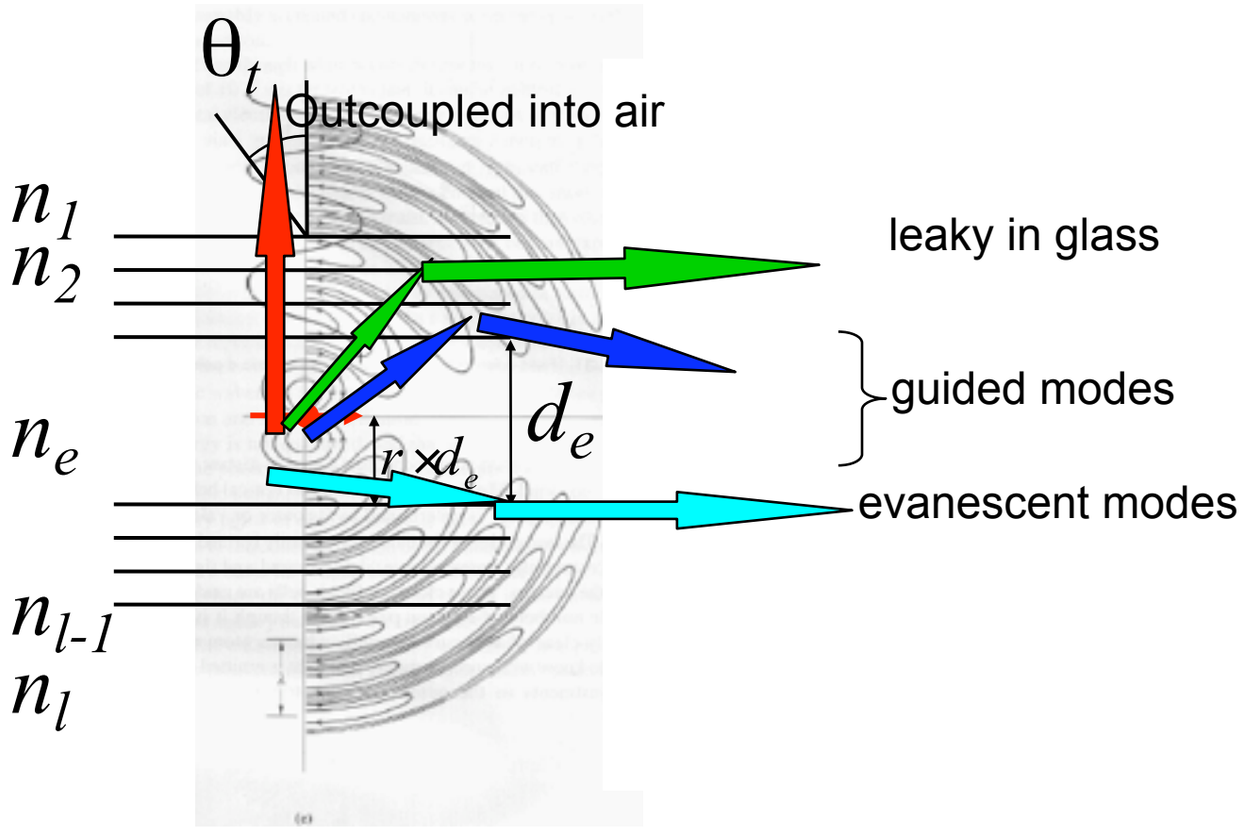
Light emission: dipole model

Dipole emission model with dependence on

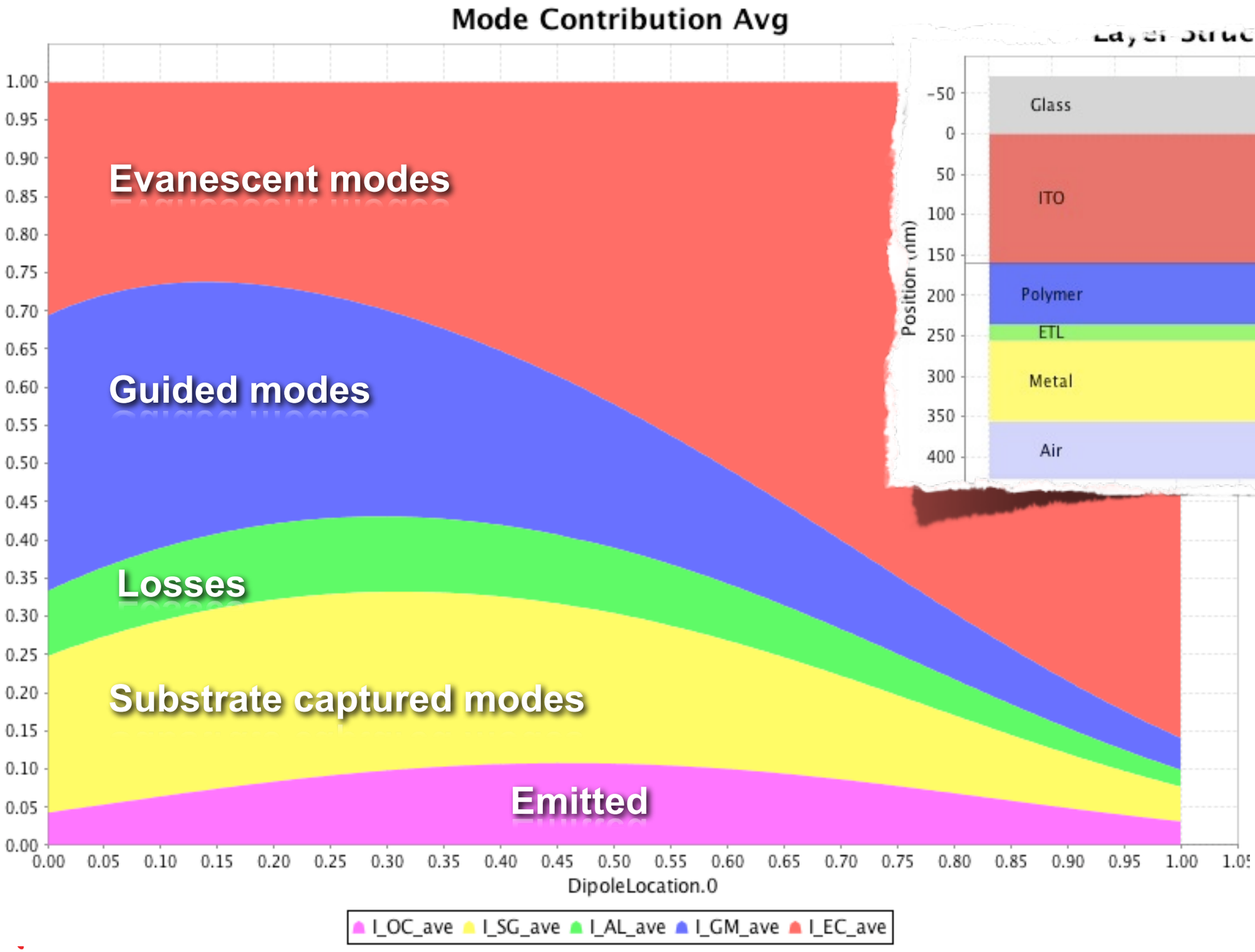
› viewing angle
› polarization
› dipole position
› dipole orientation

- **setfos** ***software allows:***

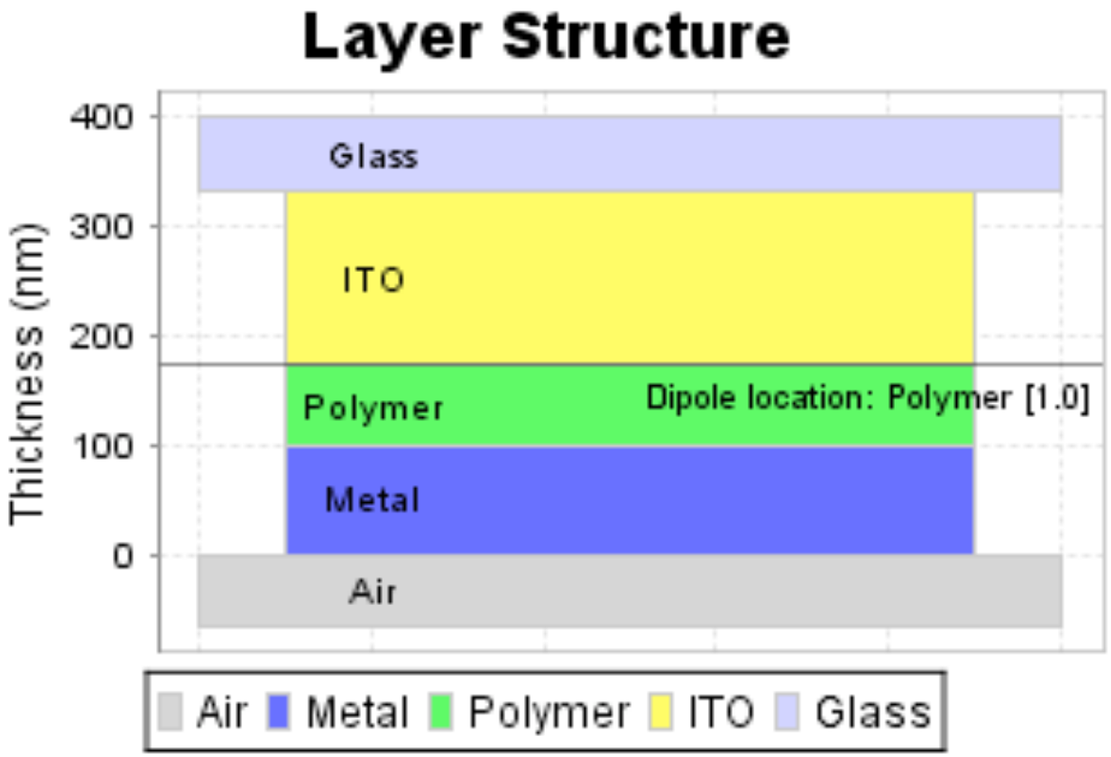
› multiple dipoles
› mode analysis
› performance figures:
CIE coord., CRI, SEIR, SIA etc.

