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Computational Physics

International Conference on Simulation of Organic Electronics and Photovoltaics 2018

Zurich University of Applied Sciences

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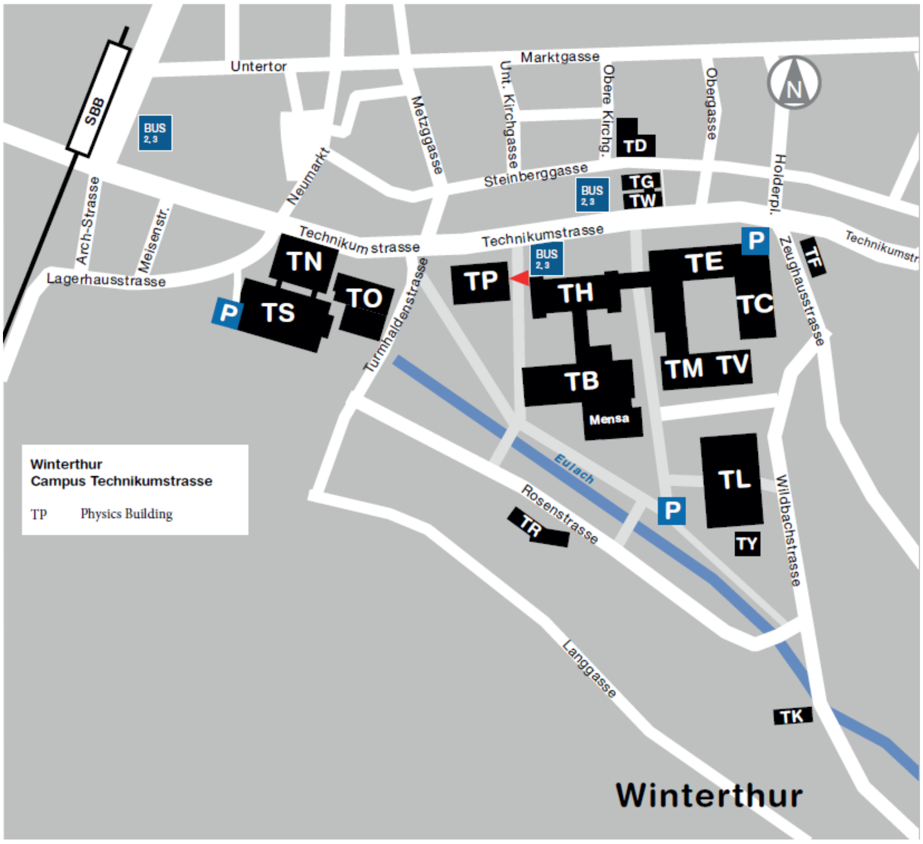
Site Plan

Conference: Building TP, Room 406. Please enter building TP through the doors at Technikumstrasse, walk up to the first floor to reach the conference lecture room 406. Coffee break refreshments and buffet lunch is served in the hallway in front of the lecture room.

Fluxim Workshops: Building TP, Room 404

Conference Dinner: Mensa



Scientific Program

Program SimOEP 2018 as of 27.8.18

	04.09.18			05.09.16			06.09.18		
	OLED	PSC/OPV	ND	OLED	PSC/OPV	ND	OLED	PSC/OPV	ND
08.45 - 09.00									
09.00 - 09.15					A. Tiwari				C. Shih
09.15 - 09.30									
09.30 - 09.45					M. AufderMaur				P. Barnes
09.45 - 10.00									
10.00 - 10.15	Fluxim Workshop: LA-Large-Area PV/OLED Simulation (LAOSS)				K. Domanski				F. Benchkeih
10.15 - 10.30									
10.30 - 10.45				**Coffee**			**Coffee**		
10.45 - 11.00									
11.00 - 11.15					P. Calado				M. Lindh
11.15 - 11.30					V. Le Corre				M. Diethelm
11.30 - 11.45					E. Knapp				S. Jenatsch
11.45 - 12.00					B. Ebenhoch				B. Blülle
12.00 - 12.15	**REGISTRATION**				A. Fischer				J. Sastre
12.15 - 12.30							A. Gagliardi		
12.30 - 12.45				**LUNCH**					
12.45 - 13.00							**LUNCH**		
13.00 - 13.15	**OPENING**								
13.15 - 13.30	C.Jungemann								
13.30 - 13.45					U. Aeberhard				
13.45 - 14.00	P. Farrell								
14.00 - 14.15					M. Neukom		Fluxim Workshop: Angular Luminescence	Fluxim Workshop: PV-Simulation (SETFOS)	
14.15 - 14.30	C. Kirsch								
14.30 - 14.45					M. Azzouzi				
14.45 - 15.00	M. Regnat				O. Sandberg				
15.00 - 15.15	N. Haase				B. Ruhstaller				
15.15 - 15.30	**Coffee**						Fluxim Workshop: OLED-Simulation (SETFOS)		
15.30 - 15.45				**Coffee**					
15.45 - 16.00	S. Gottardi								
16.00 - 16.15	S. Jenatsch			Fluxim Workshop: Characterization of PV/OLED (PAIOS)					
16.15 - 16.30	S. Züfle								
16.30 - 16.45	A. Hofmann								
16.45 - 17.00	V. Wissdorf								
17.00 - 17.15	T. Neumann								
17.15 - 17.30		B. Niesen							
17.30 - 17.45									
17.45 - 18.00	**Apéro & Fluxim Product Demo**								
18.00 - 18.15									
18.15 - 18.30									
18.30 - 18.45				**Dinner**					
18.45 - 19.00									
19.00 - 20.00									
20.00 - 22.00									

Tuesday, 4.9.2018

10.00-12.00	Fluxim Workshop *Large-Area PV and OLED Simulation (LAOSS)*	
12.00-13.00	**Registration**	
13.00-13.15	Welcome/Opening *Beat Ruhstaller, ICP ZHAW and Fluxim AG, Switzerland*	
13.15-13.45	Full Electrical Simulations of OLEDs based on the Master Equation *Christoph Jungemann, RWTH Aachen University, Germany*	6
13.45-14.15	Challenges for non-Boltzmann drift-diffusion simulations of semiconductors *Patricio Farrell, Hamburg University of Technology, Germany*	8
14.15-14.45	Electrothermal simulation of large-area semiconductor devices *Christoph Kirsch, ICP ZHAW, Switzerland*	9
14.45-15.00	Modelling the bias-dependent emission zone and its influence on the transient electroluminescence and OLED efficiency *Markus Regnat, ICP ZHAW, Switzerland*	11
15.00-15.15	Kinetic modelling of transient photoluminescence measurements of thermally activated delayed fluorescent materials *Nils Haase, Merck KGaA, Germany*	13
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15.45-16.00	Disentangling excitonic loss mechanisms in TADF-type OLEDs using kinetic Monte Carlo simulations *Stefano Gottardi, Simbeyond, Netherlands*	14
16.00-16.15	Device Performance and Degradation Analysis of a skyblue TADF-OLED *Sandra Jenatsch, Fluxim AG, Switzerland*	15
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16.45-17.00	Simultaneous Drift-Diffusion Simulation of Current Voltage and Capacitance Voltage Measurement of Hole Only Devices... *Victoria Wissdorf, Merck KGaA, Germany*	20
17.00-17.15	Computer-Aided Optimization of Multilayer OLED Devices *Tobias Neumann, Nanomatch GmbH, Germany*	21
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10.00-10.30	The Quest for Stability of Perovskite Solar Cells Understanding Degradation and Investigation Under Simulated Weather Conditions *Konrad Domanski, Fluxim AG, Switzerland*	27
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11.15-11.30	Transport layers limit the efficiency of perovskite solar cells: an experimental and theoretical study *Vincent Le Corre, University of Groningen, Netherlands*	31
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11.45-12.00	Fundamental relation of the of J-V characteristics, capacitance and charge carrier lifetimes in solar cells *Bernd Ebenhoch, Karlsruhe Institute of Technology, Germany*	34
12.00-12.30	Absorption induced heating of solar cells leads to a characteristic open-circuit voltage turnover *Axel Fischer, TU Dresden, Germany*	36
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11.15-11.30	Emission zone position in sandwich super yellow light-emitting electrochemical cells *Matthias Diethelm, EMPA, Switzerland*	49
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12.15-12.45	Charge transport in organic semiconductor materials: a numerical simulation perspective *Alessio Gagliardi, Technical University Munich, Germany*	57
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15.15-16.45	Fluxim Workshop Simulation of OLEDs and PV	

Full Electrical Simulations of OLEDs based on the Master Equation

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Institute of Electromagnetic Theory, RWTH Aachen University, Kackertstr. 15-17,
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The three-dimensional (3-D) master equation (ME) approach for organic diodes has been established[1] with the benefit of its higher efficiency and stability than the 3-D Monte-Carlo (MC) method and closer relation to the underlying physics of organic materials than the one-dimensional (1-D) drift-diffusion (DD) model. We have shown that it is feasible to perform DC[2], AC[3] and noise[4,5] analyses of OLEDs based on the ME model. Existing MC simulations[6] of IV characteristics for unipolar and bipolar devices were reproduced by our ME model (Fig. 1), and the small-signal analysis offered a nice fitting of both the differential capacitance and susceptance measurements of a polymer LED from Martens *et al.*[7] (Fig. 2). Moreover, the noise analysis could be validated by the Nyquist theorem and showed the enhanced effect of trap-induced fluctuation (Fig. 3). More recently excitonic processes have also been included to build up a full picture of all the particles' behavior in OLEDs[8]. In this contribution, we will show how all the measurements of IV characteristics and luminous efficacy (LE) roll-off of a green phosphorescent OLED[9] (Fig. 4 and 5) doped with various emitter profiles of $Ir(ppy)_3$ can be matched with consistent parameters for charge carriers and excitons. The simulation includes all the excitonic processes, i.e. inter-system crossing, Förster and Dexter transfer, radiative and nonradiative decay, field-induced dissociation into free charge carriers, exciton-polaron quenching and exciton-exciton annihilation. Hence the device efficiency can be improved based on the ME simulations.

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[1] C. Jungemann, J. Comput. Electron., vol. 14, iss. 1, pp. 37-42, Mar. (2015)
[2] W. Zhou *et al*. International Conference on Simulation of Semiconductor Processes and Devices (SISPAD) 2015, Washington, DC, USA, Sep. 9th – 11th, (2015)
[3] W. Zhou *et al*. IEEE Trans. Electron Devices, vol. 63, no. 12, pp. 4919-4923, Dec. (2016)
[4] W. Zhou *et al*. International Conference on Simulation of Semiconductor Processes and Devices (SISPAD) 2016, Nuremberg, Germany, Sep. 6th – 8th, (2016)
[5] W. Zhou *et al*. International Conference on Noise and Fluctuations (ICNF) 2017, Vilnius, Lithuania, Jun. 20th – 23rd, (2017)
[6] R. Coehoorn *et al*. Phys. Rev. B., vol. 80, no. 085302, Aug. (2009)
[7] H. C. F. Martens *et al*. Appl. Phys. Lett., Vol. 77, p. 1852, (2000)
[8] W. Zhou *et al*. Organic Light Emitting Materials and Devices XXI, San Diego, USA, Aug. 6th – 10th, (2017)
[9] M. Bösing *et al*. Materials Research Society (MRS) Symposium B Proceedings, vol. 1154, (2009)

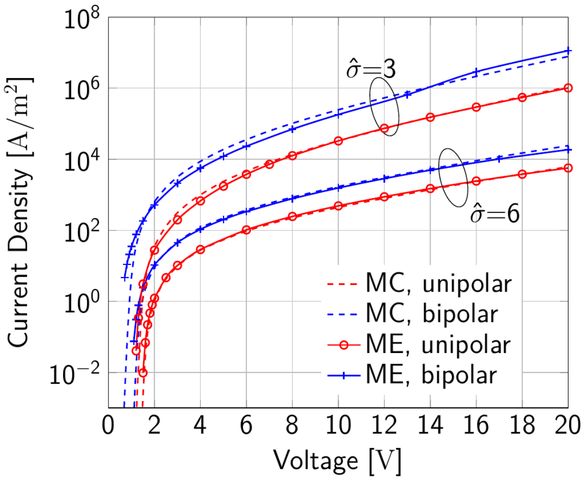

Fig. 1 IV characteristics of the unipolar and bipolar devices using 3-D ME[2] (symbols and solid lines) and from 3-D MC[6] (dashed lines).

