Zurich University
of Applied Sciences

School of
Engineering

ICP Institute of
Computational Physics

Next Generation (Organic) PV: Modeling and Simulation

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Cleantech Day on 3rd Gen PV
CSEM Basel, 19. August 2009

ICP Team at ZHAW Winterthur

- Interdisciplinary team of 8 phycisists, 4 mathematicians and 3 engineers

1996 Section NMSA
2002 CCP
2007 ICP

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

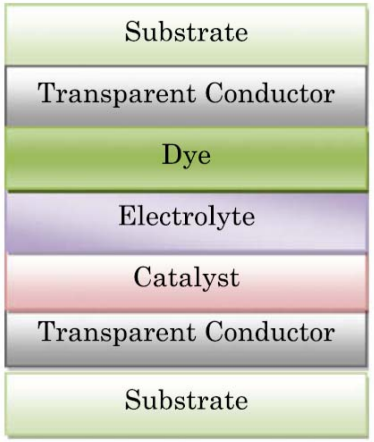
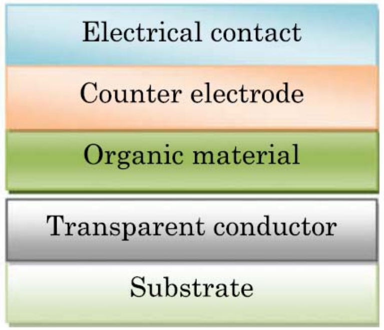
Content

- Motivation
- Organic Solar Cells (OSC)
- Dye-sensitized Solar Cells (DSSC)
- Outlook & Summary

Why modeling solar cells?

- Understand the physical processes during device operation
- Identification and quantification of loss mechanisms
- Interpretation of measured data
- Develop novel experiments for extraction of parameters
- Optimization of the solar cell
- Understand fresh and aged cell!

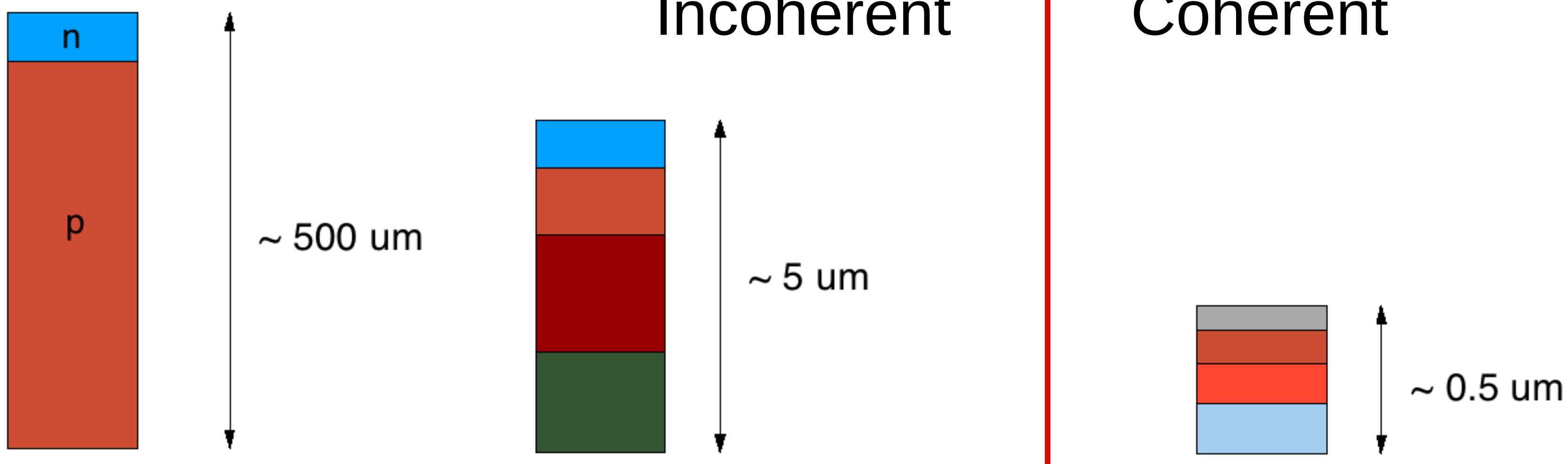
DSSC vs. OSC

	Dye-SC	Organic SC
• Device structure:		
• Transport:	Diffusion-driven	Drift-diffusion
• Active layer:	Dye-sensitized TiO2	Bulk-heterojunction (BHJ)
• Light-scattering:	yes	no
• Efficiency:	~11 %	~6%
• Printable:	yes	yes

Coherence of light is an issue in thin PV

Coherence length of
sunlight ~ 1 um

Incoherent | Coherent



crystalline
solar cell

thin film solar cell
(a-Si, CIGS, DSSC,…)

organic solar cell

+ exploitation of scattering for light trapping!