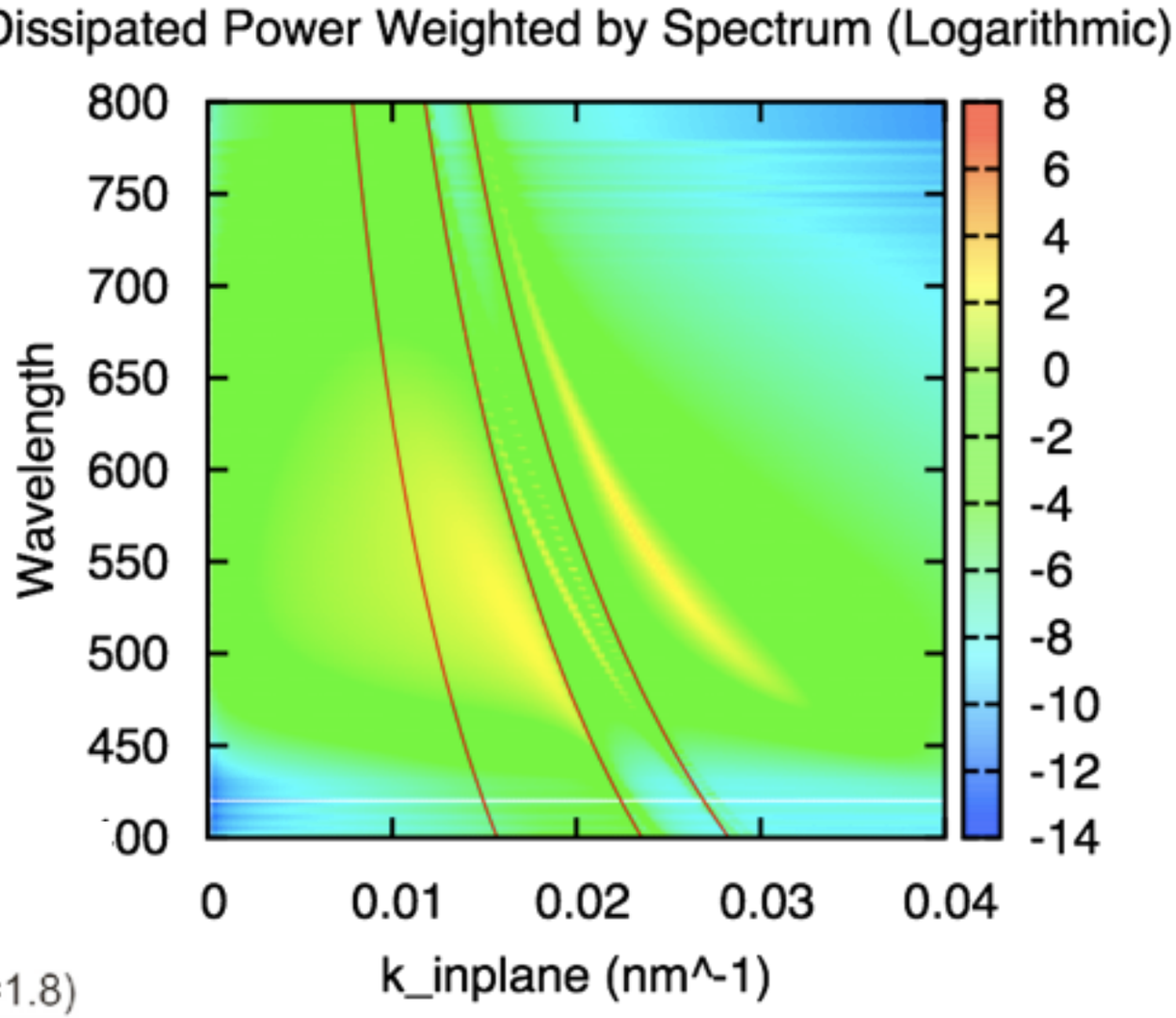


Mode analysis

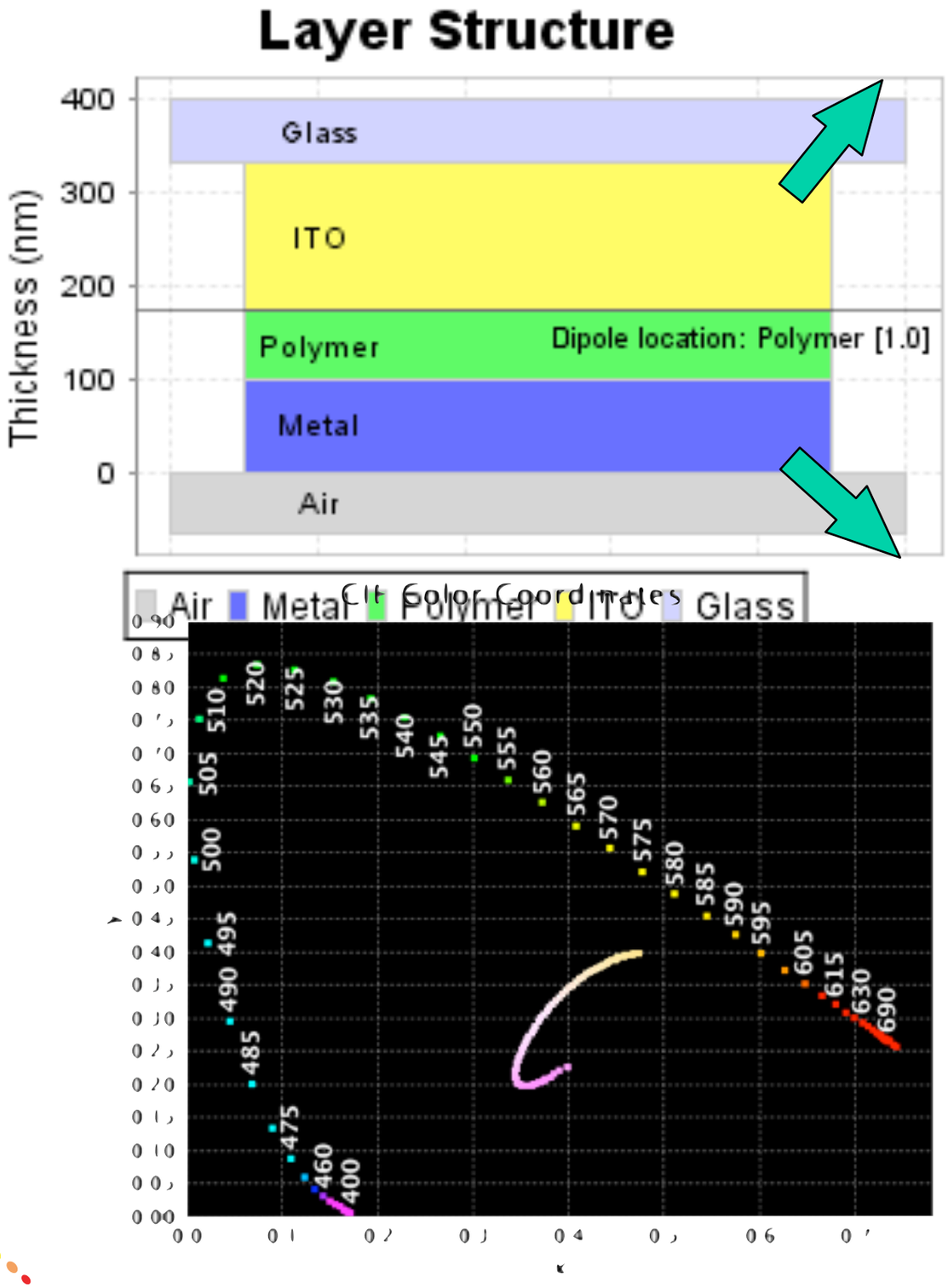


Outcoupling channels

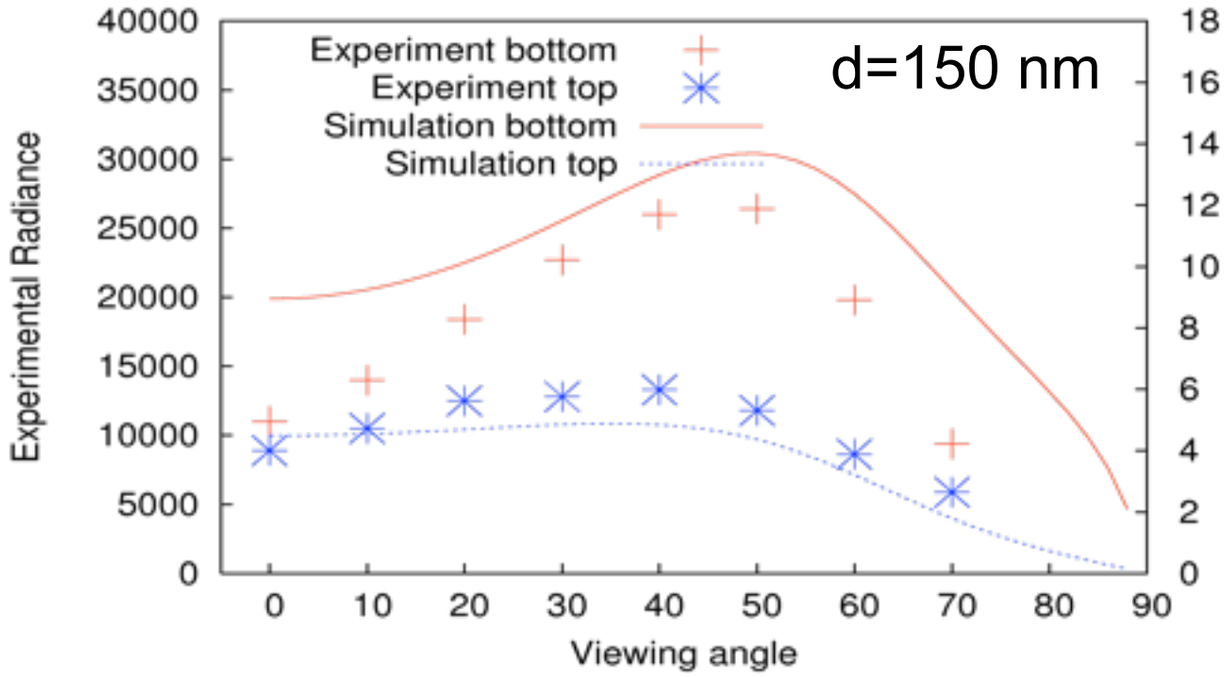




Forward and backward emission

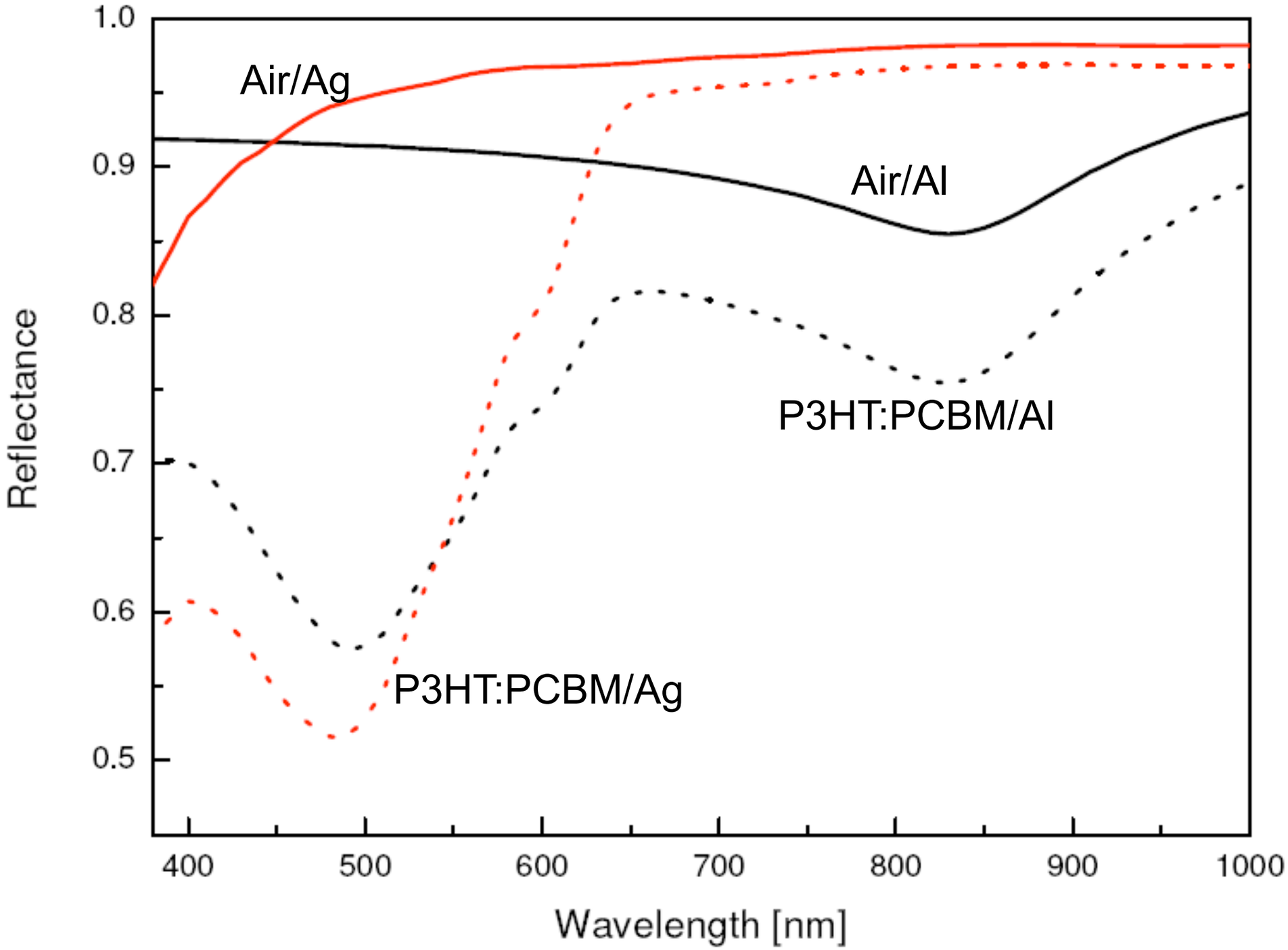