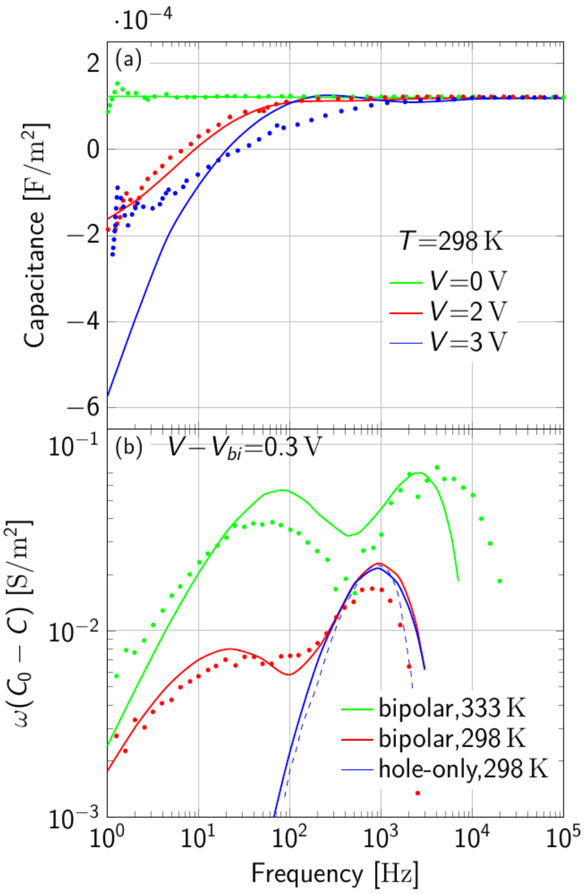

Fig. 2 Frequency-dependent (a) differential capacitance with various voltages and (b) relative susceptance (C_0 indicates the geometric capacitance) with various temperatures for a polymer LED. Dots: measurements[7]. Solid lines: 3-D ME simulations[3].

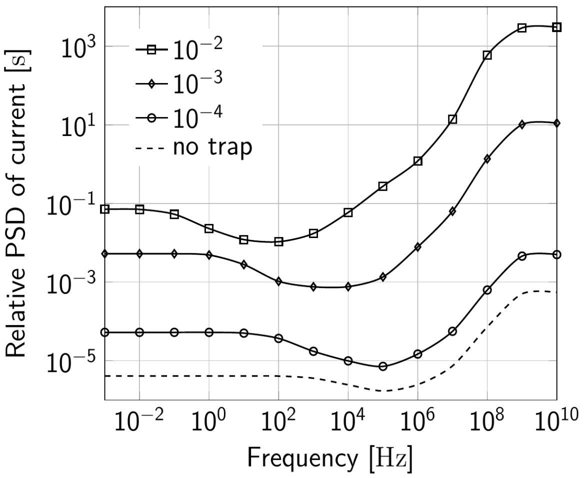

Fig. 3 Frequency-dependent relative power spectral density (PSD) of the terminal current with different trap concentrations of a bipolar diode[5].

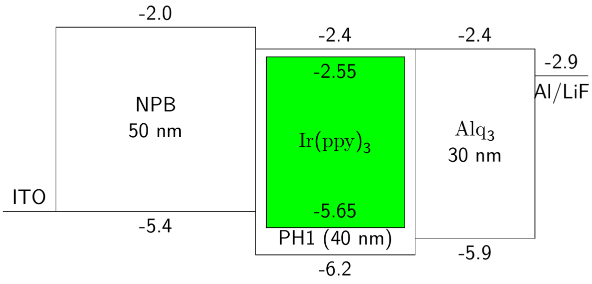

Fig. 4 Energy diagram of a green OLED[9] doped by Ir(ppy)$_3$ in the emission layer.

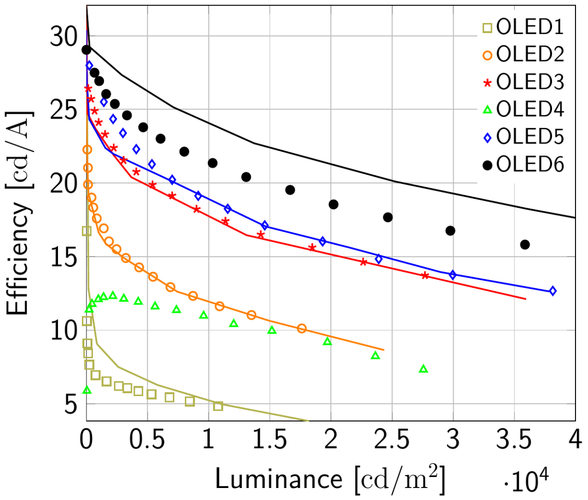

Fig. 5 Measured[9] (symbols) and 3-D ME-simulated (solid lines) luminous efficacy (LE) of the OLED in Fig. 4 with various emitter profiles. Results of OLED4 is discarded due to short-circuit problems in the experiment.

Challenges for non-Boltzmann drift-diffusion simulations of semiconductors

Patricio Farrell, Dirk Peschka
Institute of Mathematics, Hamburg University of Technology, Am Schwarzenberg-Campus 3,
D-21073 Hamburg, Germany

The thermodynamically consistent Scharfetter-Gummel flux approximation has been proven to be a very effective tool in finite volume drift-diffusion simulations of semiconductor devices[1]. Recently, its basic limitations to Boltzmann statistics have been overcome[2] [3] [4]. In this talk, new thermodynamically consistent schemes are presented which can be employed when it is no longer sufficient to assume Boltzmann statistics, for example when the device operates at low temperatures or organic semiconductor materials are used. In the latter case, the Blakemore or Gauss-Fermi functions most accurately reflect the physical statistics. Furthermore, we discuss the impact of three additional challenges which may slow down the convergence of the numerical solution: boundary layers at Ohmic contacts, discontinuities in the doping profile and corner singularities. Differences between the proposed finite volume method and a finite-element based will be examined[5].

---

[1] D. Scharfetter and H. Gummel, “Large-signal analysis of a silicon Read diode oscillator”, IEEE Transactions on Electron Devices, vol. 16, pp. 64-77, 1969.

[2] M. Bessemoulin-Chatard, “A finite volume scheme for convection-diffusion equations with nonlinear diffusion derived from the Scharfetter-Gummel scheme”, Numerische Mathematik, vol. 121, no. 4, pp. 637-670, 2012.

[3] T. Koprucki, N. Rotundo, P. Farrell, D.H. Doan, and J. Fuhrmann, “On thermodynamic consistency of a Scharfetter-Gummel scheme based on a modified thermal voltage for drift-diffusion equations with diffusion enhancement”, Optical and Quantum Electronics, vol. 47, no. 6, pp. 1327-1332, 2015.

[4] M. Patriarca, P. Farrell, J. Fuhrmann, T. Koprucki, “Highly accurate quadrature-based Scharfetter-Gummel schemes for charge transport in degenerate semiconductors”, submitted, 2018.

[5] P. Farrell and D. Peschka, “Challenges for drift-diffusion simulations of semiconductors: A comparative study of different discretization philosophies”, submitted, 2018.

Electrothermal simulation of large-area semiconductor devices

S. Altazin[1], T. Beierlein[2], M. Diethelm[1,2,3], R. Ferrini[4], R. Hiestand[1],
C. Kirsch[2], T. Offermans[4], L. Penninck[1], M. Regnat[2], B. Ruhstaller[1,2]
[1]Fluxim AG, Winterthur, Switzerland; [2]ZHAW, Winterthur, Switzerland;
[3]Empa, Dübendorf, Switzerland; [4]CSEM SA, Muttenz, Switzerland

The lateral charge transport in thin-film semiconductor devices is affected by the sheet resistance of the various layers. This may lead to a non-uniform current distribution across a large-area device resulting in inhomogeneous luminance, for example, as observed in organic light-emitting diodes (OLEDs)[1]. On the one hand, the resistive loss in electrical energy is converted into thermal energy via Joule heating, which results in a temperature increase inside the device. On the other hand, the charge transport properties of the device materials are also temperature-dependent, such that we are facing a two-way coupled electrothermal problem. It has been demonstrated that adding thermal effects to an electrical model significantly changes the results[2].

For computational efficiency we use coupled zero-dimensional (0D) and two-dimensional (2D) models instead of a full three-dimensional (3D) model to describe the electric current density and the heat flux in a large-area semiconductor device. Our coupled model consists of

- two 2D models for the top (t) and bottom (b) electrodes; these are second-order partial differential equations (PDEs) for the electric potentials ψ_t, ψ_b [V] and for the temperatures T_t, T_b [K]. The coefficients of these PDEs are the reciprocals of the electrical and thermal sheet resistances $R_\square^{\text{el}}$ [Ω/□] and $R_\square^{\text{th}}$ [KW^{-1}/□].
- a 0D model for the semiconductor stack which yields the electric current density j_s [Am^{-2}] as a function of the voltage across the stack, $\psi_t - \psi_b$ [V], and the heat flux q_s [Wm^{-2}] as a function of the temperature difference across the stack, $T_t - T_b$ [K].

Such a dimensional reduction in the modeling of thin films is common, for example, in mechanics and electromagnetics and it has been used previously for large-area OLED simulations[2].

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[1] K. Neyts, M. Marescaux, A. U. Nieto, A. Elschner, W. Lövenich, K. Fehse, Q. Huang, K. Walzer, K. Leo: “Inhomogeneous luminance in organic light emitting diodes related to electrode resistivity”. J. Appl. Phys. 100, 114513 (2006)

[2] M. Slawinski, D. Bertram, M. Heuken, H. Kalisch, A. Vescan: „Electrothermal characterization of large-area organic light-emitting diodes employing finite-element simulation“. Org. Electron. 12, 1399–1405 (2011)

The two-way electrothermal coupling is divided into two directions with different physical effects: for the electrical→thermal coupling we consider Joule heating in the semiconductor stack and in the electrodes, i. e. ohmic losses are converted into heat. For the thermal→electrical coupling we assume an Arrhenius-type temperature dependence of the electric current density j_s in the semiconductor stack.

Our coupled 0D-2D electrothermal model finally consists of a set of four nonlinearly coupled PDEs for ψ_t, ψ_b, T_t, T_b. These equations are completed by boundary conditions and solved numerically using the finite element method. We use state-of-the-art techniques such as adaptive mesh refinement to obtain numerical solutions with a prescribed accuracy. After successful tests using a MATLAB prototype the electrothermal model presented here was incorporated into the simulation software Laoss by Fluxim AG[3].

The large-area simulation allows us to investigate, for example, the influence of various electrode designs on the electric current and on the temperature distribution (Fig. 1) inside the device[4], or we may analyze the pixel crosstalk in AMOLED displays[5]. We also observe negative differential resistance due to the electrothermal coupling (Fig. 2). This phenomenon has been simulated and also measured in OLEDs recently[6].

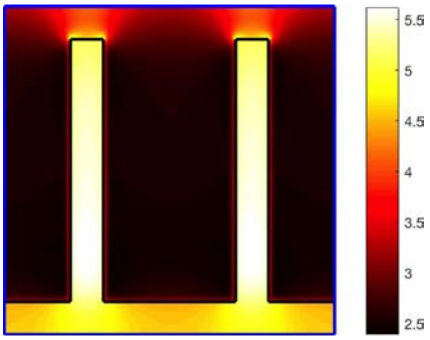

Fig. 1 Temperature distribution inside a 5 cm x 5 cm OLED module with a busbar and two metal fingers. The values indicate the temperature above the ambient temperature of 300 K.

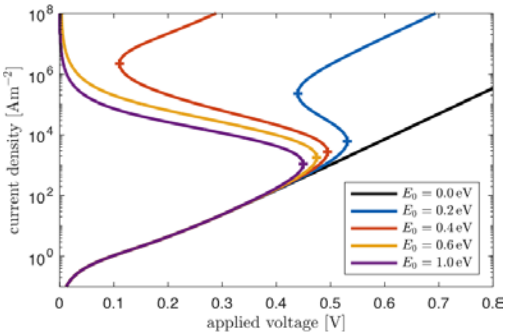

Fig. 2 S-shaped current-voltage characteristics of an OLED device (for different values of the activation energy E_0), indicating negative differential resistance. This is due to the positive feedback by the thermal→electrical coupling.

Acknowledgement This research was funded by the Swiss Commission for Technology and Innovation within the “Large Area Organic Semiconductor Software” (LAOSS) project (18737.1 PFNM-NM).