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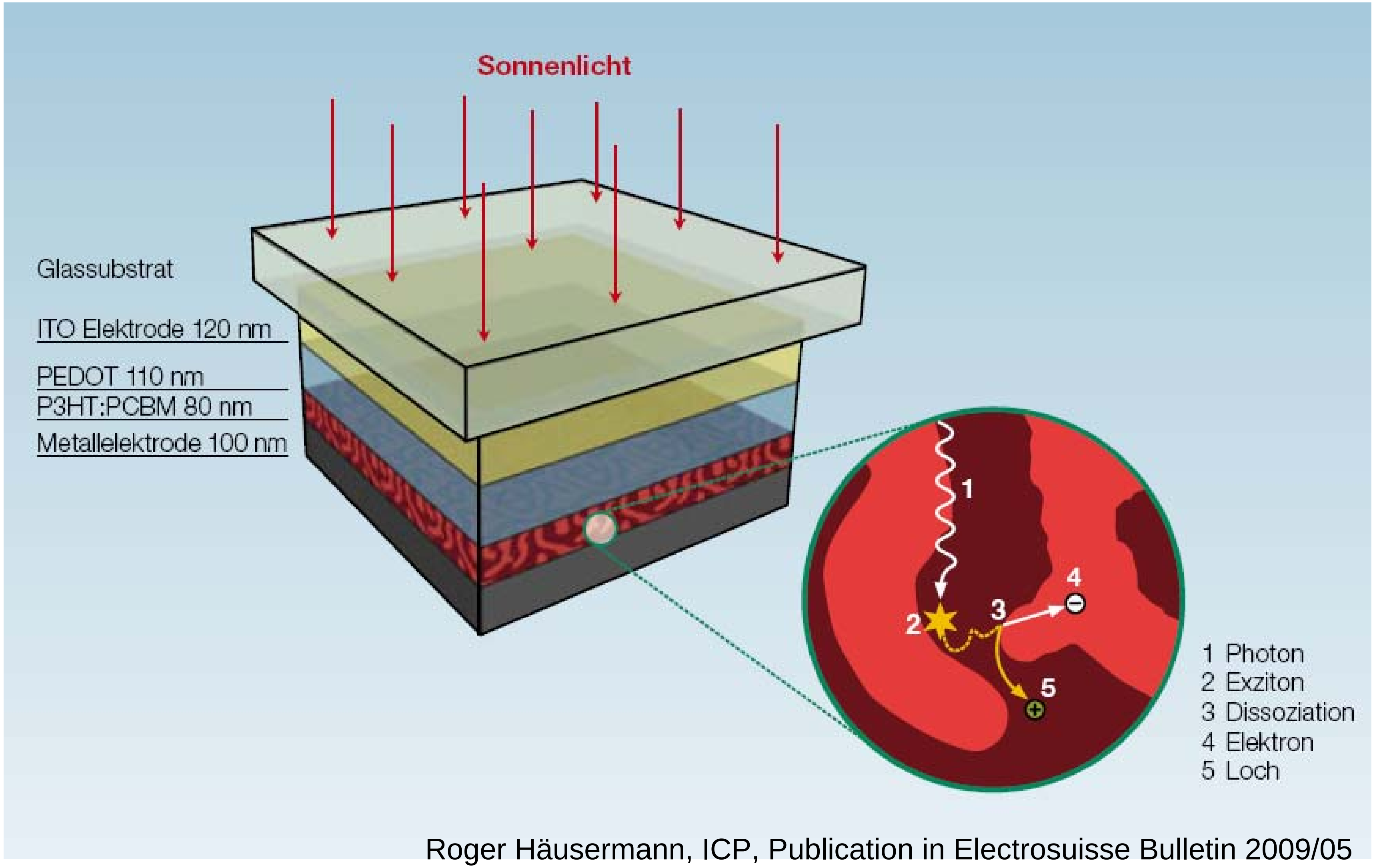
Organic Solar Cell Operation



Roger Häusermann, ICP, Publication in Electrosuisse Bulletin 2009/05

Charge Separation & Transport

The generated charges are incoupled into a drift diffusion model (only electrons are shown here):

Poisson Equation:

$$\vec{\nabla}\vec{E} = \frac{q}{\varepsilon\varepsilon_0}(p-n)$$

Current:

$$\vec{J}_n = q \cdot \mu_n \cdot n(x) \cdot E(x) + D_{\mu,T} \cdot \vec{\nabla} n$$

Continuity e⁻ :

$$\frac{dn}{dt} = \frac{\vec{\nabla}\vec{J}_n}{q} - r_{eff} \cdot R + k_d \cdot S$$

Recombination

Continuity CT-Excitons :

$$\frac{dS}{dt} = r_{eff} \cdot R - k_f \cdot S + g_{eff} \cdot G(x) - k_d \cdot S$$