Comparison with experiment

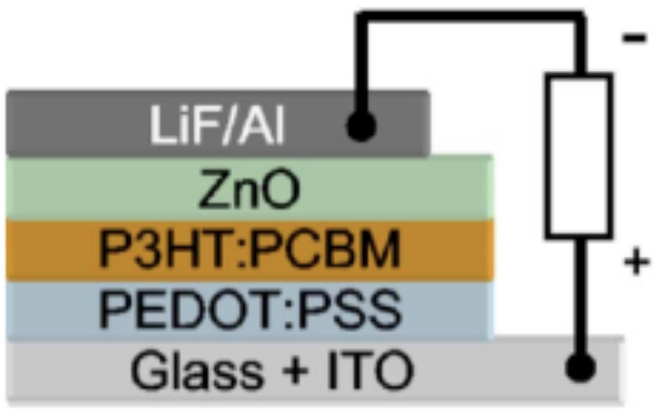


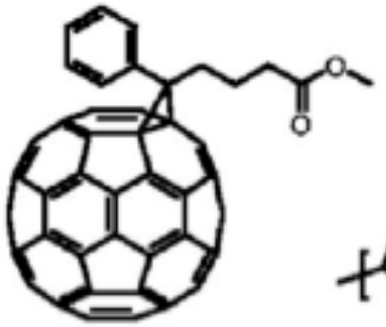
(Device: Al(15 nm)/PEDOT(60 nm)/
[76% PVK+19% PBD+5%
CGR-Red(x nm)] /
Ba(1 nm)/Al (15 nm))