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[3] http://www.fluxim.com/laoss

[4] C. Kirsch, S. Altazin, R. Hiestand, T. Beierlein, R. Ferrini, T. Offermans, L. Penninck, B. Ruhstaller: „Electrothermal Simulation of Large-Area Semiconductor Devices“. Int. J. Multiphys. 11 (2), 127–136 (2017)

[5] M. Diethelm, L. Penninck, S. Altazin, R. Hiestand, C. Kirsch, B. Ruhstaller: “Quantitative analysis of pixel crosstalk in AMOLED displays”. J. Inf. Disp. 19 (2), 61–69, (2018)

[6] M. Liero, J. Fuhrmann, A. Glitzky, T. Koprucki, A. Fischer, S. Reineke: „3D electrothermal simulations of organic LEDs showing negative differential resistance“. Opt. Quant. Electron 49, 330 (2017)

Modelling the bias-dependent emission zone and its influence on the transient electroluminescence and OLED efficiency

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[3]FLUXIM AG, Winterthur, Switzerland

Organic light emitting devices (OLEDs) for lighting applications need high luminance values, which can be achieved by e.g. driving the OLED at high currents. At this driving level however OLEDs show an efficiency roll-off, which is nowadays one of the mayor challenges for high-efficient phosphorescent OLEDs. The main processes causing the efficiency roll-off are non-radiative exciton quenching processes, such as triplet-polaron quenching and triplet-triplet annihilation. At high bias, high exciton and charge carrier densities can be present in the emission zone leading to an increase of the non-radiative exciton decay rates and hence to a decrease of the OLED efficiency. A common method to determine the non-radiative exciton quenching rates is measuring the transient photo-/electroluminescence for increasing biases and fitting the initial luminance decay time, which is inverse proportional to the sum of radiative and all non-radiative contributions.

In this study we investigated the influence of the bias-dependent emission zone on the transient electroluminescence (EL) decay and on the OLED efficiency for a three-layer phosphorescent OLED. In this OLED, a strong emission zone shift for increasing bias was found in a previous study[1].

Figure 1a shows the measured EL decays for various biases. For applied voltages up to 8 V the EL decay time increases and then starts to decrease. We show that the increase correlates with a shift of the maximum emission away from the cathode towards the anode side of the emission layer where the Purcell factor is lower. At high bias the measurements show a decrease of the EL decay time, which is an indication of non-radiative exciton quenching.

Figure 1b shows the measured and simulated current efficiency. For biases up to 9 V, the OLED efficiency increases before it decreases again. Considering the bias-dependent emis-

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[1] M. Regnat, K. P. Pernstich, S. Züfle and B. Ruhstaller, „Analysis of the bias-dependent split emission zone in phosphorescent OLEDs", manuscript submitted to ACS Applied Materials & Interfaces

sion zone shift as well as exciton quenching in the electro-optical model[2], very good agreement between simulation and measurement was achieved.

We will present a detailed analysis on how the emission zone shift and the exciton quenching parameters influence the EL decay and the current efficiency.

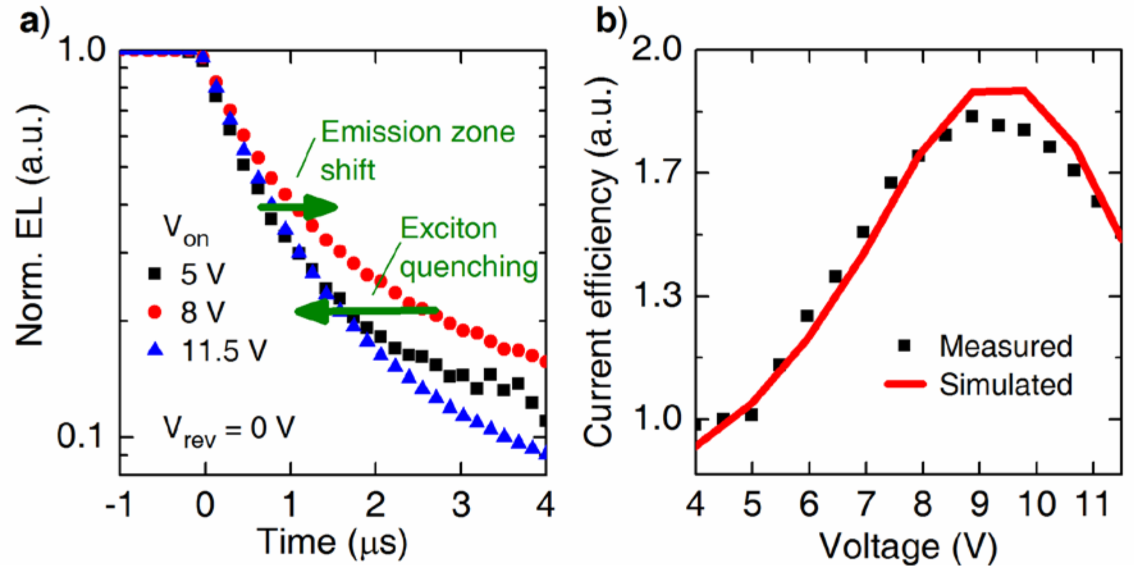

Fig. 1 (a) Measured ELdecays for increasing on-voltage, showing an increase of the decay time up to a bias of 8 V and then a decrease for further increased biases. **(b)** Measured and simulated current efficiency for increasing bias, showing an efficiency increase up to 9 V, followed by a decrease.

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[2] B. Perucco, N.A. Reinke, D. Rezzonico, E. Knapp, S. Harkema, B. Ruhstaller, “On the exciton profile in OLEDs-seamless optical and electrical modeling”, Organic Electronics 13 (2012) 1827–1835

Kinetic modelling of transient photoluminescence measurements of thermally activated delayed fluorescent materials

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[a]Merck KGaA, Display Solutions, Frankfurter Straße 250, 64293 Darmstadt, Germany
[b] University of Durham, Physics Deparment, South Road, Durham, DH1 3LE, UK

Thermally activated delayed fluorescence (TADF) is an established mechanism for harvesting triplet excitons in "metal-free" OLEDs[1] which gives a maximum attainable internal quantum efficiency of 100%. By minimizing the energy gap between the lowest lying singlet and triplet states, a conversion of slowly relaxing triplet states to faster relaxing singlet states via reverse intersystem crossing rate (rISC) is promoted. Although several highly efficient TADF emitters have been discovered, a reliable determination of the reverse intersystem crossing rate as a key parameter for the characterization of TADFs has not been provided yet.

In this work, we present a kinetic model for the TADF process which allows to extract not only rate constants but also time dependent state populations from transient photoluminescence experiments. Using this model, we obtain temperature dependent rISC rates from which we calculate the activation energy for the TADF process.

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[1] H., Uoyama; K., Goushi; K., Shizu; H., Nomura; C., Adachi; Nature 492 (2012), 234–238.

Disentangling excitonic loss mechanisms in TADF-type OLEDs using kinetic Monte Carlo simulations

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Mechanistic modeling of organic light-emitting diodes (OLEDs) using Kinetic Monte Carlo (KMC) provides a true molecular-scale and nanosecond-resolved view of the relevant processes occurring inside a device, including the actual spatial non-uniformity of the current density and emission[1], a decomposition of the efficiency loss in terms of fundamental loss processes such as exciton-polaron quenching and exciton-exciton annihilation, and a prediction of the device lifetime based on including molecular degradation[2].

The efficiency and operational stability of new generations of OLEDs are to a large extent determined by the detailed balance of generation and transfer of singlet and triplet excitons among the different materials inside the device's emitting layer. In TADF-based OLEDs, short living singlet excitons are generated by triplet-harvesting TADF molecules via the reverse intersystem crossing mechanism. A further improved OLED device can be designed by including high quantum-yield fluorescent molecules, to which singlet excitons generated on the TADF molecules are transferred, leading to hyperfluorescence. This is achieved by selecting material pairs that can facilitate efficient Förster energy transfer from the TADF molecule to the assisting dye. For optimal efficiency the average TADF-to-dye distance should be sufficiently large, so that short-range Dexter-type triplet transfer is unlikely, and at the same time sufficiently small so that the rate of longer-range Förster-type transfer is still large.

In this talk, we demonstrate how KMC simulations[3] can be used to successfully analyze, predictively model, and ultimately enhance the quantum efficiency of thermally-assisted delayed fluorescence (TADF)-based OLEDs and its roll-off at large current densities. We will show how the concentration of the fluorescent dye affects the device performance and how this material can be modified to boost the device efficiency.

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[2] R. Coehoorn et al., Adv. Funct. Mater. 25, 2024 (2015)

[3] Bumblebee KMC software (Simbeyond B.V.), https://simbeyond.com/bumblebee/

Device Performance and Degradation Analysis of a skyblue TADF-OLED

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The further establishment of OLED-based products requires the enhancement of device efficiency and moreover their long-term stability. Especially the achievement of blue color is challenging in commercially available products such as displays. Blue phosphorescent emitters are not stable enough due to the combination of long triplet lifetimes and the high bandgap. Therefore, most applications still make use of blue fluorescent emitters despite their intrinsic efficiency limitation due to the singlet-triplet factor. Thermally activated delayed fluorescent (TADF) emitters can harvest both singlet and triplet excitons for emission and exhibit shorter triplet lifetimes due to the efficient reverse intersystem crossing rate (k_{risc}).

In a first part, we analyze the behavior of a skyblue TADF-OLED. The emission zone and the emitter orientation are determined by combining angular emission spectra, measured with Phelos[1], with optical simulations in Setfos[1]. The determined emission zone (Figure 1d)) agrees well with rough sensing layer experiments and suggests emission originating from both sides of the emission layer (EML) and some dependence on current density. The characterization of OLED devices with systematically varied hole and electron transport layers (HTL and ETL) using steady-state, transient and impedance measurements allows to gain further insight into device operation.

In the second part, we focus on the degradation of the same skyblue TADF-OLED. During interrupted constant current stressing, a serious of measurements including I-V, TEL, C-f, C-V, spectral intensity and CELIV were carried out using Paios[1]. Several hypotheses for device degradation were analyzed based on the stress-time dependent behavior in the above men-

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[1] Phelos, Setfos, Paios by Fluxim AG, www.fluxim.com

tioned measurements. On the one hand, signatures of the commonly reported formation of trap states and increasing number of non-radiative quenching sites[2], which would lead to higher non-radiative recombination could not be observed. On the other hand, indications were found which suggest a reduced hole transport in the degraded device. Using electro-optical device simulations in Setfos[1] this could be further ascribed to a hole injection barrier increase or a HTL mobility decrease. However, these electrical parameters alone would not be sufficient to explain the current efficiency decrease during degradation. The elucidation of the remaining components responsible for device degradation is the topic of further investigations.

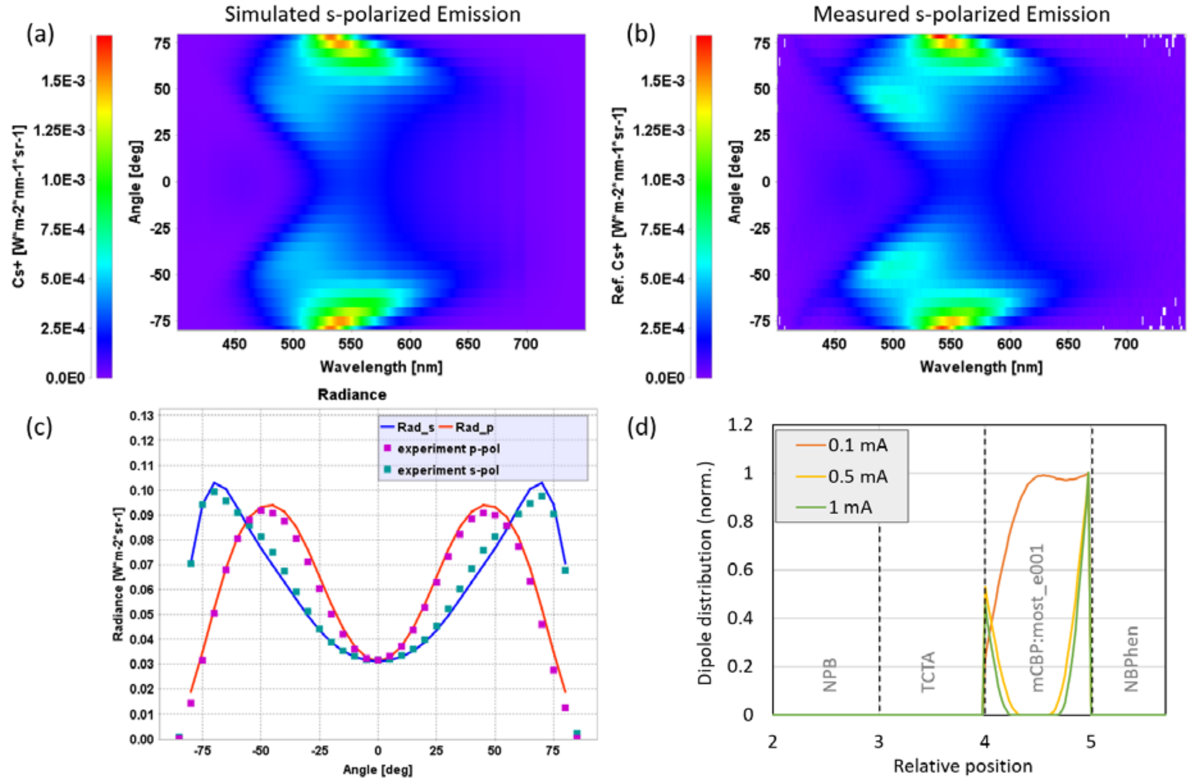

Fig. 1 (a) Simulated and (b) measured s-polarized emission spectrum of the studied skyblue TADF OLED at 0.1 mA. (c) Measured (squares) and simulated (lines) s- and p-polarized radiant intensity at a current density of 0.1 mA. (d) Determined emission zone profiles for different applied current densities indicated in the legend.