Optical CT-Exciton Generation

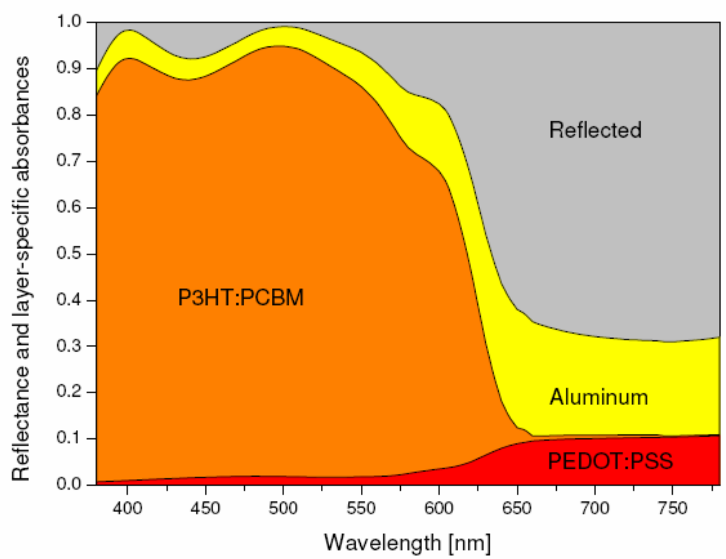
CT-Exciton dissociation

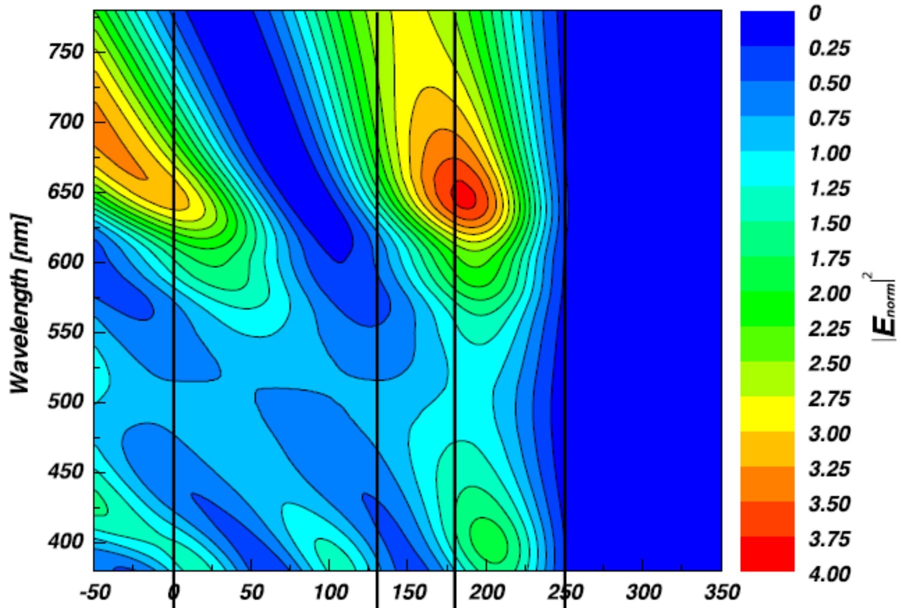
Time Iteration

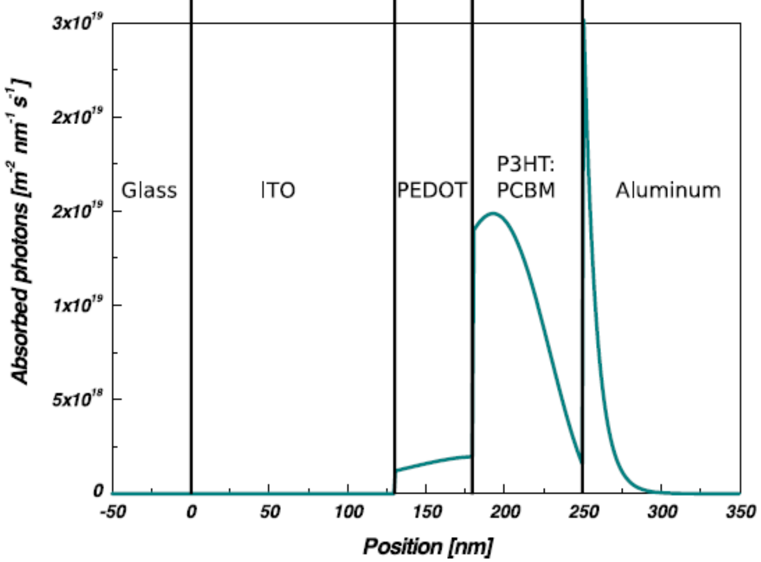
Implemented in the SETFOS Simulator

Light Incoupling in Organic Solar Cells

- Bulk-hetero-junction with P3HT-PCBM