Non-measurable parameters

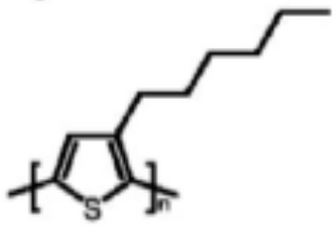


Organic solar cells

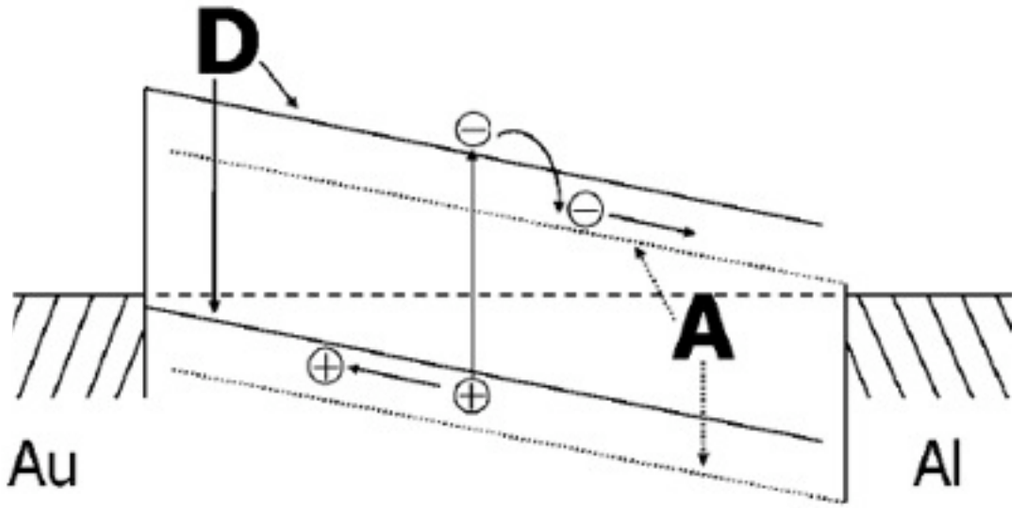




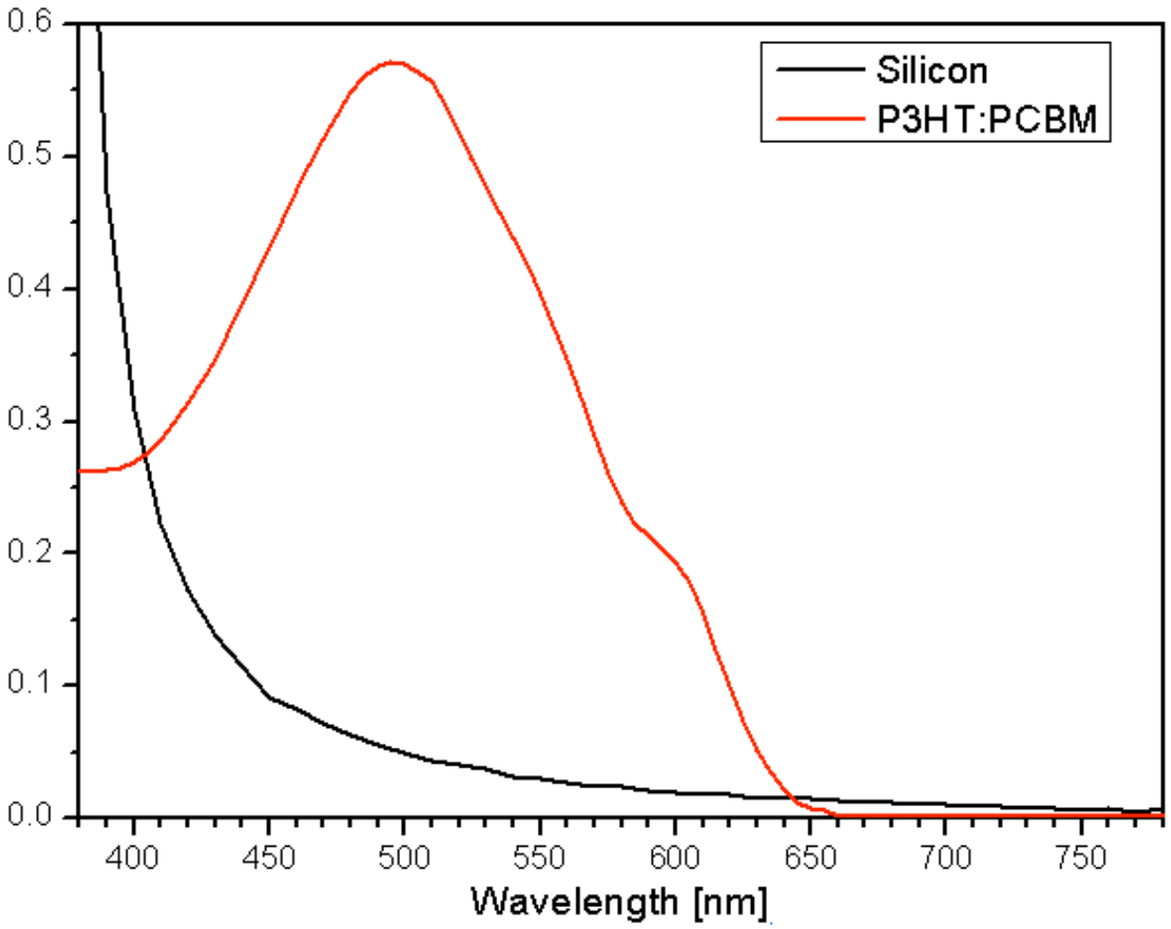
PCBM

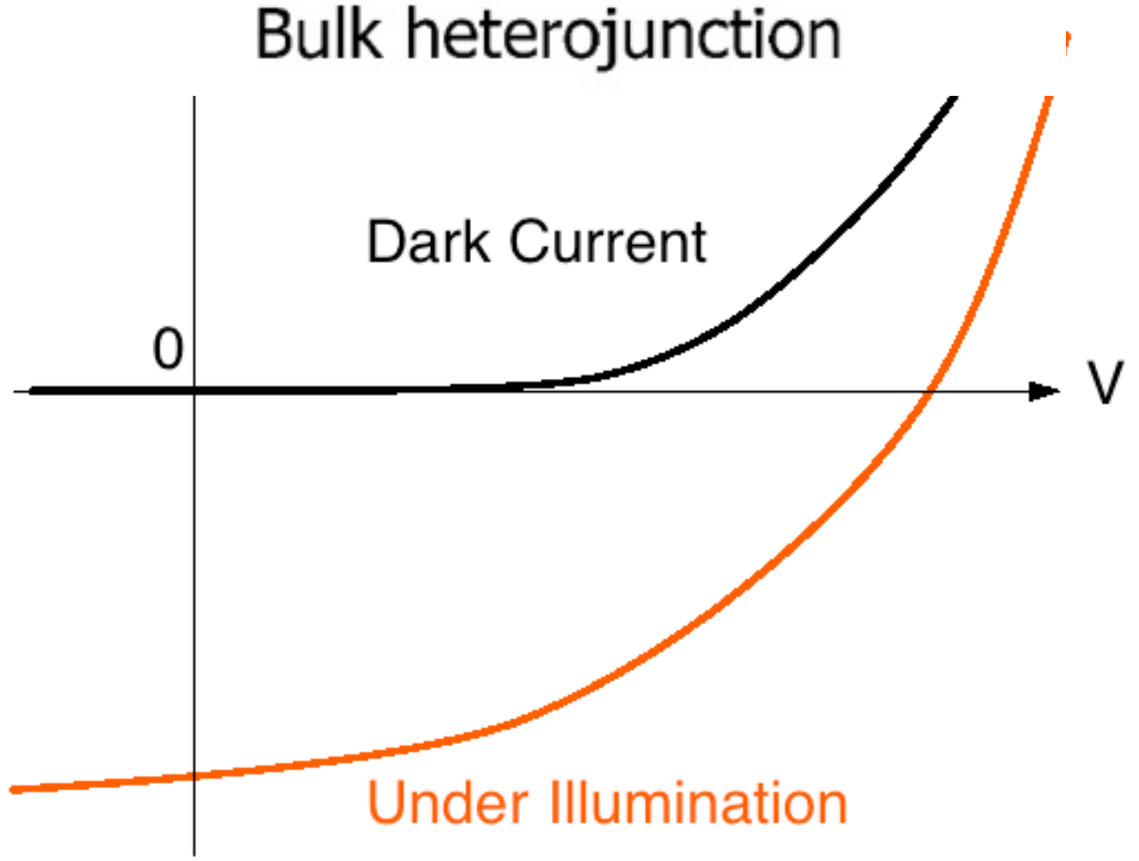