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[2] A S. D. Sandanayaka, T. Matsushima, and C. Adachi, “Degradation Mechanisms of Organic Light-Emitting Diodes Based on Thermally Activated Delayed Fluorescence Molecules”, J. Phys. Chem. C 119, 23845 (2015)

The use of polar OLEDs and MIS devices for parameter analysis

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Many commonly used electron transport materials for OLEDs form a permanent macroscopic polarization orientation upon deposition. This leads to the observation that, in a bilayer ETL/HTL configuration, holes are already injected into the hole transport layer below the built-in voltage and accumulate at the internal interface with the ETL.
We show that these polar bilayer devices behave as metal-insulator-semiconductor devices in accumulation regime, which have become popular in the last years for dedicated parameter analysis. Due to the energetic alignment it is possible to investigate only one charge carrier type at a time.
Using a drift-diffusion modeling approach[1] we can understand specific signatures of the polar layer that are found in impedance-frequency and capacitance-voltage experiments as well as in CELIV (charge carrier extraction by linearly increasing voltage) measurements[2]. The MIS-CELIV experiment can indeed be performed for these devices to determine the hole mobility. Again by employing simulation we investigate whether the thermal activation of the charge transport can be deduced from temperature-dependent experiments. We find that this is possible when combining the MIS-CELIV and the capacitance-frequency measurements. While the CELIV peak gives the mobility, the transition frequency of the C-f-T contains contributions of both the injection barrier and the mobility thermal activation[3].

Polar bilayers are therefore well-suited for parameter analysis, and the used materials and fabrication processes are widely accessible, which can be an advantage over standard MIS architectures. Furthermore it allows to employ fully operative devices with optimized processing and thicknesses for parameter analysis.

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[1] Setfos 4.4 by Fluxim AG

[2] Züfle et al., Journal of Applied Physics 121,175501 2017

[3] Züfle et al., Journal of Applied Physics 122,115502 2017

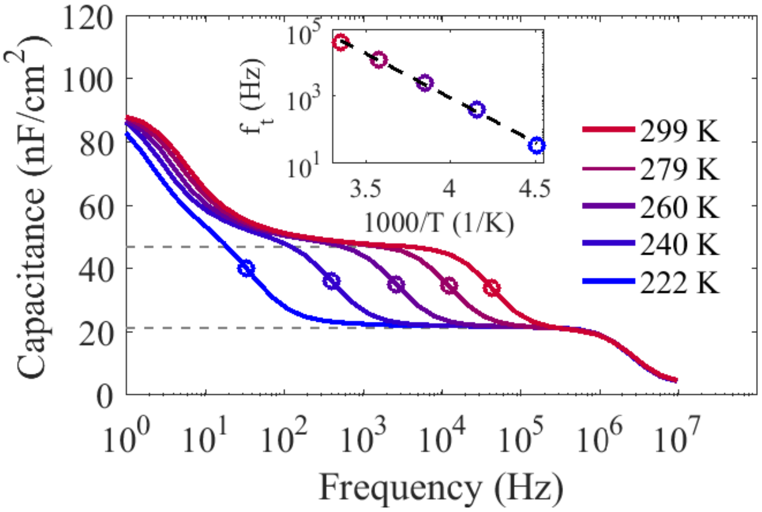

Fig. 1 Capacitance-frequency-temperature measurements of a polar bilayer OLED showing the thermal activation of holes into the hole transport layer.

Manipulation of injection barriers by dipolar doping

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The strong dipole moment of polar organic materials like tris-(8-hydroxyquinolate) aluminum Alq_3, if not oriented perfectly isotropic, can lead to the buildup of a spontaneous orientation polarization (SPO) inside the organic film. Its magnitude strongly depends on the growth conditions of the organic layer and is involved in the degradation process of OLEDs[1]. It is also responsible for the giant surface potential (GSP) of the polar layer, with a magnitude reaching a few 10 mV/nm. Both, SOP and hence GSP, not only occur in neat films but also in polar guest-host systems. We have studied "dipolar doping" of polar molecules diluted into a non-polar host material and could shed light on the orientation of guest molecules and the resulting GSP[2] as well as the influence of the GSP's magnitude on electron injection and therefore device performance independently[3]. In this contribution, the effect of dipolar doping on hole injection is elucidated. As we have shown previously[4], it is possible to apply the CELIV (Charge Extraction by Linearly Increasing Voltage) method on polar diodes to determine the charge transport activation energy. Combined with impedance spectroscopy, this technique can be used to measure the injection barrier of the underlying metal-semiconductor interface[5]. We applied this approach to polar diodes with varying GSP to measure the electrical injection barriers. Additionally, ultra violet photoelectron spectroscopy as an established method of determining injection barriers was conducted on suitable devices for comparison. We have applied the techniques to the prototypical organic system *N*,*N*'-Di(1-naphthyl)-*N*,*N*'-diphenyl-(1,1'-biphenyl)-4,4'-diamine (NPB) and Alq_3 in different dilutions and show the dependence of the determined barrier on the dilution ratio.

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Noguchi et al., Applied Physics Letters **96**, 143305 (2010)

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[3] Altazin et al., Organic Electronics, **39**, 244–249 (2016)

[4] Züfle et al., Journal of Applied Physics **121**, 175501 (2017)

[5] Züfle et al., Journal of Applied Physics **122**, 115502 (2017)

Simultaneous Drift-Diffusion Simulation of Current Voltage and Capacitance Voltage Measurement of Hole Only Devices Containing N,N'-Di(1-naphthyl)-N,N'-diphenyl-(1,1'-biphenyl)-4,4'-diamine (NPB)

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Drift-Diffusion simulations are widely used to describe the device characteristics of Organic Light Emitting Diodes (OLEDs). In comparison to other theoretical models such as kinetic Monte Carlo or Master Equation approaches they have the big advantage of less time-consuming calculations under the consideration of macroscopic layer parameters such as intrinsic transport levels and charge carrier mobilities. Therefore, they allow fitting of electrical device characteristics and enable the extraction of layer parameters. The determination of such parameters is a crucial step towards an advanced understanding of the physical processes that determine the performance of OLEDs. Even though drift-diffusion simulations are the method of choice, a parameter extraction is by far means not trivial: It highly depends on the mobility or injection model assumed, the measurement technique used and can be inaccurate due to a strong parameter correlation. To reduce this correlation, it is essential to combine several measurement techniques[1]. A common method for the extraction of charge carrier mobilities is for example the CELIV method[2], whereas injection barriers can be determined from the detailed evaluation of the peak position of capacitance voltage measurements as proposed by Mensfoort et al.[3].

Within this study we present a novel approach for the extraction of material parameters by combining both steady state and dynamic device characteristics. We first discuss the current voltage and capacitance voltage characteristics of hole only devices containing the well-known hole transport material N,N'-Di(1-naphthyl)-N,N'-diphenyl-(1,1'-biphenyl)-4,4'-diamine (NPB) for different layer thicknesses and different ac-frequencies for dynamic impedance spectroscopy measurement. For the theoretical description of these electrical device characteristics we use a unipolar drift-diffusion approach based on the work by Kühn et al.[4]. We keep our model as detailed as necessary but as simple as possible to describe the device characteristics. By simultaneously fitting both measurements we can extract material parameters such as hole mobility and hole injection barrier as well as device parameters such as the series resistance. Furthermore, we compare the extracted mobility with values reported in literature and the photo electron spectroscopy measurements performed for the corresponding hole transport material.

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Computer-Aided Optimization of Multilayer OLED Devices

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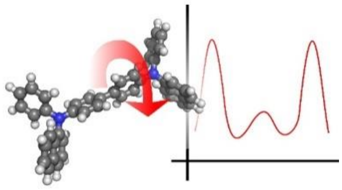
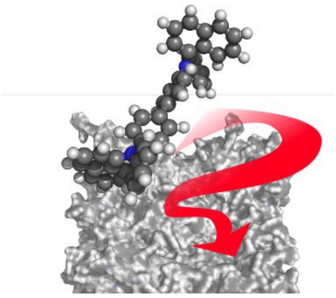
While computer simulations are widely used in organic electronics to support experimental R&D, established methods such as drift diffusion are based on parametric models and simulations rely on experimental input for parameters such as energy levels or charge carrier mobilities. This prevents the design of novel materials and optimization of devices fully in the computer. Therefore, industrial R&D relies on time consuming and costly trial and error approaches.

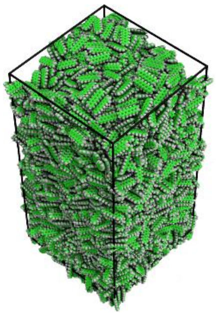
We overcome this barrier with a bottom-up multiscale modeling approach starting on the quantum mechanical level that maps single molecule properties to the device scale without the use of external parameters, e. g. from experiment. By including relevant effects and processes on the microscopic scale, this approach (i) generates insight on information that is not accessible by experiments (artificial microscope), (ii) allows researchers to analyze the impact of specific microscopic effects on device performance and (iii) enables the parameter-free ab-initio parametrization of continuum models (e.g. drift diffusion). This enables a straightforward and systematic identification of bottlenecks and allows the targeted development of compounds tailored for specific purposes and the optimization of layer architectures, fully in the computer.

In order to compute properties on the device level, we construct a digital twin of the device in the computer. This is done in four simulation steps:

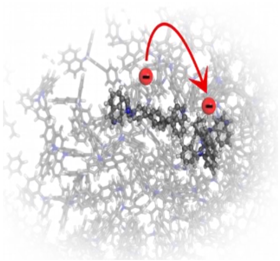
1. Geometries and electronic properties of single molecules (the constituents of e. g. HTL or ETL, host materials, dopants) are computed using quantum mechanical ab initio methods. Customized force-fields describing inter and intra-molecular interactions are generated automatically for each molecule for the simulation of the thin film formation.



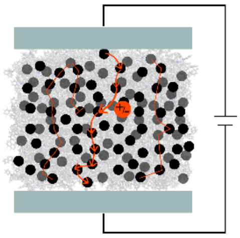




2. Based on the customized force-fields, molecular thin-films with atomic resolution are generated. Parallelized, grid-based force-field evaluation allows the fast deposition of morphologies on the 10 nm scale. By mimicking physical vapor deposition, experimentally observed features, such as inhomogeneities and anisotropies are exhibited in these structures. [1]



3. Atomistic morphologies are then analyzed on full quantum mechanical level. Electronic information necessary to compute charge and energy transfer rates (such as local energy levels or intermolecular electronic coupling) is calculated. Environmental effects are taken into account exclusively on quantum mechanical level, enabling the analysis of pristine layers, doped systems and specific interface effects. Distributions of electronic properties on the 10nm scale are mapped on the device scale to enable full device simulation.[2][3][4][5][6][7]



4. Based on the electronic structure in the molecular layers, charge transport on the device level, from single layers to multi-stack devices, is calculated using a kinetic Monte-Carlo approach. Rates for the individual processes are computed according to Marcus theory based on the electronic structure calculations of step 3.[8] Taking into account relevant excitonic and charge transport processes, these simulations allow the detailed analysis of microscopic bottlenecks in device performance.

This approach was applied to several systems that highlight how computer simulations can support R&D efforts in OE. Here we demonstrate its applicability and impact using a multi-layer OLED device, where fundamental reasons for limited IQE and roll-off are identified with the aid of charge carrier and exciton simulations.