- Simulations:
  - › Spectral EM Field Penetration
  - › Charge Generation Profile
  - › Layer-specific Absorbances







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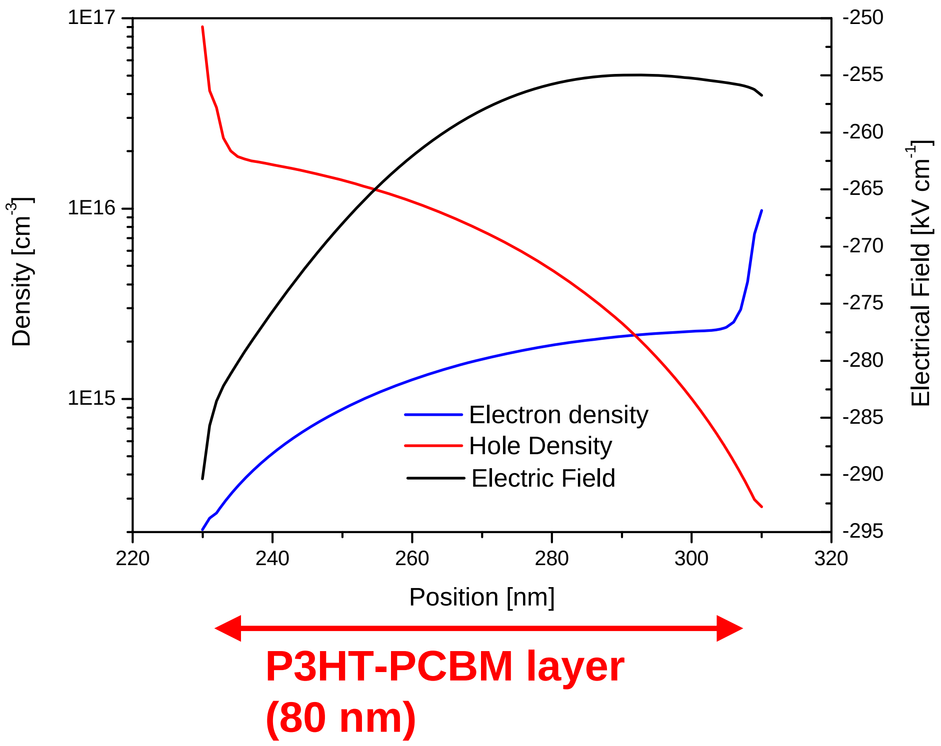
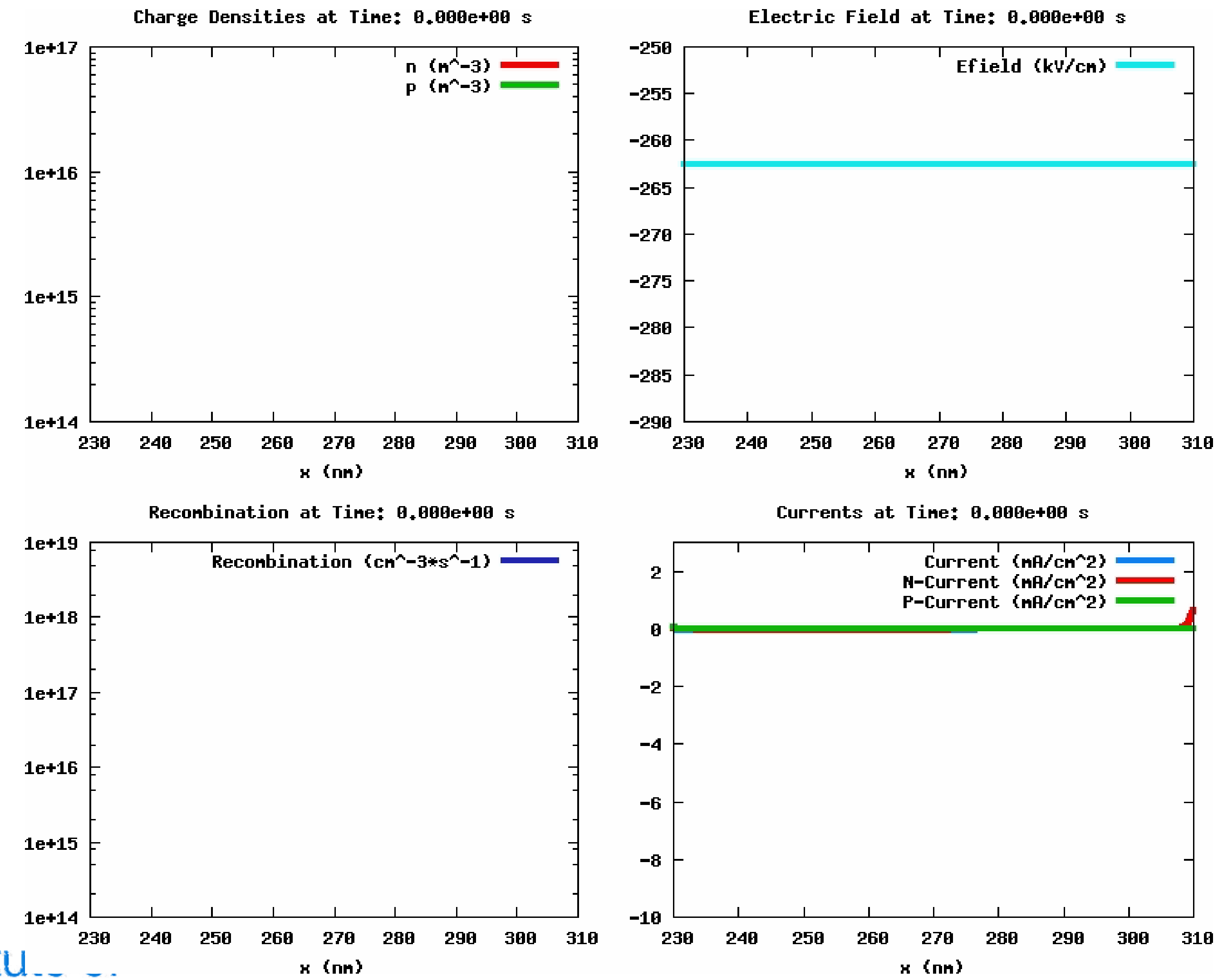
Electronic processes in OPVs I