P3HT



Bulk heterojunction

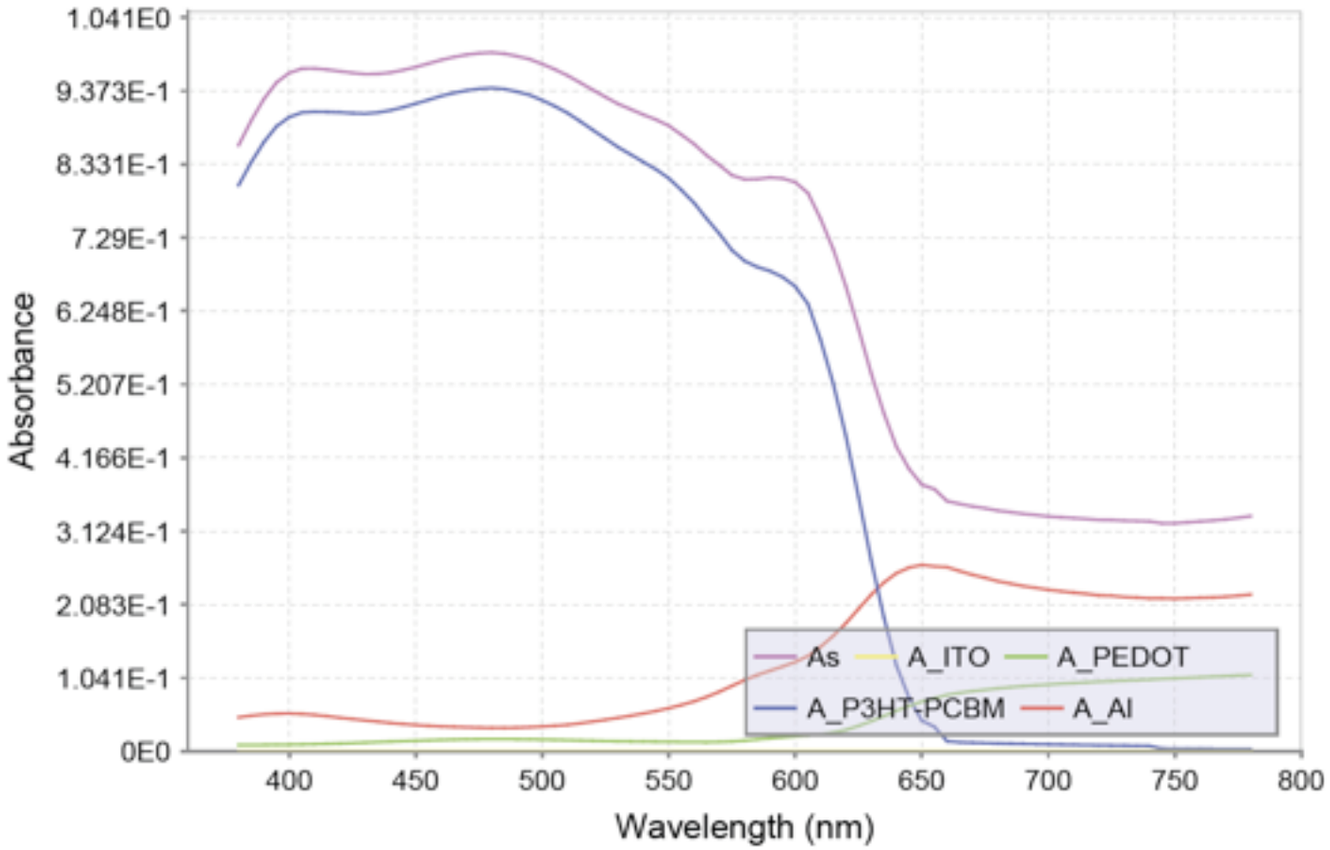


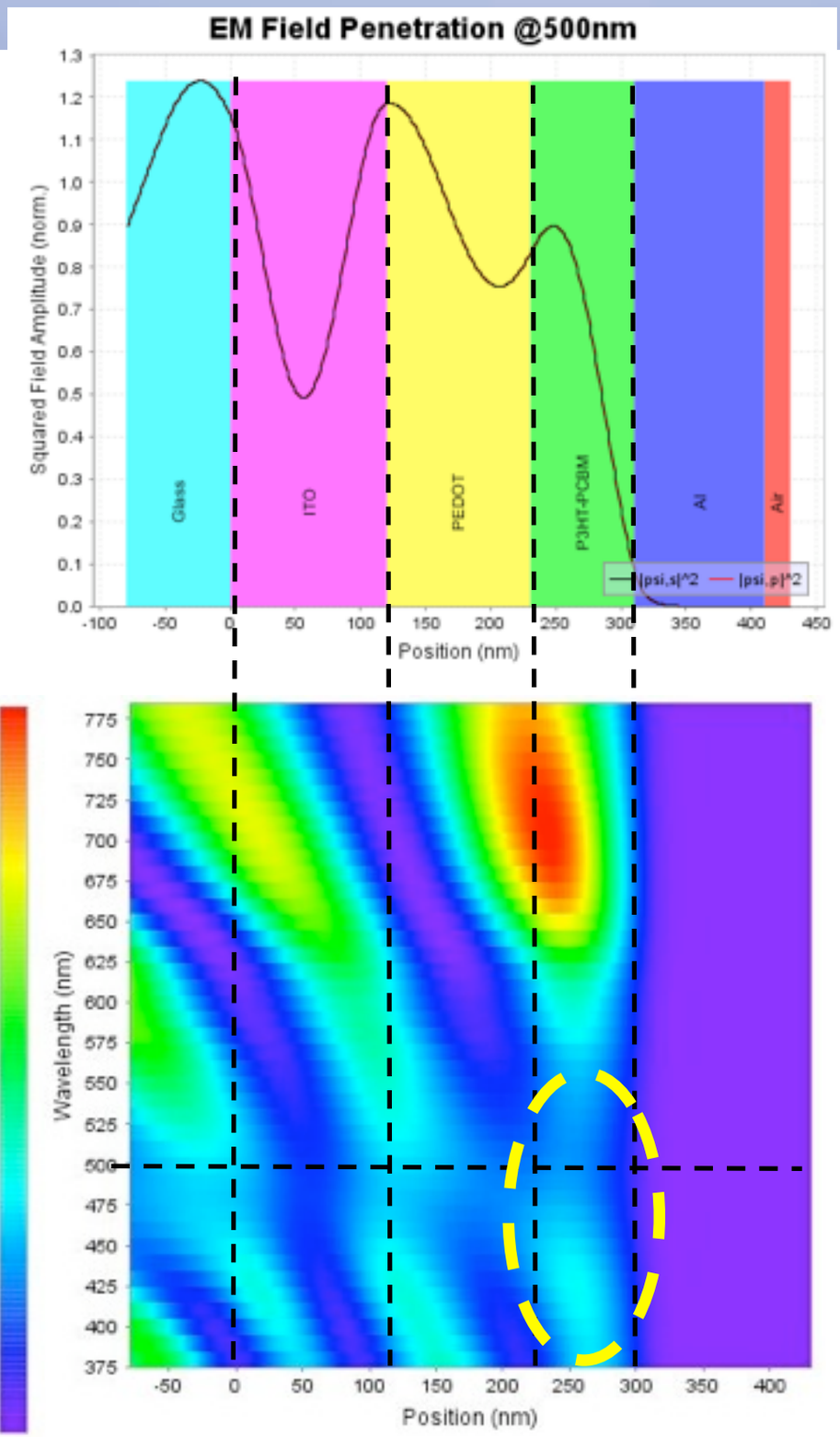


OPV Light-harvesting

Bulk-hetero-junction with
P3HT-PCBM
Simulation:

- *Spectral EM field penetration*
- *Layer-specific absorbances*

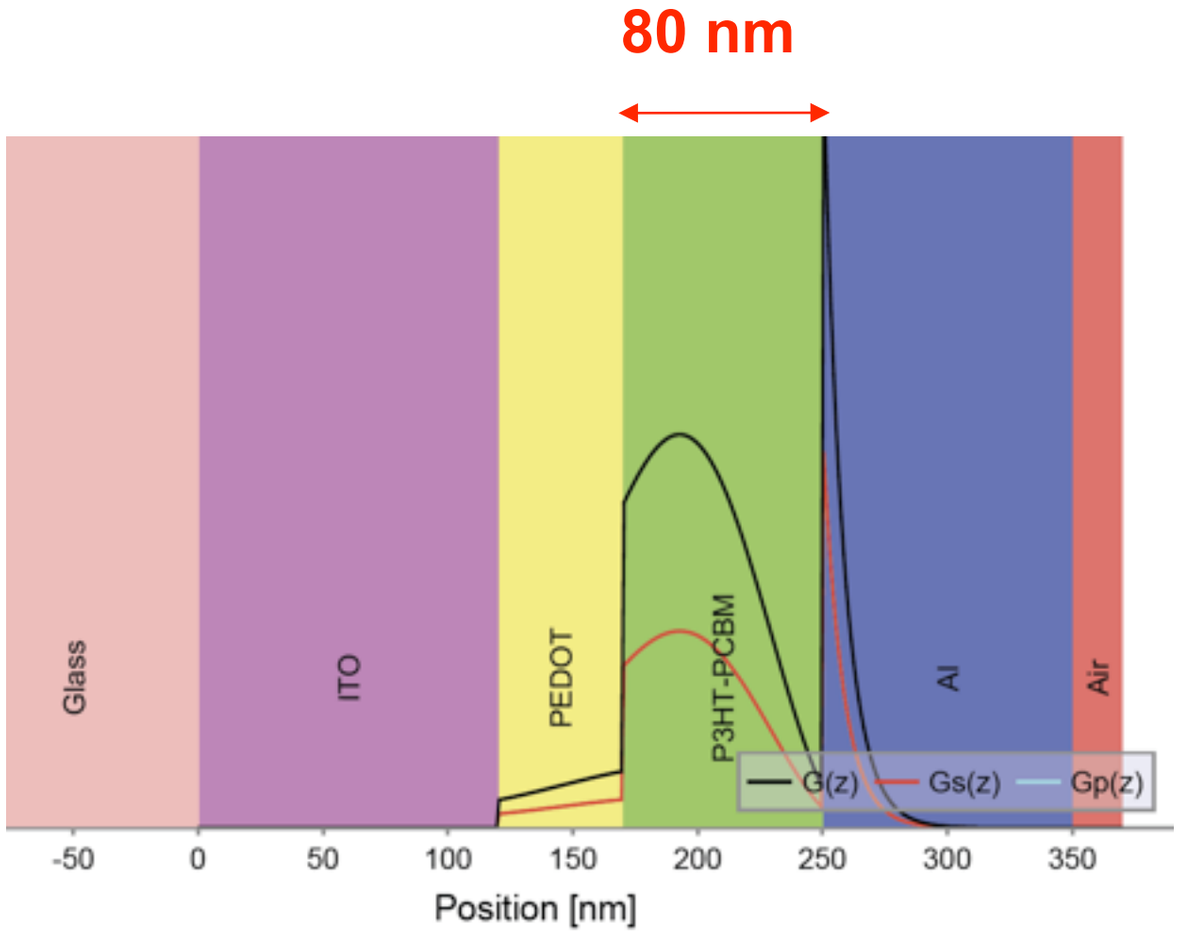


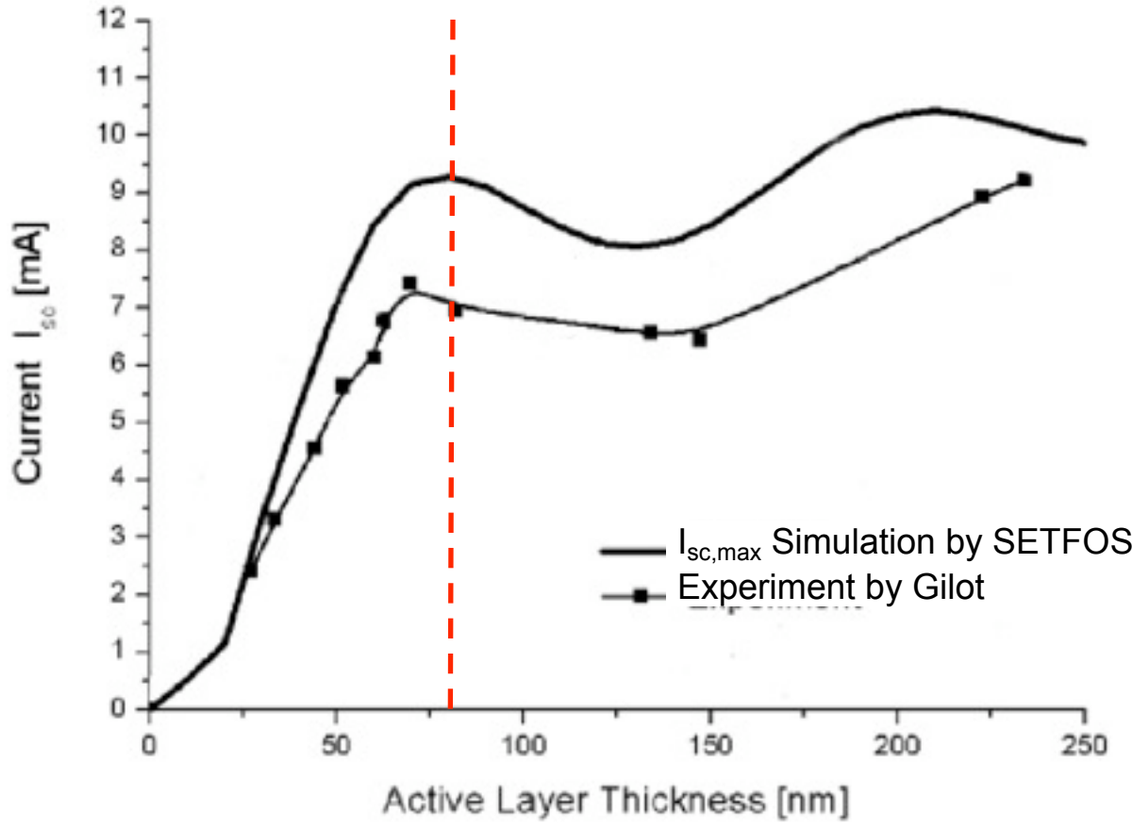


OPV Light-harvesting

Photon Absorption Profile

- Photocurrent Thickness Scaling
  - › 80 nm is optimum!

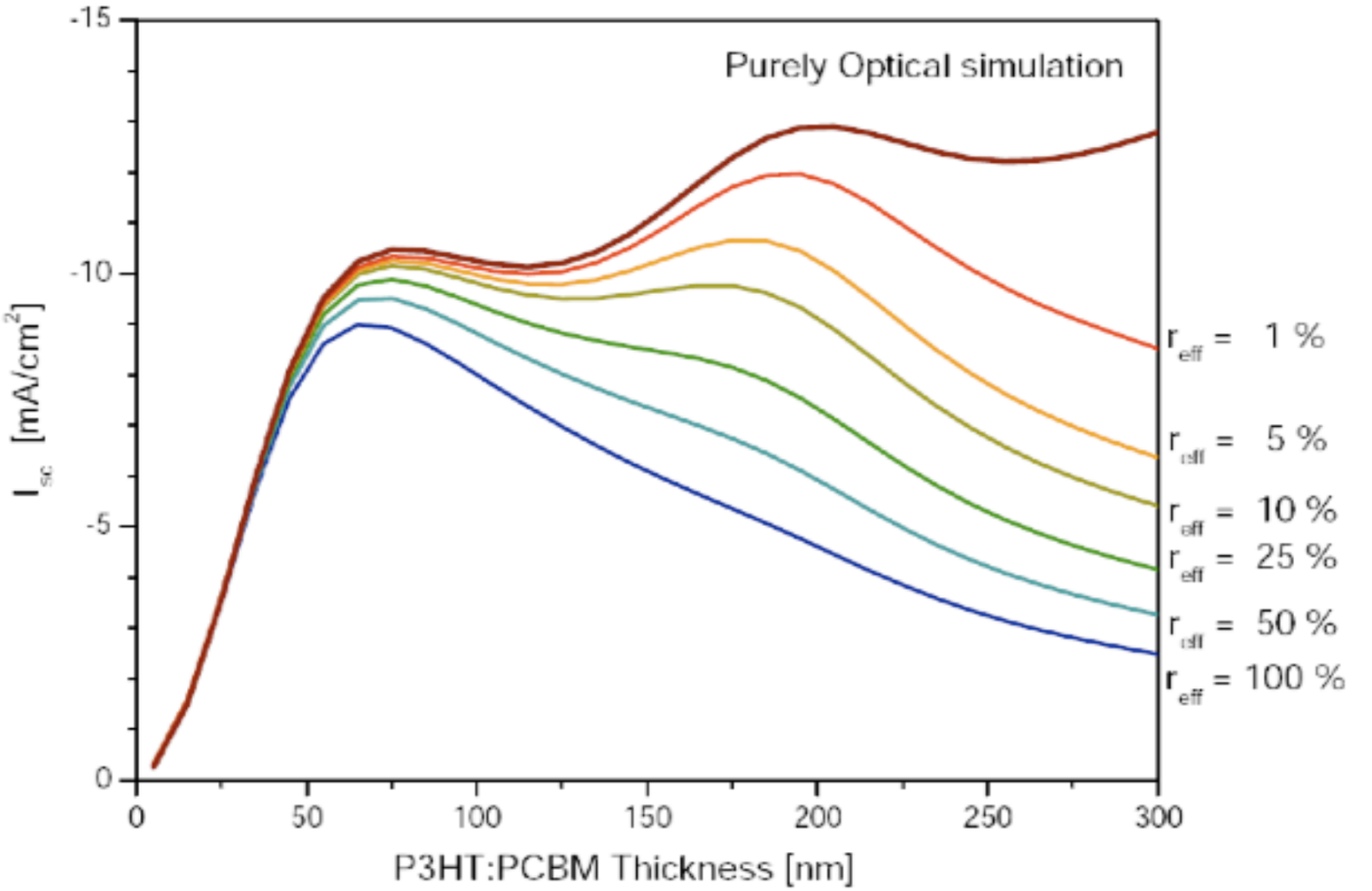




Experiment: J. Gilot, I. Barbu, M. M. Wienk, R. A. J. Janssen, Applied Physics Letters 91, 113520 (2007)

Opto-electronic Simulation of OPV

Short-circuit current vs. thickness of active layer

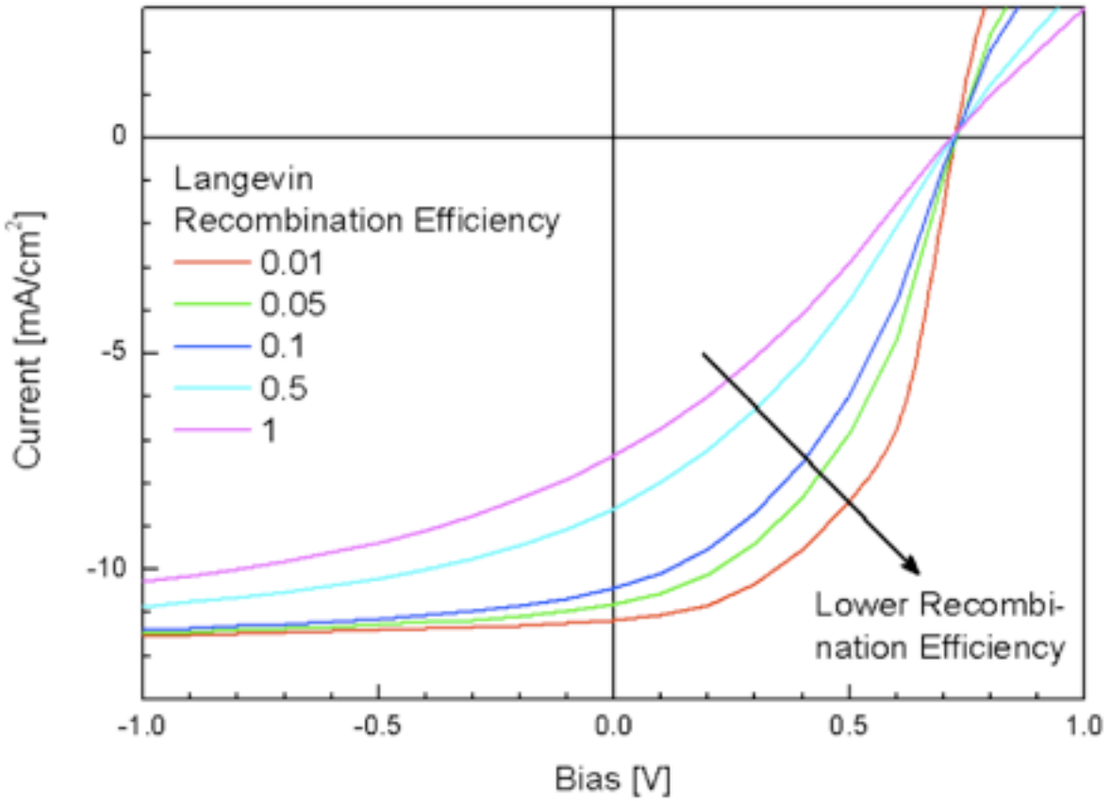


(Roger Häusermann)