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Light management for perovskite/silicon tandem solar cells with efficiency >25%

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Crystalline silicon solar cells are about to reach their efficiency limit, requiring disruptive approaches to further improve performance and lower the cost of photovoltaic electricity. One of the most promising solutions to overcome this limit relies on stacking several absorber materials with different bandgaps in a tandem cell. For example, an established technology such as crystalline silicon can be combined with a low-cost, wide-band gap top cell. With their tunable band gap, low material costs, and a high performance of up to 22%, perovskite solar cells are highly promising for tandem solar cells.

Based on a near-infrared-transparent perovskite cell processed at low temperature, we developed monolithic perovskite/silicon tandem cells with efficiencies of up to 25.2% [1]. In this tandem cell configuration, the perovskite top cell is deposited onto the silicon bottom cell, using an intermediate recombination layer between both sub cells. Optical losses in such tandem cells are mostly due to reflection losses and parasitic absorption in the transparent electrodes and top cell charge transport layers. We present how both types of losses were addressed to optimize the performance of our tandem cells, with optical simulations [2-4] guiding this development. These simulations consider both ray-optical scattering at the random-texture wafer surface as well as coherent thin-film optics in the conformal layers of the tandem cell. Parasitic absorption was minimized by using a perovskite top cell in the p-i-n polarity, which allows us to use a thin fullerene layer at the front side, reducing losses in the UV/blue part of the solar spectrum. In addition, a high-mobility transparent conductive oxide was employed as the front electrode, reducing free-carrier absorption in the near-infrared. Reflection losses were minimized by optimizing layer thicknesses in the top cell and using an intermediate recombination layer with a high refractive index to reduce interference effects [5]. Furthermore, we show how reflection losses can be further strongly reduced by utilizing both-sides textured wafers [1,4]. The deposition of the perovskite top cell is challenging on such textured wafers with micron-sized pyramidal surface structures. By choosing appropriate deposition techniques for every layer in the top cell stack, a conformal coating is achieved, resulting in high optical and electrical tandem cell performance. Moreover, light management in tandem solar cells involves the distribution of current between both sub cells. This is especially important in the monolithic tandem configuration, where the current is limited by the sub cell which produces the lower photocurrent. We present pathways to obtain current matching by tuning the top cell absorber layer band gap and thickness [4-6].

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Development of Perovskite/CIGS thin film solar cells and opportunities with lightweight flexible devices

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$Cu(In,Ga)Se_2$ (CIGS) thin film solar cells and modules have been developed on glass as well as metal foil and polymer film substrates. Manufacturing of flexible and light-weight solar modules is challenging but offers numerous advantages and opportunities. Recent advancements show promising potential for solar cell efficiency enhancements but might limit to 25% due to material and interface properties of the stack. The approach of tandem solar cell is an attractive option for the development of super high efficiency (>30%) thin film photovoltaic devices. Perovskite and CIGS compounds allow band gap engineering over a wide composition range making them attractive for multi-junction solar cells. Our group has developed semi-transparent perovskite solar cells with combined high efficiency and near infrared transparency enabling us to achieve 22.7% Perovskite/CIGS tandem device in 4-terminal configuration. Further efficiency improvements will depend on the reduction of optical and electronic losses in stacks with diverse layers and interfaces.

Simulation study of the effects of ferroelectric domains in perovskite solar cells

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This work is focused on understanding the role that ferroelectric domains in methylammonium lead halide perovskite ($MAPbI_3$) can have on the performance of solar cells built from this material. We study 2D and 3D systems considering different polarization domain patterns, inspired by measurement data, by proposing a polarization model based on the knowledge of the crystalline structure, symmetry considerations and electrical simulations. We compute charge carrier transport by solving a drift-diffusion model, in which the Poisson equation for the electrostatic potential calculation explicitly includes the polarization field.

We show that the presence of polarization domains has a strong impact on charge separation, thus leading to a decrease of recombination losses and formation of current pathways at domain interfaces[1]. Specifically, the decrease of Shockley-Read Hall recombination losses improves the open-circuit voltage, while the low resistivity current pathways lead to improved transport and an increase of the short-circuit current. The achieved results demonstrate that the presence of ordered ferroelectric domains, even with weak magnitude of polarization, can actually affect the performance of the solar cell in terms of enhanced power conversion. Moreover, from the comparison between our results and experimental IV characteristics of $MAPb(I,Cl)_3$ devices we conclude that the polarization model proposed can effectively reproduce the solar cell operation.

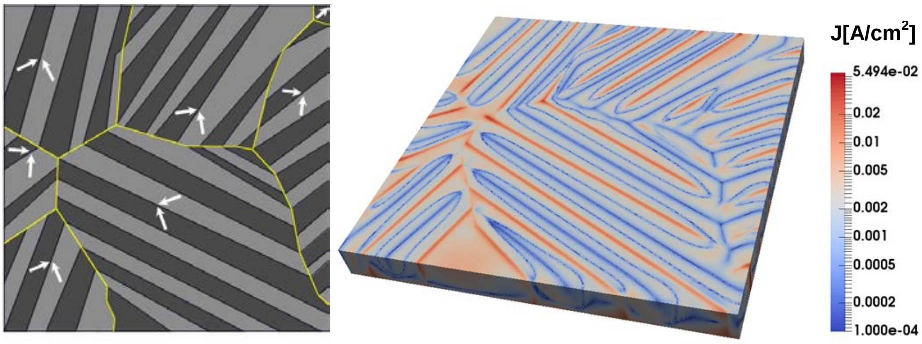

Fig. 1 Perovskite sample with multiple grains, and differently oriented polarization domains (left), the simulated current density pattern (right).

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The Quest for Stability of Perovskite Solar Cells – Understanding Degradation and Investigation Under Simulated Weather Conditions

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[2]EPFL, Lausanne, Switzerland

Perovskite solar cells have achieved power-conversion efficiency values approaching those of established photovoltaic technologies, making the reliable assessment of their operational stability the next essential step towards commercialization. Although studies increasingly often involve a form of stability characterization, they are conducted in non-standardized ways, which yields data that are effectively incomparable. Furthermore, stability assessment of a novel material system with its own peculiarities might require an adjustment of common standards. This talk will firstly explore, how different experimental conditions impact the ageing behaviour of perovskite solar cells and which parameters are important to control during ageing experiments.[1] At the end of the day, however, only energy yields that can be achieved under real-world, long-term operation matter. Hence, secondly, this talk will analyse the performance of 20%-efficient perovskite solar cells under simulated weather conditions based on real temperature and irradiance data of selected days during the course of a year at a location in central Europe.[2] Combining measurement with simulation and comparing it to the performance to a silicon heterojunction cell, it will be shown that the perovskite cell, shows a much lower decrease of efficiency with temperature and light intensity, maintaining almost optimum values for dominant weather conditions. Therefore, the resulting year-averaged efficiency is close to the value measured under standard operating conditions. Whereas the maximum-power-point voltage of silicon and perovskite solar cell is differently affected by the weather conditions, the current scales linearly with light intensity for both devices. This finding is particularly important when considering integration of perovskites into current-matched monolithic 2-terminal tandem solar cells with silicon, which are believed to be the way towards a successful commercialization of the perovskite technology.

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[2] Performance of Perovskite Solar Cells Under Real Weather Conditions in the Lab. **Tress, Domanski et al.** *Submitted*

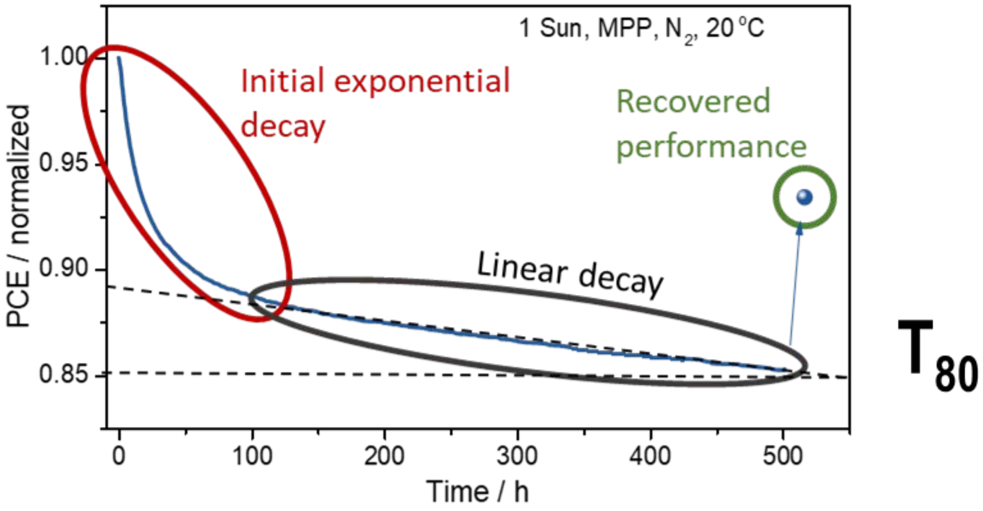

Fig. 1 Degradation behaviour of a perovskite solar cell under maximum power point tracking, showing an initial reversible degradation component, followed by a slow, linear, irreversible one

Identifying recombination mechanisms in perovskite solar cells using transient ideality factors

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The ideality factor of a solar cell, derived from the open circuit voltage V_{OC} dependence on light intensity ϕ, has classically been used to identify the dominant recombination mechanism in photovoltaic devices.[1] However, applying this 'Suns-V_{OC}' technique to perovskite cells is problematic since open circuit voltage values change with time owing to the presence of mobile ionic charge in the perovskite layer. This V_{OC} evolution depends on the previously applied bias V_{pre}, the light intensity ϕ, and the device architecture. Here we show that the dominant recombination mechanism in perovskite devices can be identified from the signature of the transient ideality factor $n_{id}(t)$ following application of a forward bias in the dark. $n_{id}(t)$ is measured by monitoring the evolution of the open circuit voltage as a function of time at different light intensities (**Fig. 1a**). The ideality factor is then extracted using the slope of the V_{OC} versus log(ϕ) plot at each point in time throughout the measurement (**Fig. 1b**).

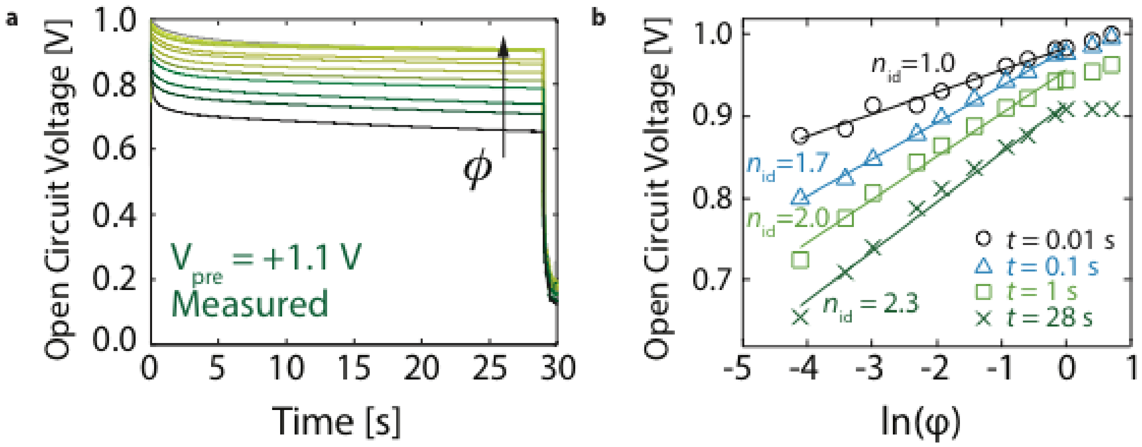

Figure 1. Example transient Suns-V_{OC} measurement. (a) Open circuit voltage evolution for increasing light intensity ϕ for a FTO/compact-TiO_2/mp-Al_2O_3/$CH_3NH_3PbI_3$/Spiro-OMeTAD/Au perovskite solar cell following preconditioning in the dark for 60 s with a forward bias of V_{pre} = +1.1 V. **(b)** Transient ideality factor n_{id}, inferred from the same transient Suns-V_{OC} measurement.