- Photon absorption couples to drift-diffusion
  - photon -> charge-pair
- Short-circuit profiles of charges and field



Animation

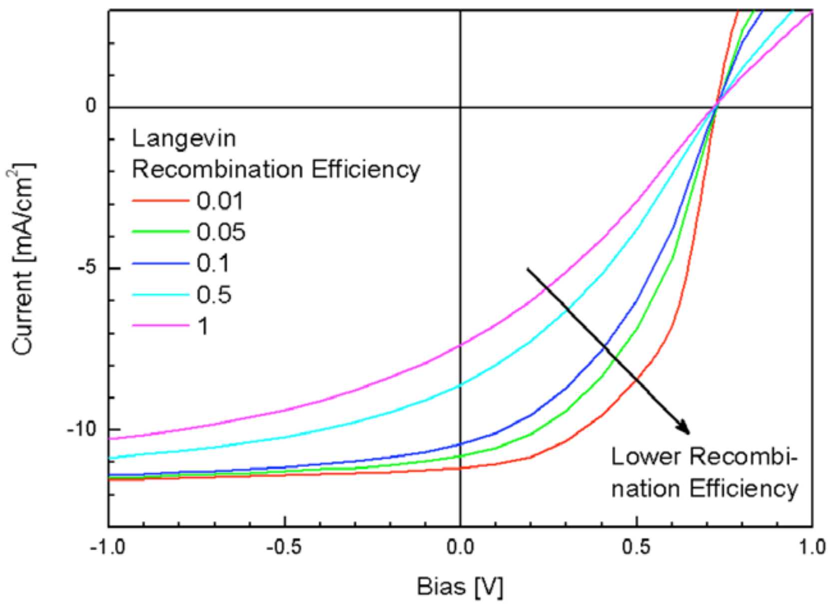
Example: OPV turn-on dynamics

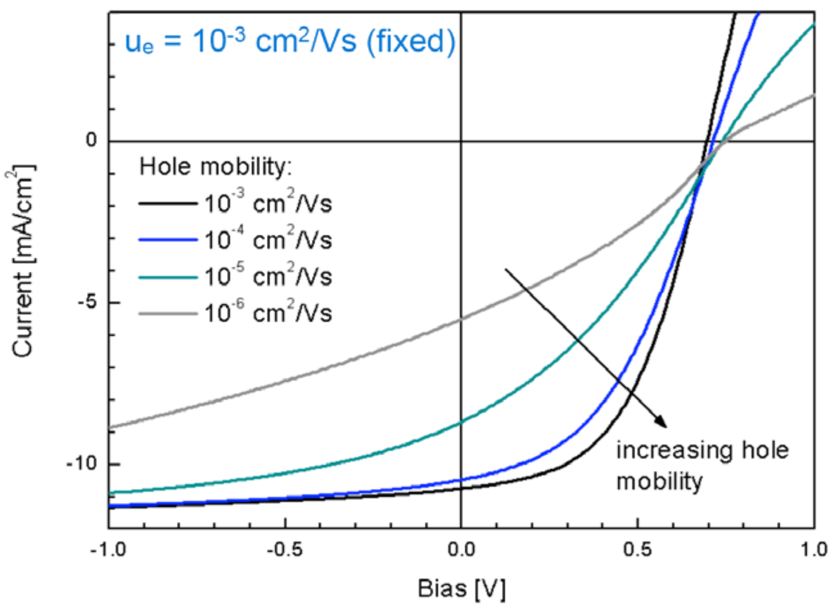


Electronic processes in OPVs II

OPV Current-voltage Curves

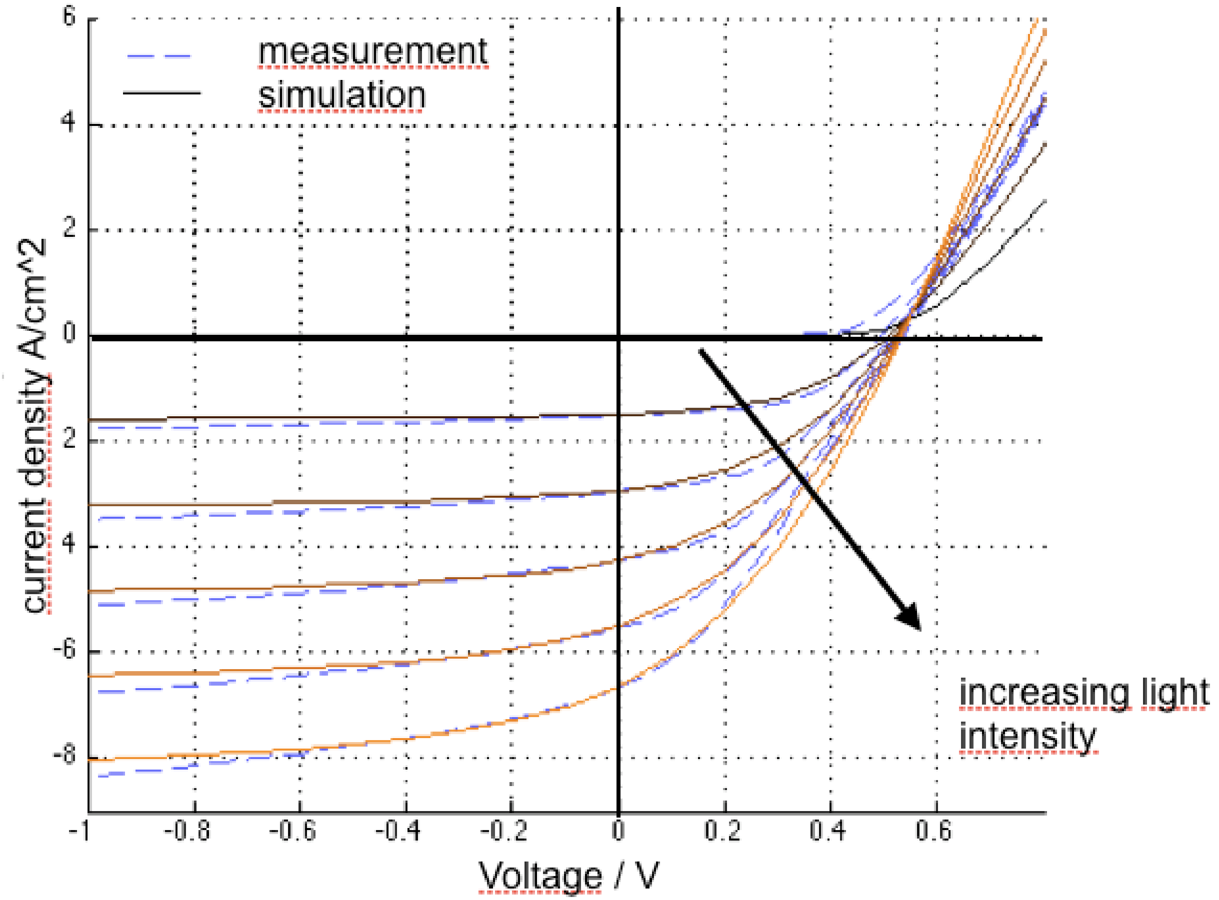
- Variation of the Langevin recombination prefactor
- Variation of the charge mobility





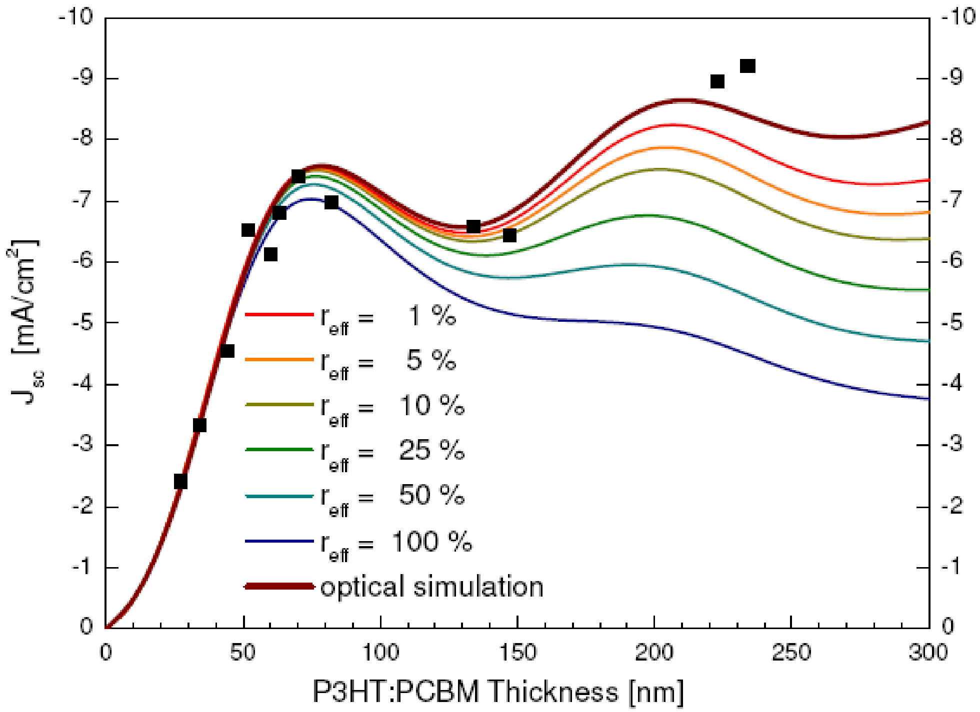
Must reduce recombination losses and increase the mobility!