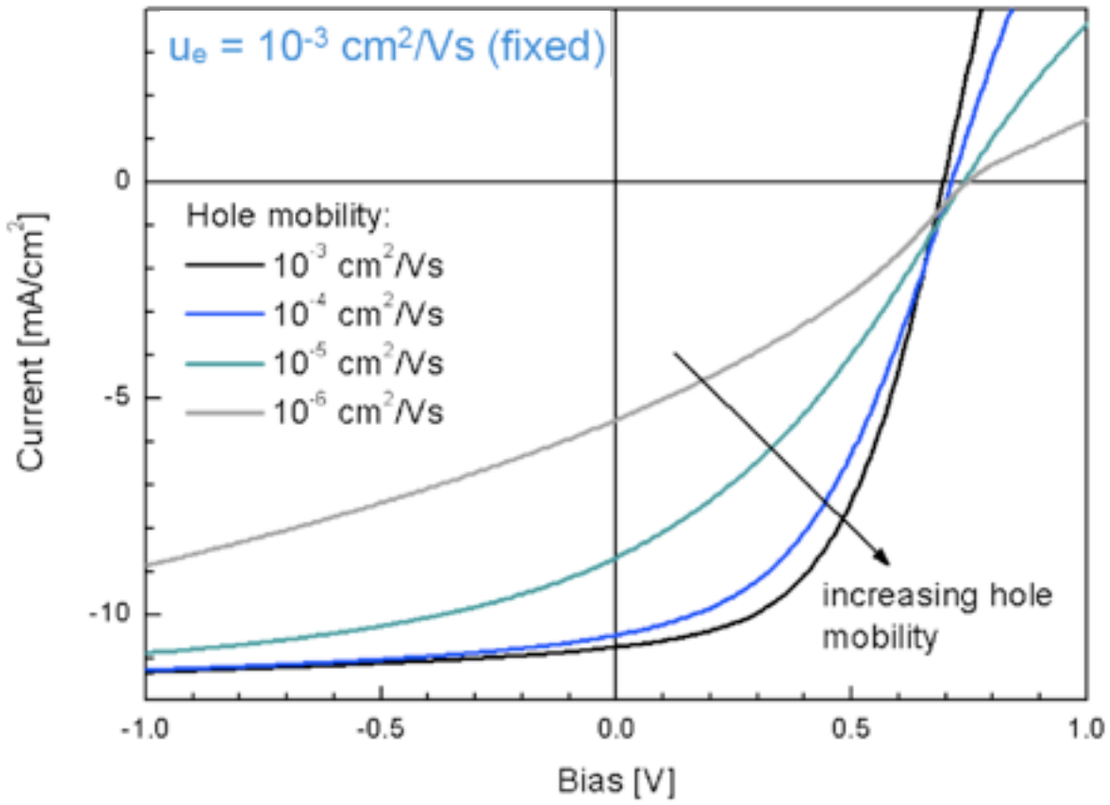
Electronic processes in OPVs

OPV Current-voltage Curves

Variation of the Langevin recombination prefactor

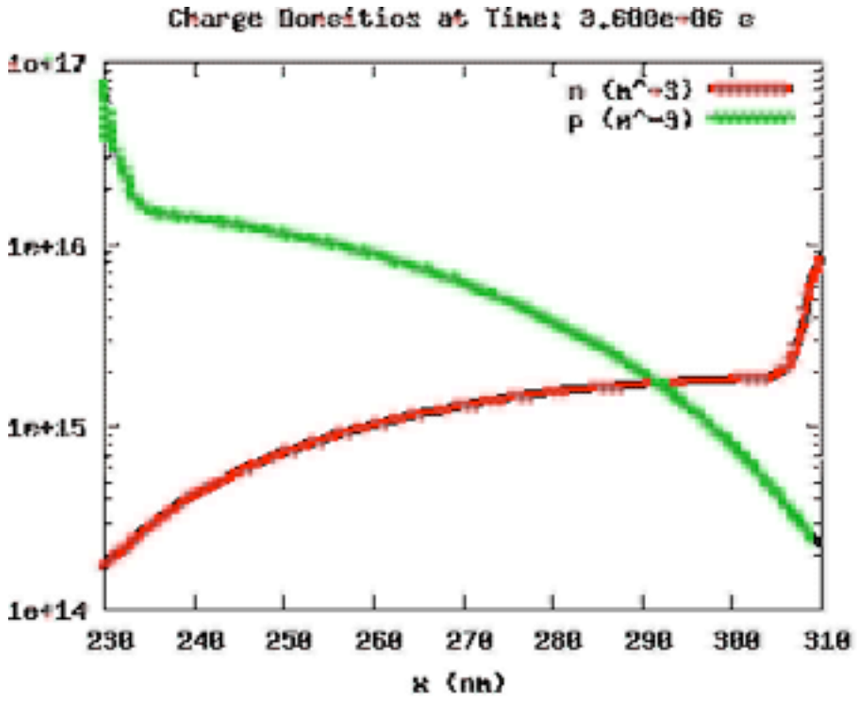


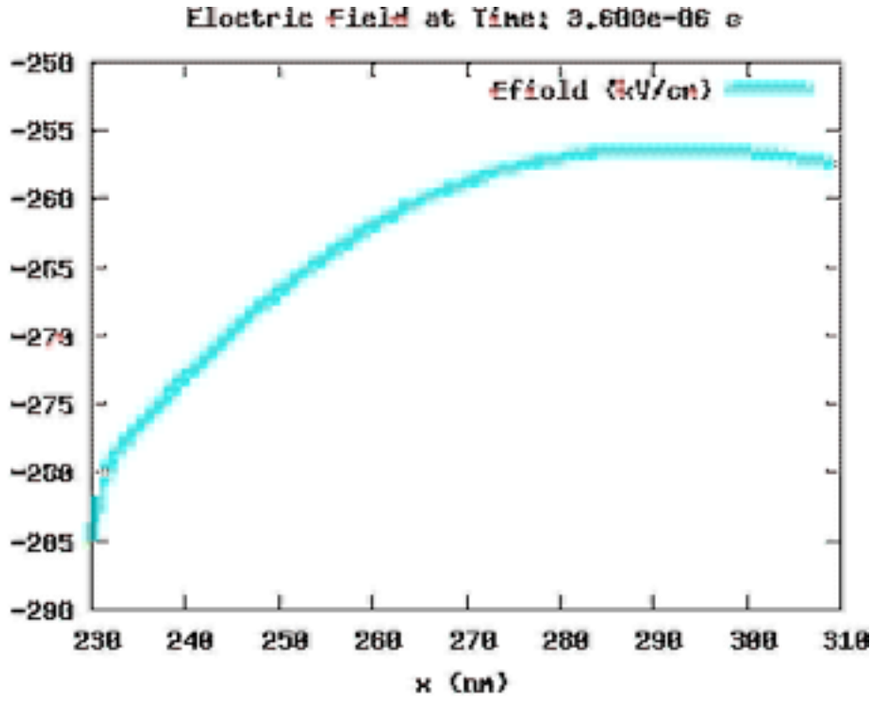
- Variation of the charge mobility

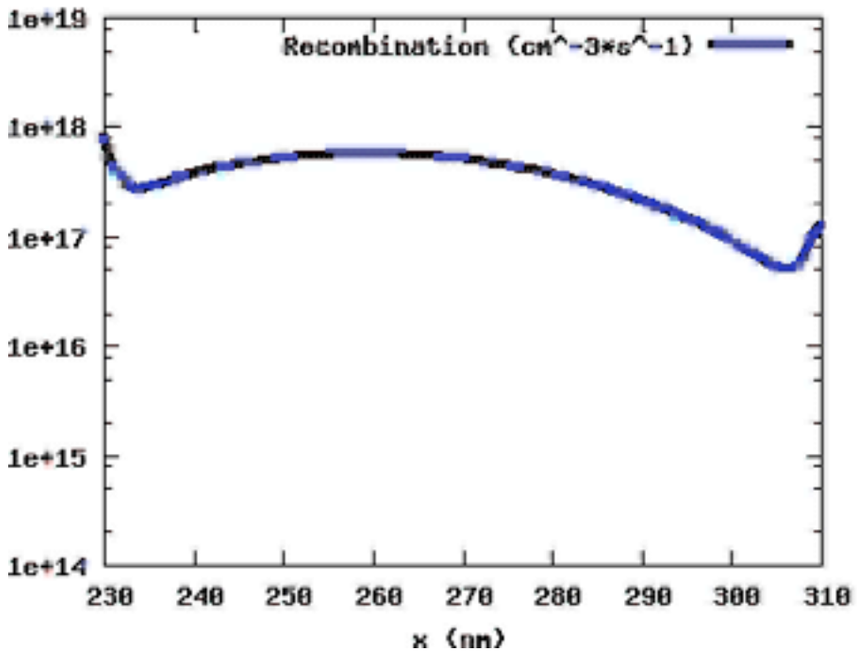


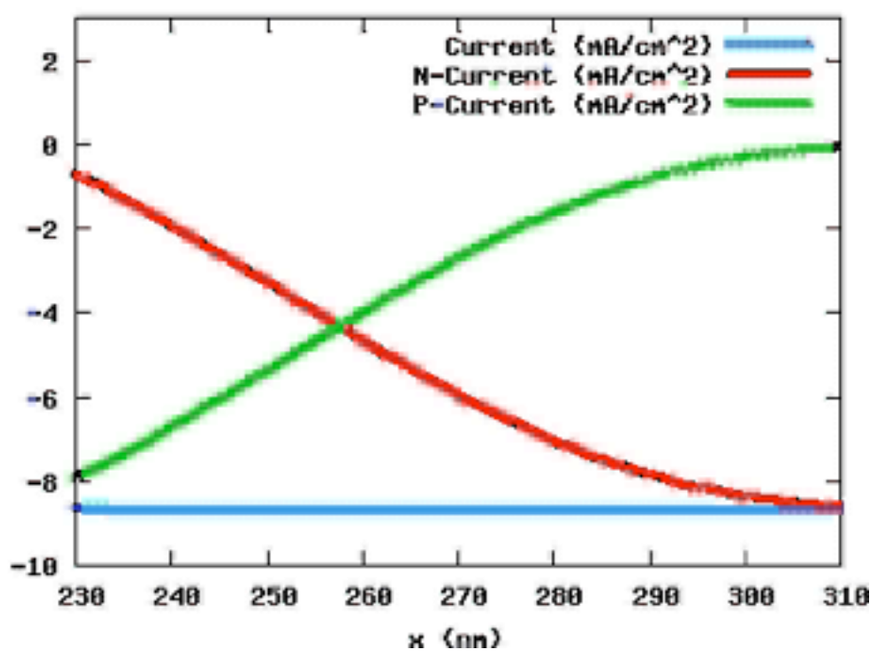
Must reduce recombination losses and increase the mobility!