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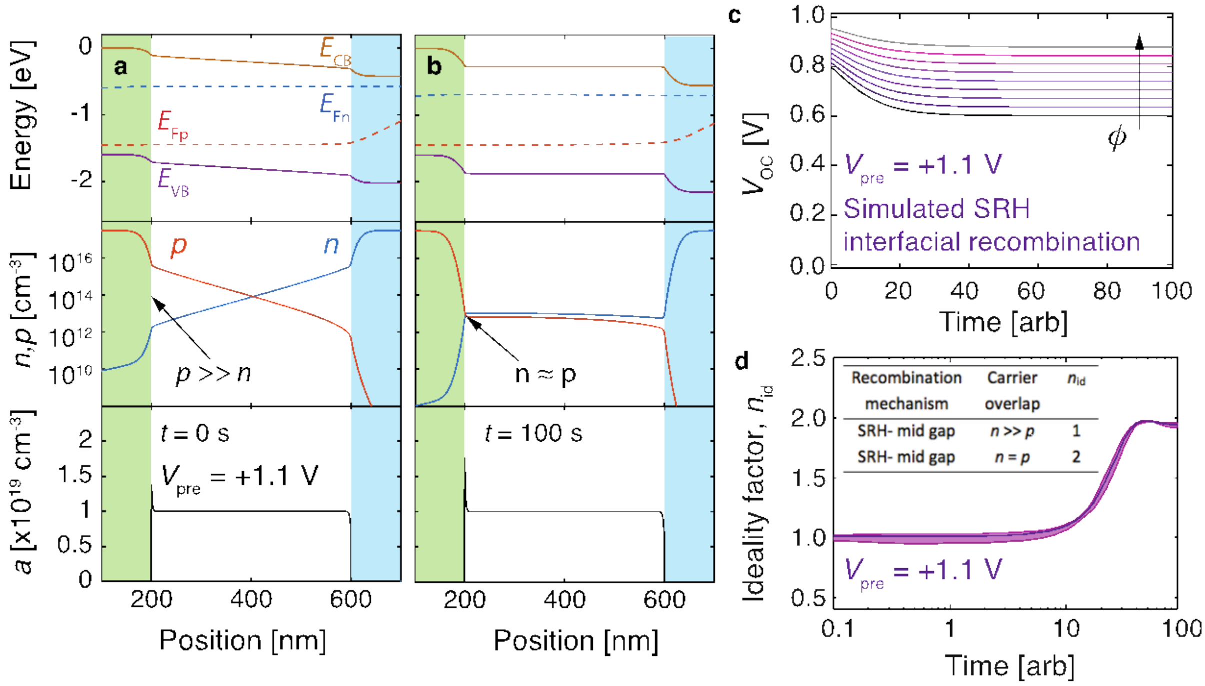
[1] Thomas Kirchartz, Florent Deledalle, Pabitra Shakya Tuladhar, James R. Durrant, and Jenny Nelson. On the Differences between Dark and Light Ideality Factor in Polymer:Fullerene Solar Cells. *Journal of Physical Chemistry Letters*, 4 (14):2371–2376, 2013.

Using a one-dimensional drift-diffusion model[2] we investigate the effect of mobile ionic charge carriers on the transient ideality factor of simulated *p-i-n* devices with a range of recombination schemes. We show changes in the overlap of electron and hole populations (**Figs. 2a – 2d**) owing to slow mobile ion redistribution can account for the transient ideality factors observed in perovskite devices: a change in the dominant recombination process is not required.



Recombination mechanism	Carrier overlap	n_{id}
SRH- mid gap	$n >> p$	1
SRH- mid gap	$n = p$	2

Figure 2. Simulated Energy level diagram, charge densities and transient V_{OC} evolution for a *p-i-n* device at open circuit. Energy level diagram, electron *n*, hole *p* and mobile ionic charge *a* densities for a simulated device dominated by SRH recombination at the interfaces after preconditioning at V_{pre} = +1.1 V and being switched to open circuit at **(a)** t = 0 s and **(b)** t = 100 s. **(c)** Simulated open circuit voltage transients following illumination at increasing light intensity for the same device. **(d)** The transient ideality factor changes from 1 to 2 following preconditioning at V_{pre} = +1.1 V due to the change in charge carrier overlap consistent with zero-dimensional theoretical predictions (inset table).

Following this analysis we show that the signature evolution of the ideality factor following preconditioning at forward bias can be correlated to theoretical predictions for different recombination types. The results show that a standard architecture $CH_3NH_3PbI_3$ device with an inert mesoporous (mp) Al_2O_3 scaffold is dominated by interfacial recombination through deep level trap states, whereas a similar device employing a mp-TiO_2 scaffold is dominated by recombination throughout the mesoporous region.

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[2] DRIFTFUSION is a MATLAB-based code developed at Imperial College London, available to download and contribute at: https://github.com/barnesgroupICL/Driftfusion

Transport layers limit the efficiency of perovskite solar cells: an experimental and theoretical study.

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Prof.Dr. Dieter Neher[2] and Prof.Dr. L. Jan Anton Koster[1]

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Perovskite solar cells (PSCs) are the current rockstar of photovoltaic research attracting more and more attention. With efficiency now reaching up to 23% PSCs are on the way of catching up with classical inorganic solar cells. However, PSCs have not reached their full potential yet. In fact, their efficiency is limited, on the one hand, by non-radiative recombination, mainly via trap states located either at the grain boundaries or at the interface between the perovskite and the transport layers. On the other hand, it is limited by losses due to the poor transport properties of the commonly used transport layers. Indeed, state-of-the-art transport layers (e.g. TiO2, PCBM and Spiro-OMeTAD…) suffer from rather low mobilities, typically within 10^{-4} – 10^{-2} cm^2 V^{-1} s^{-1}, when compared to the high mobilities, 1 – 10 cm^2 V^{-1} s^{-1}, measured for perovskite using field-effect transistors or space-charge-limited-current measurement.

In this work, the effect of the mobility, thickness and doping density of the transport layers was investigated by means of a combined experimental and modeling analysis. For the experiment, two sets of devices made of a triple-cation perovskite were studied, including n-i-p and p-i-n structures demonstrating efficiencies of up to 20%. For the two structures, the thickness and doping density of one of the transport layers were varied in order to understand their effect on the performance and especially on the FF. In addition, we performed a transient extraction experiment to look at the influence of the transport layers properties on the rate of extraction. The experimental results were then reproduced using drift-diffusion simulations to explain how and by how much every single parameter influences the extraction and the performance. A new and simple formula was also introduced to easily calculate the amount of doping necessary to counterbalance the low mobility of the transport layer.

In conclusion, this work presents a comprehensive analysis of the effects of the different properties of a transport layer on the efficiency of PSCs. We also present general guidelines on how to optimize a transport layer to avoid losses.

Modeling negative capacitance and inductive loop in perovskite solar cells

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Negative capacitance and inductive loops in impedance spectroscopy at low or intermediate frequencies in perovskite solar cells have been described in several recent reports [1-4]. The origin of these observations, however, remained unknown so far and is under debate. There are suggestions that the negative capacitance and inductive loop are related to one another as they appear in the same samples but at different applied biases. A direct correlation between the observation of the negative capacitance and a corresponding decrease in performance of the solar cell was reported recently [3]. Similarly, we have demonstrated that ion migration is present even in high-efficiency low-hysteresis perovskite cells [5].

In this contribution, we shed light on the physical mechanisms behind these observations. For this purpose, we employ a 1D model that includes electronic transport as well as ionic transport. The model is able to simulate current-voltage curves, transient responses and impedance spectra and naturally produces inductive loops and negative capacitance.

We investigate which factors influence the occurrence of the negative capacitance and the inductive loop by systematically varying the model parameters. The simulations allow us to analyze the charge carrier and ion distributions at different applied bias where the negative capacitance and an inductive loop appear.

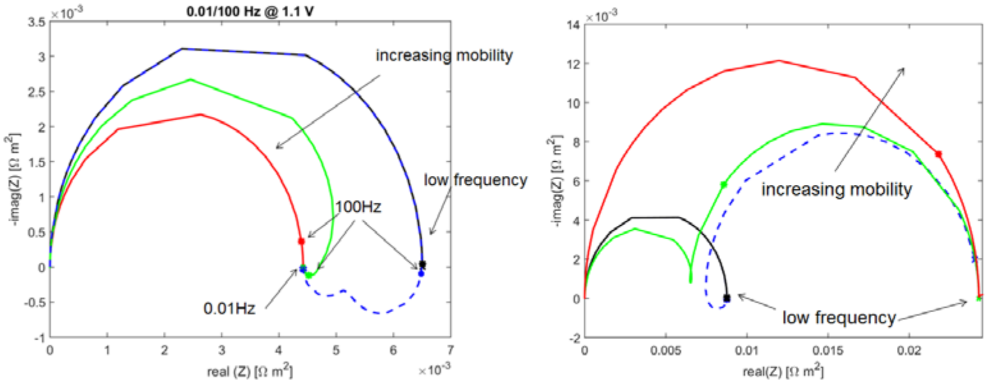

Fig. 1 Simulation of impedance of a perovskite solar cell for varied ion mobility: a) negative capacitance is obtained for bias of 1.1 V below Voc, b) inductance loop is observed at 0 V.

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Fundamental relation of the of *J-V* characteristics, capacitance and charge carrier lifetimes in solar cells

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The recombination of free charge carriers is the dominating loss mechanism in solar cells and reduces the open-circuit voltage, fill factor and short-circuit current and thus limits the power conversion efficiencies. To achieve high power conversion efficiencies, charge carriers must be extracted to the electrodes before they recombine. Charge carrier recombination is thus commonly described by an associated charge carrier lifetime. With the purpose of getting a deeper understanding of the limiting recombination factors, charge carrier lifetimes are widely measured using various optical and electrical measurement techniques, and empirical relations of the charge carrier lifetimes to parameters of the current-voltage (*J-V*) characteristics are found. [1,2]

Recently, however, it was demonstrated that the charge carrier lifetimes obtained by optoelectronic techniques are severely disturbed by capacitive effects in thin film organic solar cells. [3,4] But a complete understanding of the device physics is still lacking.

In this presentation we demonstrate that the charge carrier lifetimes, as measured by optoelectronic techniques, in silicon and organic solar cells are inherently linked to the *J-V* characteristics by the discharge of the electrode capacitance. As a function of voltage, the charge carrier lifetimes are determined by the capacitance and the differential resistance of the *J-V* characteristics. Thus, we conclude that the *J-V* characteristics and the charge carrier lifetimes are inherently linked, and that optoelectronic measurements of the charge carrier lifetimes become obsolete as they do not provide a deeper understanding of the underlying processes. Meaningful insight into the charge carrier dynamics can only be obtained on electrode-free samples, *e.g.* by spectroscopic techniques such as transient absorption.

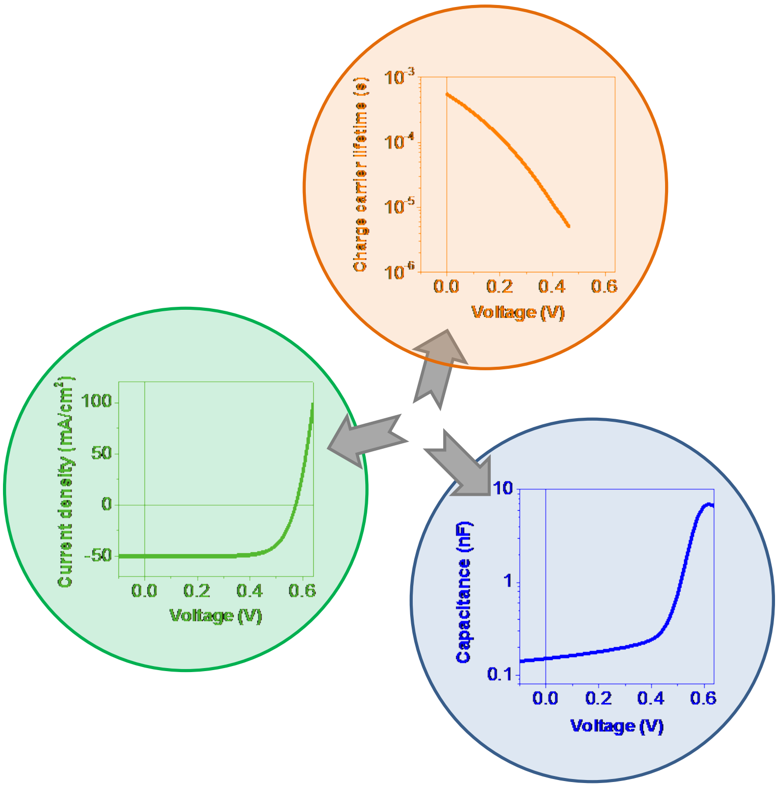

Fig. 1 In solar cells, charge carrier lifetimes are determined by the internal discharge of the capacitance. The capacitance, *J-V* characteristics and charge carrier lifetimes can be calculated from each other.