Validation with Experiment: IV-Curves



Opto-electronic Simulation of OPV

- Short-circuit current vs. thickness of active layer



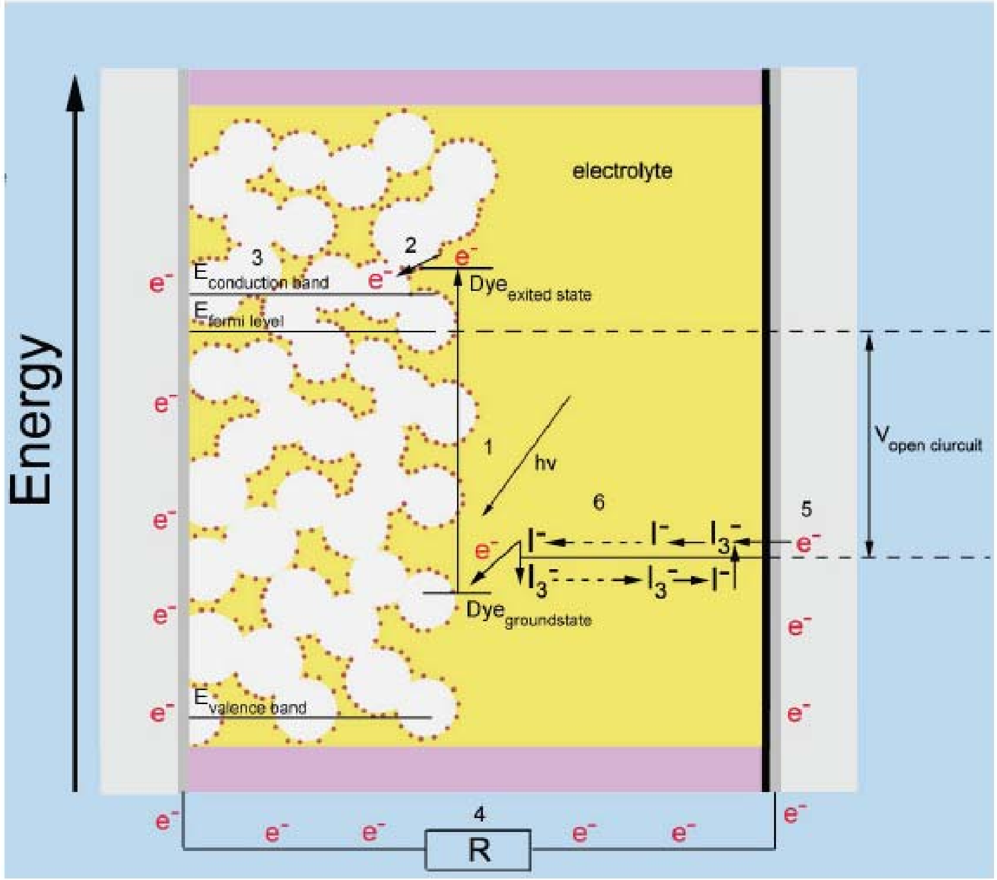
Experiment by J. Gilot, I. Barbu, M. M. Wienk, R. A. J. Janssen, Applied Physics Letters 91, 113520 (2007)

Simulation by Roger Häusermann, ICP

- We can estimate the recombination losses and dissociation efficiency!

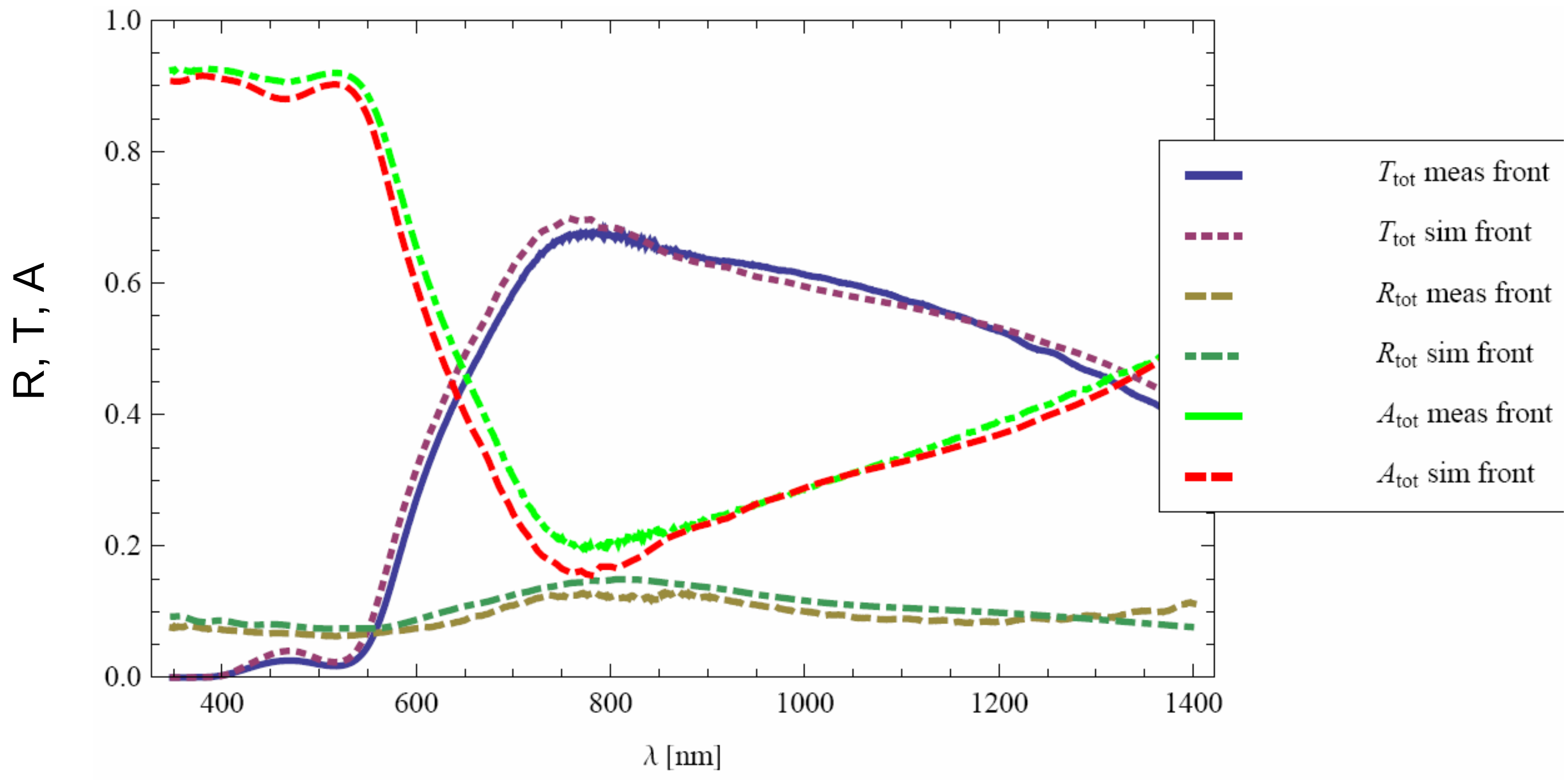
DSSC Device Operation

- (1) A photon is absorbed by the dye.
- (2) The excited electron in the dye is injected into the conduction band of the TiO_2.
- (3) Electrons diffuse to the anode through the network of TiO_2 nanoparticles.
- (4) External circuit.
- (5) At the cathode tri-iodide ions are reduced: $I_3^- + 2e^- \rightarrow 3I^-$.
- (6) The dye is reduced by iodide ions: $2D^+ + 3I^- \rightarrow 2D + I_3^-$