Example: OPV dynamics









Fluxim and the ICP

zh aw

FLUXiM

2004 2005 2006 2007 2008 2009

OLED

etfos

etfos 1.2

etfos 1.3

etfos 1.4

setfos

setfos 2.1

Semiconducting

OPV

Fluxim AG is a spin-off of the
Zurich University for Applied Sciences, ZHAW
Switzerland

ICP Team

Interdisciplinary team with Physicists,

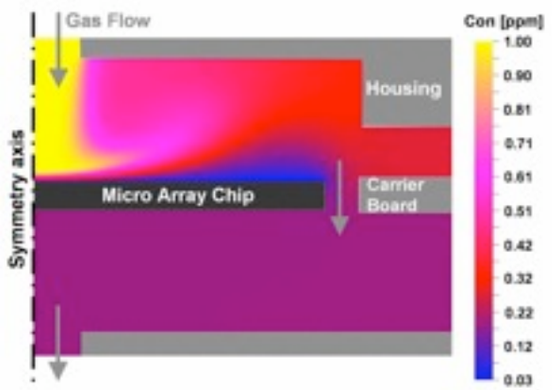
Mathematicians and Software developers

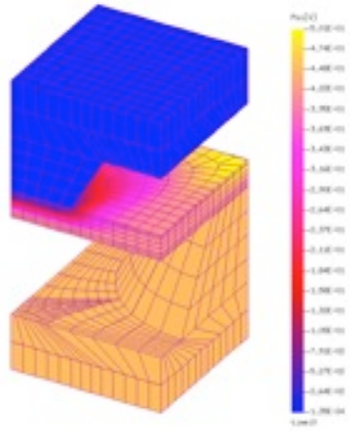
1996 Fachgruppe NMSA
2002 Gründung CCP
2007 Gründung ICP

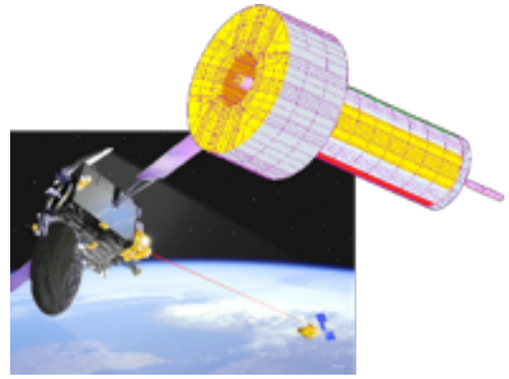
Spin-offs:
Numerical Modeling GmbH, www.nmtec.ch
Fluxim AG, www.fluxim.com

www.icp.zhaw.ch

ICP research fields







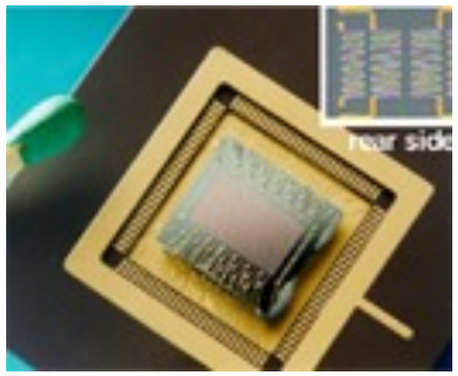
4 main areas of application oriented R&D

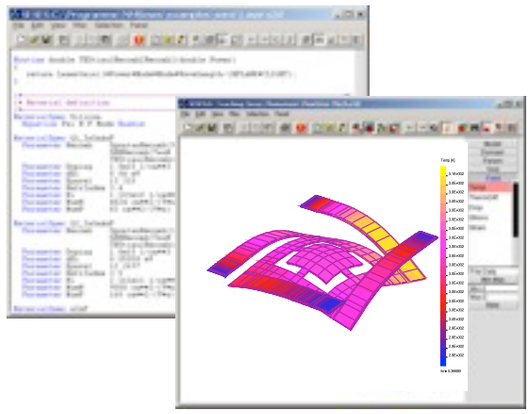
› microsystems, sensors und actuators

› fuel cells

› organic optoelectronics and photovoltaics

› multi-physics simulation software development





Acknowledgments

Research Partners

- *ICP, ZHAW, Winterthur*
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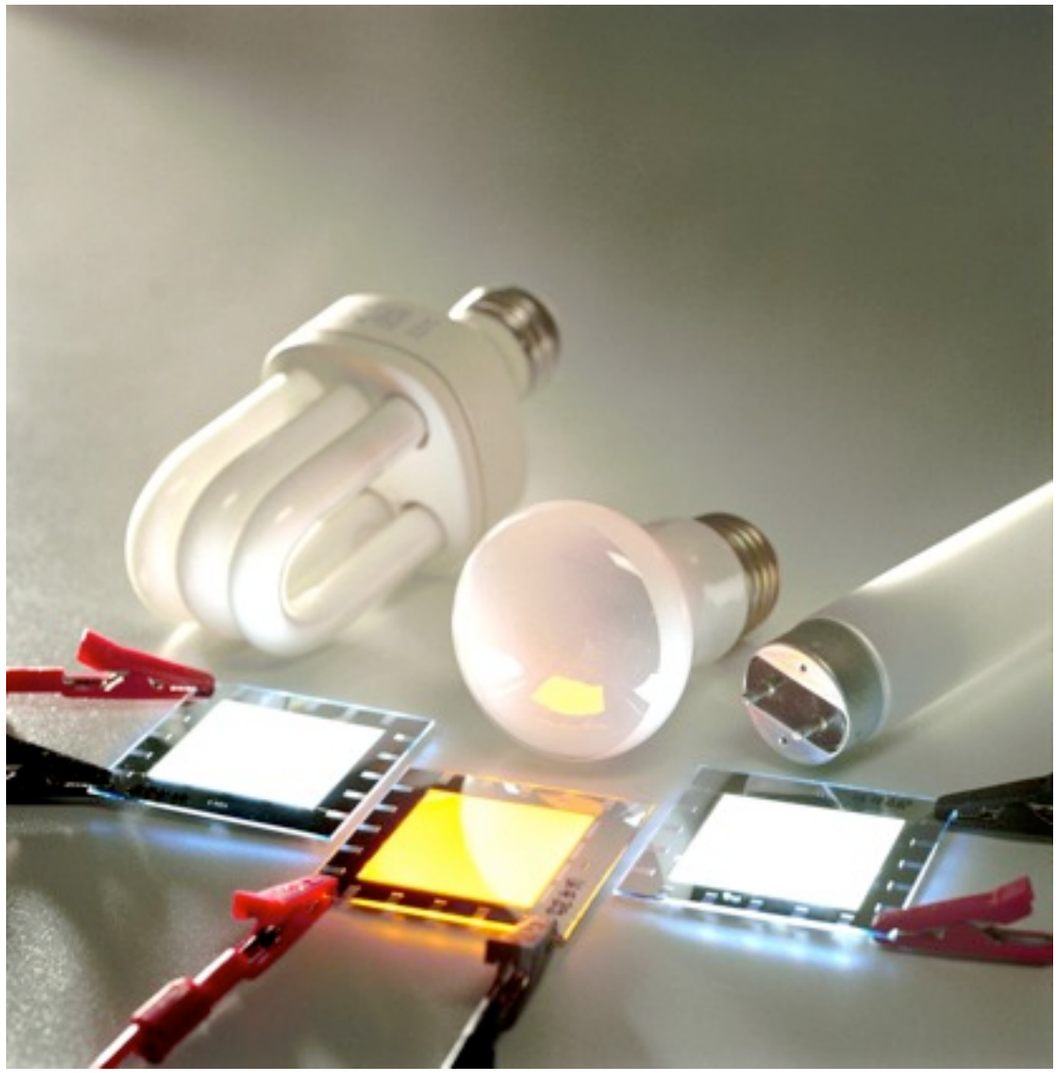
- *CSEM SA, Basel*
- *Philips Research, Eindhoven*
- *ETH Zurich, TU Eindhoven*

Funding

- *Swiss Federal Commission for Technology and Innovation (CTI)*
- *European Union, FP7 Project "AEVIOM"*

Thanks for your attention!



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