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Absorption induced heating of solar cells leads to a characteristic open-circuit voltage turnover

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The open-circuit voltage (V_{oc}) of a solar cell is known to increase with the intensity of the incident light. However, the absorption of photons heats up the sample, especially if no charge carrier can leave the device. Any temperature increase is known to decrease V_{oc}. Solving these recombination current related dependencies self-consistently leads to the result that the open-circuit voltage has a turnover for increasing light intensity[1].

The proposed effect is measured for different material systems, such as perovskite, small molecules, polymers, and silicon. We find a good agreement between the model and the experimental data and the fit allows to access several parameters: The effective bandgap over which free charge carriers recombine, a global invariant ideality factor, and a thermal resistance related to the sample geometry.

A benefit of our method is the determination of these parameters from a single measurement curve at ambient conditions which would also suit to large-area devices where other methods using external temperature control are not applicable. The results further demonstrate that a turnover of V_{oc} does not necessarily stem from surface recombination, but can often easily be explained by absorption induced sample heating, which leads to a similar mathematical behavior as observed for electrothermal feedback in systems with temperature-activated conductivity[2].

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Microscopic simulation of charge carrier transport and recombination at hetero-interfaces in solar cells

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Hetero-interfaces are ubiquitous in modern solar cell architectures, be it at carrier selective contacts (electron/hole blocking layers) or at window and passivation layers. Since key physical processes such as charge carrier transport and recombination are severely affected by the presence of hetero-interfaces, the latter need to be considered adequately in any computational device engineering approach. In conventional semi-classical and macroscopic device simulation, band offsets induce abrupt variations in the carrier density. Furthermore, the local density of states entering the computation of interface recombination reflects neither the effects of the barrier potential nor the large electric fields associated with the strong band bending that is often present in the interface region. On the other hand, such deviations from the semiclassical flat-band bulk picture can be captured by a microscopic device simulation framework on the level of quantum-kinetic theory[1].

Motivated by the large impact of local fields and heterostructure potentials revealed by quantum-kinetic simulations in ultrathin GaAs solar cells[2,3] and silicon heterojunction devices[4], we apply the formalism to the situation of perovskite absorber architectures, where the recombination in the hetero-contact regions is increasingly considered as a major loss factor[5]. The investigation of defect-mediated recombination in a quantum-transport model is enabled by recent progress in the extension of the non-equilibrium Green's function theory of recombination via multiphonon relaxation[6] to non-bulk-like environments in spatially-resolved device simulation, which will be briefly reviewed in the presentation.

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Opto-electronic characterization of third-generation solar cells

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We present an overview of opto-electronic characterization techniques for solar cells including light-induced charge extraction by linearly increasing voltage, impedance spectroscopy, transient photovoltage, charge extraction and more. Guidelines for the interpretation of experimental results are derived based on charge drift-diffusion simulations of solar cells with common performance limitations. It is investigated how nonidealities like charge injection barriers, traps and low mobilities among others manifest themselves in each of the studied cell characterization techniques. Moreover, comprehensive parameter extraction for an organic bulk-heterojunction solar cell comprising PCDTBT:PC70BM is demonstrated. The simulations reproduce measured results of 9 different experimental techniques. Parameter correlation is minimized due to the combination of various techniques. Thereby a route to comprehensive and accurate parameter extraction is identified.

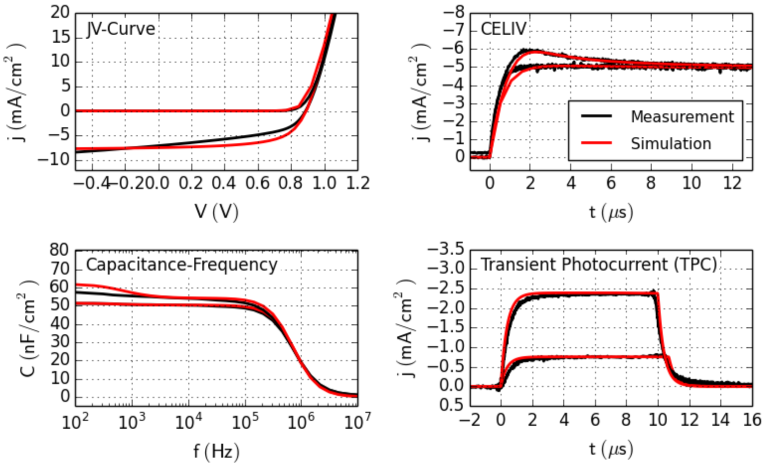

Fig. 1 **Simulation and measurement of an organic bulk-heterojunction solar cells. a) JV-curve in the dark and under illumination. b) Photo-CELIV currents with two different light intensities. c) Impedance spectroscopy data in the representation of capacitance versus frequency for two different offset-voltages. d) Transient photocurrents with two different light intensities.**

Revisiting the use of transient photovoltage measurements as a probe of recombination in thin film solar cells

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Transient photovoltage (TPV) measurements have been frequently used to study the recombination lifetime of thin-film solar cells. TPV uses the decay of a small optically-induced voltage perturbation to probe the charge dynamics of devices at open circuit. The transient response to a short pulse of light in modelled devices was simulated using a drift diffusion model. Whilst for high mobility systems the lifetime inferred from the simulated TPV measurement matches well with the input lifetime, in cases where charge-carrier mobilities in the active layer are lower than 10^{-3} $cm^2V^{-1}s^{-1}$, the extracted lifetime deviates strongly from the input lifetime value and is highly dependent on mobility. In such low-mobility cases, the simulated charge carrier dynamics show bi-exponential behaviour where the fast decay at early times reflects the recombination of charges in the bulk, while the second, slower decay relates to charges that accumulate near the interfaces. The inhomogeneous spatial distribution of charge carriers in a device at open circuit reduces the recombination rate close to the interfaces, making net recombination dependent on how fast charges can diffuse into the bulk to recombine. As the open-circuit voltage is related to the majority carrier quasi-Fermi levels near the interfaces, its decay is most strongly related to this second slower decay of the charges. Following this observation we developed a new technique to monitor the charge-carrier density during the TPV experiment. We applied this method alongside conventional TPV to measure the recombination dynamics in different systems, including bulk heterojunctions comprised of P3HT with both a fullerene acceptor (PCBM) and non-fullerene acceptor (O-IDTBR). We observed that while the TPV lifetime of the fullerene and non-fullerene devices were similar in magnitude (7µs and 3µs respectively), the recombination lifetime of the non-fullerene system was significantly faster at 0.1µs compared to 2µs. By studying the parameters influencing the photovoltage and charge carrier decays, we present a method to estimate the mobility of these devices, and hence estimate the diffusion length of carriers in the active layer.

Using extraction current transients to characterize device parameters relevant for charge collection in thin-film diodes and solar cells

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In order to improve charge collection in solar cell devices based on low-mobility semiconductors, such as organic solar cells, a deeper physical understanding of the processes taking place is needed. The charge collection is limited by the competition between charge carrier transport and recombination within the bulk. The charge collection in these type of devices is also sensitive to both contact-related issues, such as surface recombination, and unintentional doping giving rise to doping-induced space charge regions within the active layer[1]. However, in order to be able to quantify different loss mechanisms, new methods to characterize relevant device parameters, such as the built-in voltage, are needed. In particular methods to determine the surface recombination velocity, being a key parameter describing the charge carrier selectivity at the contacts[2,3], have been lacking for organic devices.

In the past, extraction current transients such as the charge extraction by linearly increasing voltage (CELIV) technique has been used to characterize the mobility in organic solar cell devices. In this work, we use a drift-diffusion model to extend the underlying analytical theory behind CELIV to account for effect of contacts, etc. Based on the analytical derivations and the numerical simulations, we furthermore demonstrate how the extended CELIV theory can be utilized to characterize other device parameters, such as doping concentration, built-in voltage, and surface recombination velocity at contacts in organic semiconductor devices.

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Reliable electrical characterization and modeling of organic LEDs and solar cells with doped layers and internal interfaces

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Fundamental prerequisites to understand the physics inside organic electronic devices and improve their performance are the reliable extraction of material parameters and to have a good device model to investigate the impact of the physical parameters on the device operation and performance.

An elegant way to extract material parameters is therefore the combination of numerical device simulation and multiple measurement techniques applied to a few samples. In this way one can extract all involved material parameters at the same time and extract device independent values. Hole-only devices with different thickness were characterized to reduce the number of involved material parameters compared to a full OLED. We perform steady-state and impedance simulations of pip devices with different thickness using the drift-diffusion model implemented in SETFOS.

In order to improve our device model, the physics of organic/organic interfaces was investigated and a comprehensive model based on the hopping transport theory was derived. It is able to capture the mechanisms happening in charge generation or recombination units in tandem devices. A key parameter is the doping density which can be extracted by the above method. The model is coupled with the drift-diffusion formalism away from the interface, enabling fast simulations of full devices. This approach has been implemented in SETFOS, taking advantage of state-of-the-art optical, electronic and excitonic models already implemented.

S. Jenatsch et al., J. Appl. Phys., accepted for publication (2018)

S. Altazin et al., J. Appl. Phys., accepted for publication (2018)

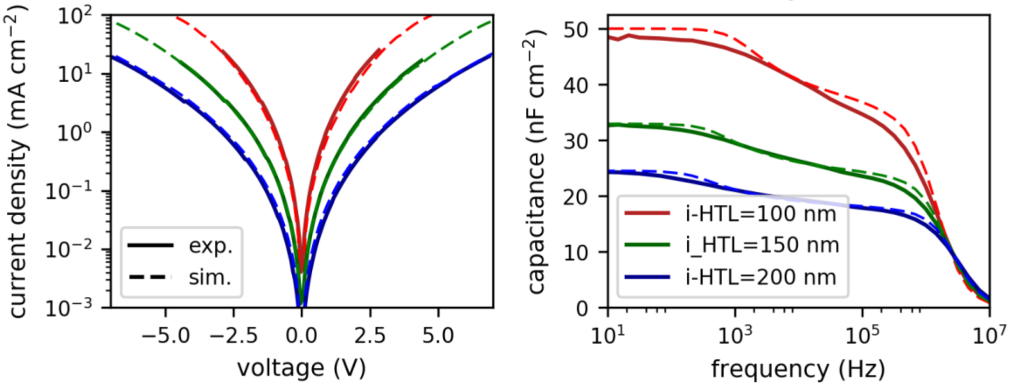

Figure 1. I-V (left) and C-f (right) measurements (full lines) and simulations (dashed lines) of hole-only pip devices with different intrinsic layer thickness.