DSSC Optical Validation

- Passive Optics (R, T, A) of DSSC



Experiment by EFPL-LPI

Electronic Model Equations of the DSSC

$$\underbrace{\frac{dj_e(x)}{dx}}_{\text{TiO}_2} + \underbrace{\frac{dj_{\text{ions}}(x)}{dx}}_{\text{electrolyte}} = 0 \qquad \text{charge conservation} \qquad (1)$$

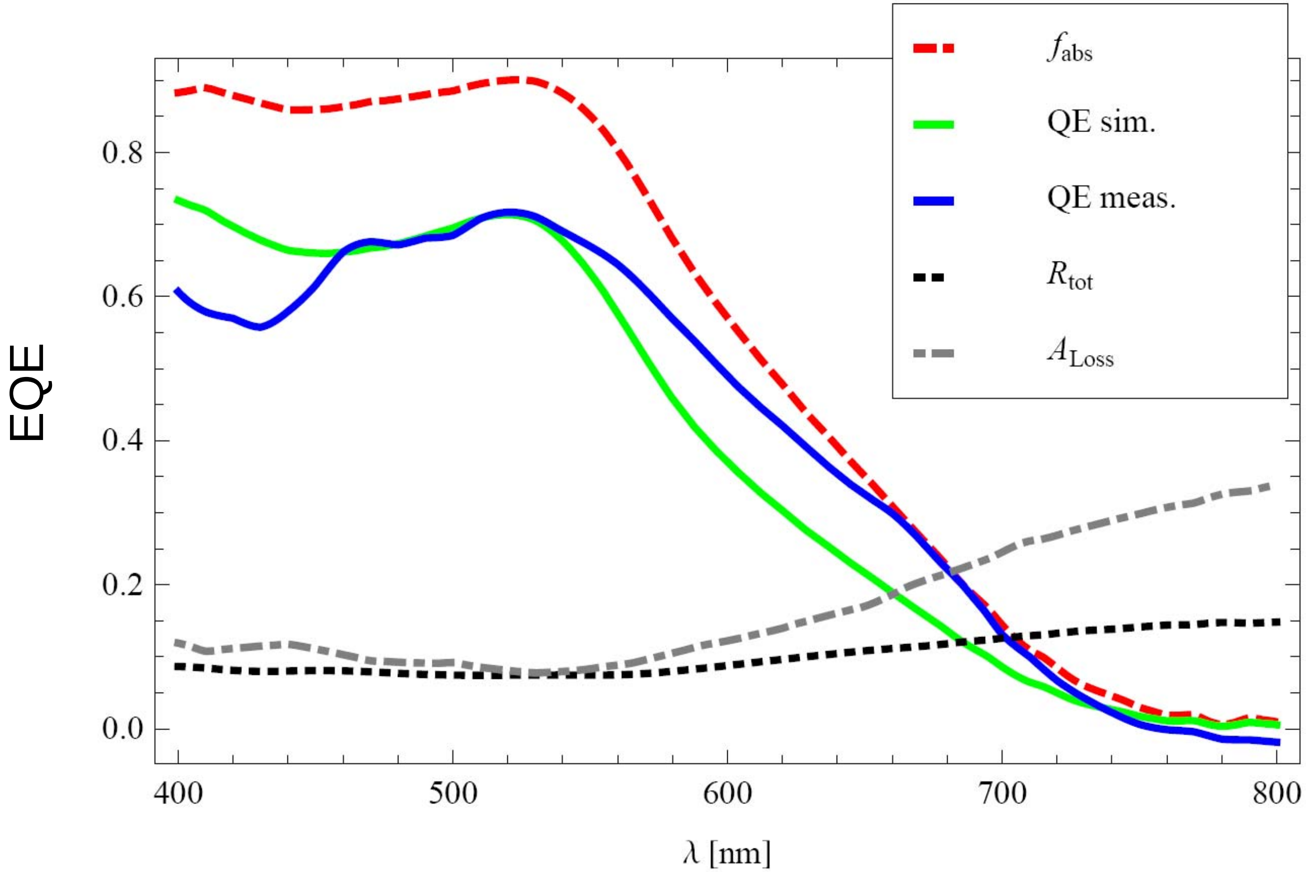
$$-\underbrace{\frac{1}{e}\frac{dj_e(x)}{dx}}_{\text{TiO}_2} = \underbrace{G(x) - U(x)}_{\text{interface}} \qquad \text{continuity equation} \qquad (2)$$

$$\frac{1}{Z_l e} j_l = \underbrace{-D_l \frac{dn_l}{dx}(x)}_{\text{diffusion}} + \underbrace{\mu_l n_l(x) E(x)}_{\text{drift}} \qquad \text{transport equations} \qquad (3)$$

- Transport in both electrolyte and TiO_2 is dominated by diffusion term.
- $l = e,\ I_3^-,\ I^-,\ K^+$.

Spectral Quantum Efficiency of DSSC

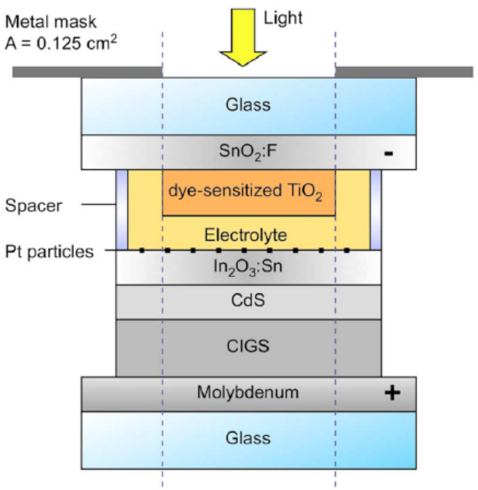
- Quantification of electrical losses!



Experiment by EFPL-LPI

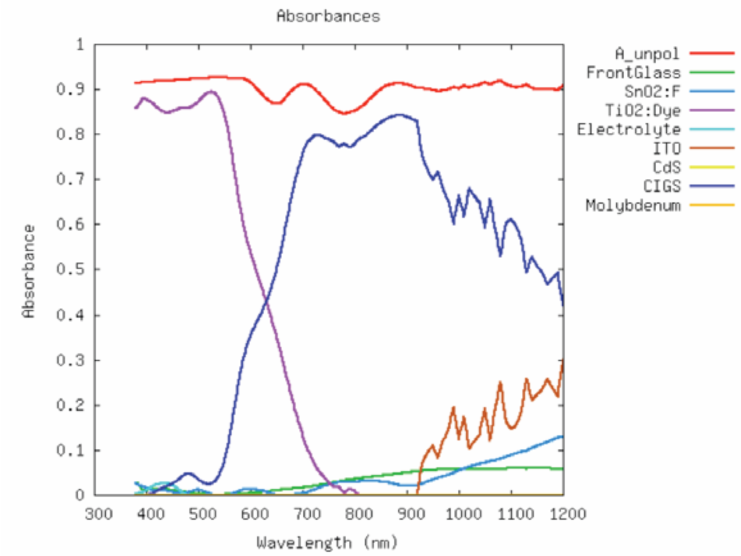
Optimization of Tandem Cells

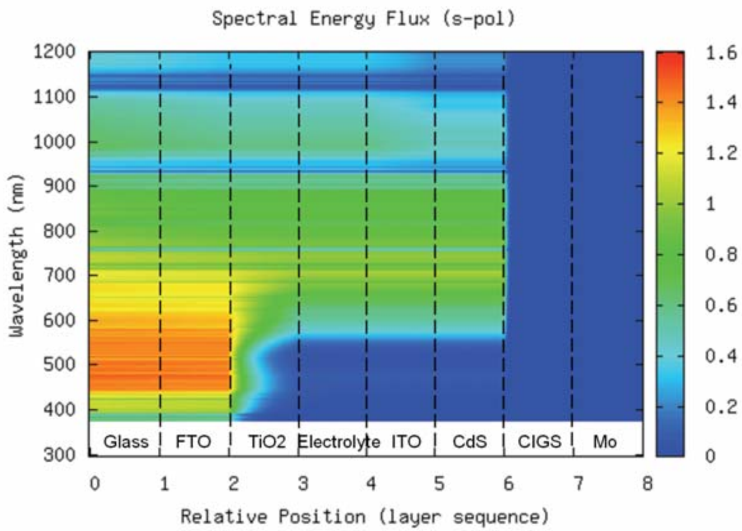
- Monolithic DSSC-CIGS tandem



Tandem structure from Wenger et al., Appl. Phys. Lett. **94**, 173508, (2009)

We simulate a combination of coherent and incoherent layers



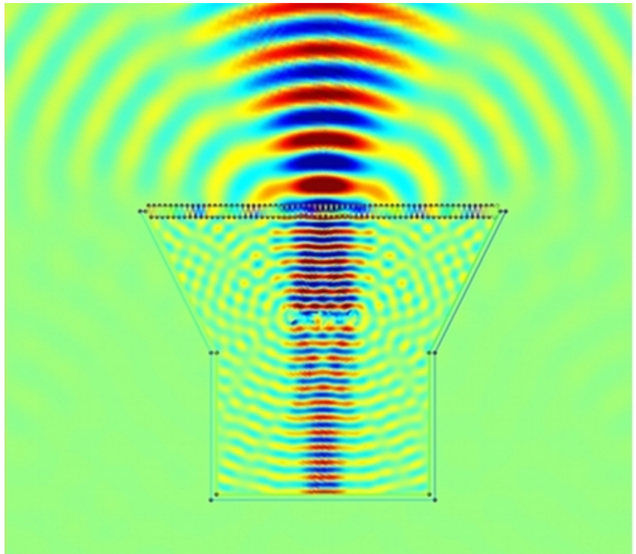


simulation by SETFOS

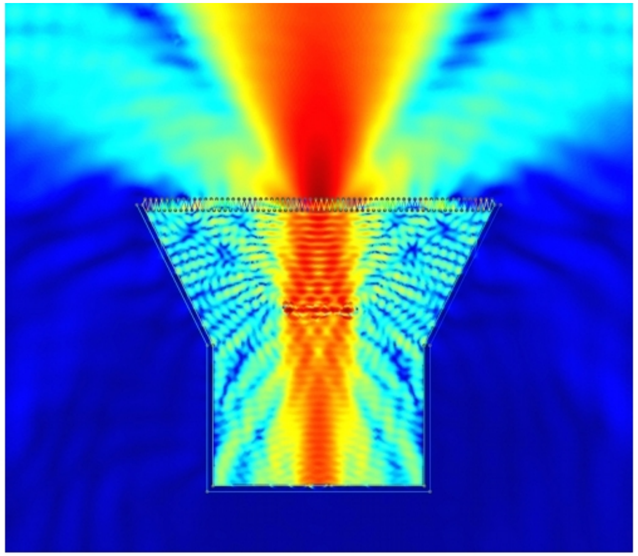
Light Scattering by Full Wave Simulations

- 2-dimensional simulation of light propagating in regularly textured device

field



intensity



Martin Loeser, ICP

- Characterization and optimization of light trapping

Summary

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aw

- Optical solar cell simulations are very reliable
- Electronic device simulation can give insight into the operating mechanisms and the limitations
- Novel dynamic experiments and parameter extraction methods need to be developed
- *We have more homework to do!*

Acknowledgements

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  - Nils A. Reinke, Martin Neukom, Roger Häusermann (OSC)
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  - **Technical University Eindhoven**
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