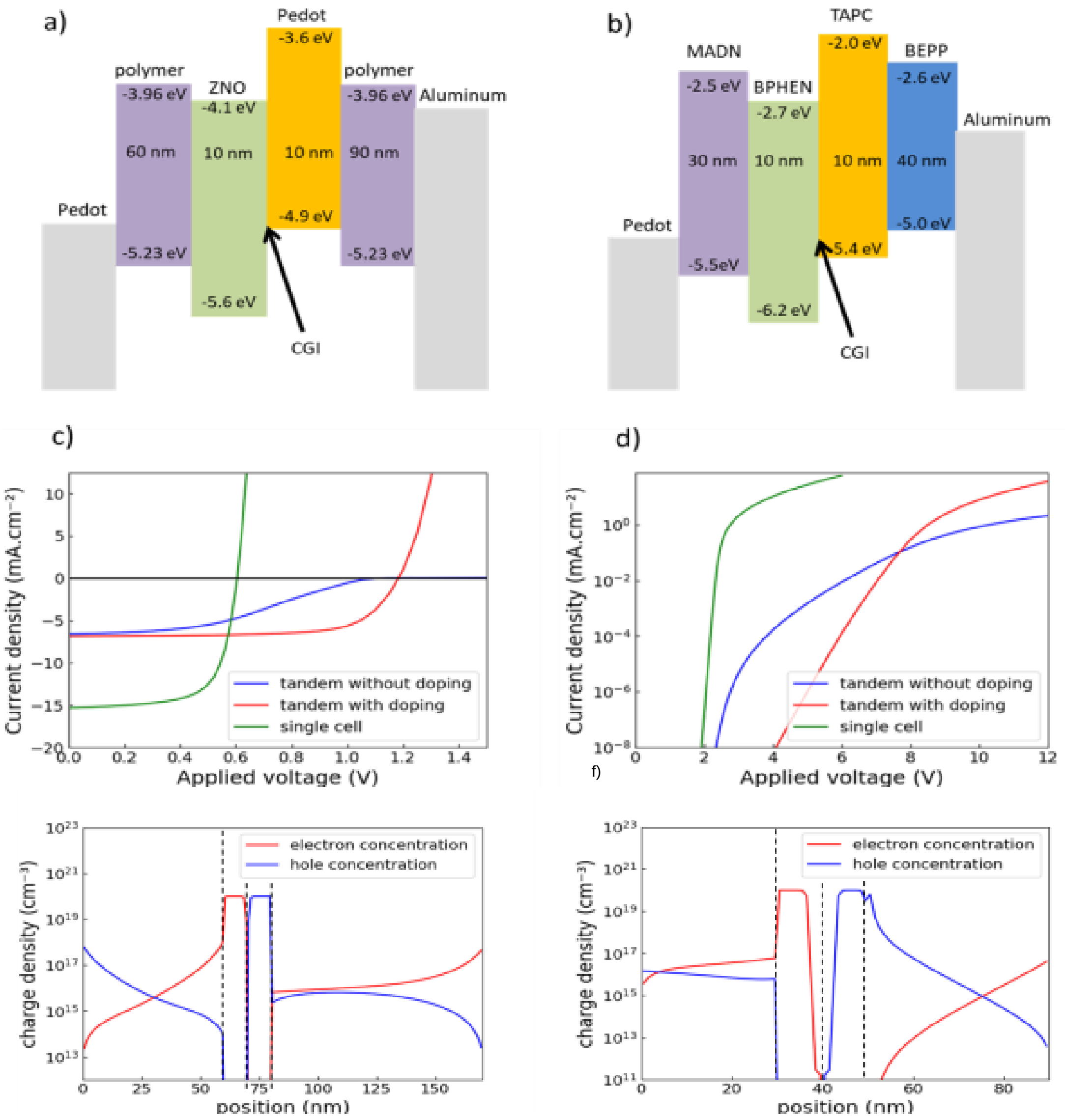

Figure 2. Energy diagram for the simulated tandem OPV composed of two sub-cells with identical active-layer material ("polymer") (a) and of a simple tandem OLED (b). Simulated IV curve of the corresponding device with and without doping the layers surrounding the CRI and CGI, respectively (c) and (d). Charge carrier density in the OPV at MPP (1V) (e) an in the OLED at 8V (f).

Monochromatic LEDs Based on Perovskite Quantum Dots: Opportunities and Challenge

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The emergence of organic-inorganic hybrid perovskite (OIHP) semiconductors has generated considerable research effort aimed at demonstrating their optoelectronic devices, including the light-emitting diodes (LEDs). In practice, an important motivation for the development of perovskite LEDs is the need of monochromatic light sources covering the entire visible range of human eye, in particular in the deep green spectral region. Among all solution-processible semiconductors, OIHPs are the only material system that can theoretically cover > 95% color gamut of the Rec. 2020 standard. In this talk, I will briefly summarize the opportunities and challenges in both fundamental and technological aspects, based on our recent work in this field[1-5].

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[5] S. Kumar, J. Jagielski, T. Tian, N. Kallikounis, W.C. Lee and C.J. Shih, Under review (2018)

Ionic-to-electronic current amplification in hybrid perovskite solar cells

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Mobile ions in hybrid perovskite semiconductors introduce a new degree of freedom to electronic devices suggesting applications beyond photovoltaics. An intuitive device model describing the interplay between ionic and electronic charge transfer is needed to unlock the full potential of the technology. We describe the perovskite-contact interfaces as transistors which couple ionic charge redistribution to energetic barriers controlling electronic injection and recombination. This reveals an amplification factor between the out of phase electronic current and the ionic current. The resulting simple equivalent circuit model, which we verified with time-dependent drift-diffusion simulations of impedance spectra, allows a general description and interpretation of perovskite solar cell behaviour. Our findings also suggest a strategy to design thin film electronic components with large, tuneable, capacitor-like and inductor-like characteristics.[1]

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[1] arXiv:1805.06446

Modeling of organic semiconductor LASERs: toward continuous wave operation and electrical current injection

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Over the past few decades, organic semiconductors have been the subject of intense research and are now being explored extensively for various optoelectronic applications such as organic photovoltaics, lighting, displays and sensing. Our group focuses on the design and development of new organic emitters for high performance organic optoelectronic devices.

In this talk, we firstly introduce recent results of our group related to new thermally activated delayed fluorescence (TADF) molecules and long persistent luminescence. Then, the demonstration of the first organic semiconductor laser (OSL) in quasi-continuous wave (CW) regime is presented.

The operation of OSLs in CW regime under optical excitation and the realization of electrically driven OSL diode is still a challenging issues. Losses caused by the generation of long-lived triplet and thermal degradation of the organic gain medium under intense long-pulse optical pumping represent severe issues for long-term laser operation.

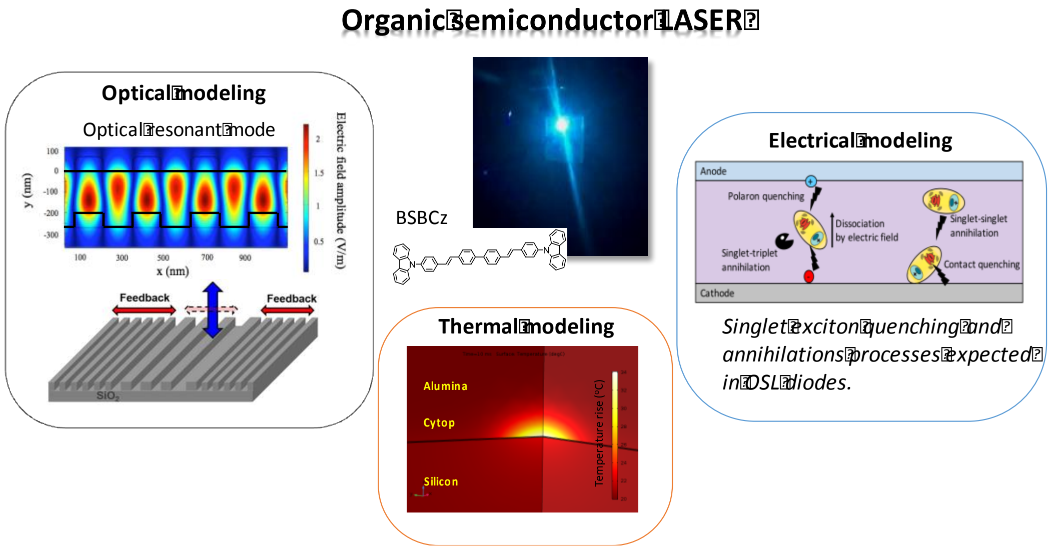

Fig. 1 Optical, thermal and electrical modeling of organic semiconductor LASER.

Recently, in our group, we demonstrated an OSL operating at 80 MHz in quasi-CW regime and still working in the long-pulse regime after 500 successive pulses of 30 ms which represents a major step toward the development of a real CW, organic, solid-state laser technology[1]. Figure 1 shows a photograph of the quasi-CW OSL.

This achievement was possible thanks to the use of 4,4′-bis[(N-carbazole)styryl]biphenyl (BSBCz) as organic gain material with high PLQY, high optical gain, and no spectral overlap between the lasing emission peak and the triplet and singlet excited-state absorption bands. The combination of this gain material with mixed-order DFB gratings allowed the achievement of low-threshold quasi-CW lasers. Optical and thermal modeling were performed in order to design the LASER and to derive conclusions about how the present devices are limited on the way toward achieving real CW operation (Figure 1). These results represent a major advance in the field of organic photonics and open new prospects toward the development of reliable and cost-effective, organic-based, CW, solid-state laser technology.

The CW operation will also facilitate the realization of electrically driven OSL diodes. In addition to the loss mechanisms present in the optically pumped LASER, further loss mechanisms are excepted in electrically driven OSL diodes. Those losses are due to the low charge carrier mobility of organic semiconductors, the presence of contacts and the accumulation of triplet excitons and polarons. Thus, investigation of the various annihilation and quenching processes in an OLED under high pulsed electrical excitation such as polaron quenching, singlet-triplet annihilations and electric field quenching, etc. is crucial to optimize the device performance and overcome the limitation processes to the achievement of an OSLD[2]. In this context, the performances of an OLED under high pulsed electrical excitation are analyzed by performing an electro-optical simulation in order to probe the effect of the various exciton annihilation and quenching processes.

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[1] A.S.D. Sandanayaka, T. Matsushima, F. Bencheikh, K. Yoshida, M. Inoue, T. Fujihara, K. Goushi, J.-C. Ribierre, and C. Adachi, ”Toward continuous-wave operation of organic semiconductor lasers“, Sci. Adv. **3**, 1602570 (2017).

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Optical modes in light-emitting electrochemical cells

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The distinguishing differences between an organic light-emitting diode and a light-emitting electrochemical cell (LEC), stem from the inclusion of an electrolyte in the emissive active layer of the latter. During operation, the electrolyte gives rise to a number of highly desirable device properties such as a (comparative) insensitivity to layer-thickness variations, relaxed requirements on the electrodes' work functions, and low-voltage driving with thick active layers. However, it also brings more involved operational physics with time-dependent *in-situ* growth of electrochemically p- and n-type doped transport regions and formation of a p-i-n junction. This process obstructs straightforward prediction of the device performance through thin-film optics- and drift-diffusion simulations. E.g., when the conductivity of the electrochemically doped regions increases during operation, the full complex refractive index dispersion evolves as a result of the (very) high polaron density in these regions.[1] We make use of a commercial thin-film optics simulation tool (setfos 4.6), and investigate the effects of electrochemical doping on the different optical modes at steady state in Super Yellow-based polymer LECs. It has been anticipated that doping-induced self-absorption will limit the performance of polymer LECs with heavily doped and/or thick active layers,[2] but is that really a limiting factor in the commonly employed thickness range, and can we learn something from these computer based experiments that can accelerate the development of LECs—from a scientific curiosity into a market-ready technology?

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[1] Lanz T. et al., On the asymmetric evolution of the optical properties of a conjugated polymer during electrochemical p- and n-type doping, J. Mater. Chem. C., 2017, (5) 4706

[2] Kaihovirta N. et al., Doping-Induced Self-Absorption in Light-Emitting Electrochemical Cells, ACS Photonics, 2014, 1(3), 182–189

Emission zone position in sandwich super yellow light-emitting electrochemical cells

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Organic light-emitting electrochemical cells (LECs) are very simple and cost-effective electroluminescent devices compared to an OLED since they consist of a single emissive organic/salt layer sandwiched between two electrodes. This is possible because an operated LEC develops a p-doped/intrinsic/n-doped (p-i-n) structure in the active layer due to movement of ions when an electric field is applied. The doped regions enable injection and transport of electronic charges to the intrinsic region where charge recombination and light emission occurs. There are still important scientific questions to answer regarding the ion, doping, emission and electric field profile inside the active layer at different points in time.

Here we investigate the impact of the emission zone (EZ) position, where excitons recombine and photons are emitted, on the performance of a super yellow (SY) LEC, a prototype emitting material which has been used for many years in this field. We fabricated well performing devices with champion (and average) values for the current efficacy of 9.8 (8.4) cd/m^2 and for the power conversion efficacy of 8.8 (7.2) lm/W with a measured thickness of 70nm and for a constant current driving of 7.7mA/cm^2. The current efficacy is increased by 30% compared to identically fabricated devices with a thickness of 110nm. This suggests that solely changing the active layer thickness is leading to a notable performance change. LECs are subject to the weak microcavity effect, which means that interference plays a crucial role in the out-coupled luminance[1,2]. Fig. 1 shows the calculated luminance for different active

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[1] E. M. Lindh, P. Lundberg, T. Lanz, J. Mindemark, and L. Edman, “The Weak Microcavity as an Enabler for Bright and Fault-tolerant Light- emitting Electrochemical Cells,” pp. 1–10, 2018.

[2] H.-C. Su, “Optical Techniques for Light-Emitting Electrochemical Cells,” Chempluschem, pp. 1–15, 2018.

layer thicknesses and positions of the EZ. The model considers the changing optical constants in the p- and n-regions due to doping as well as re-absorption of emitted light by these regions. By comparing the luminance for 110 nm with 70 nm thick devices, we find that the thin device outperforms the thicker device only for EZ positions below 0.5, if the relative EZ position is assumed to be independent of the active film thickness. From planar LECs, however, it is known that the EZ is positioned closer to the negative electrode[3]. Furthermore, our average measured device performance value of 660 Cd/m^2 for the 70nm thick device falls in the region of 0.6-0.7. This suggests that the relative EZ position is actually not independent of the layer thickness, in agreement with scattered literature results on that poorly understood topic[4].

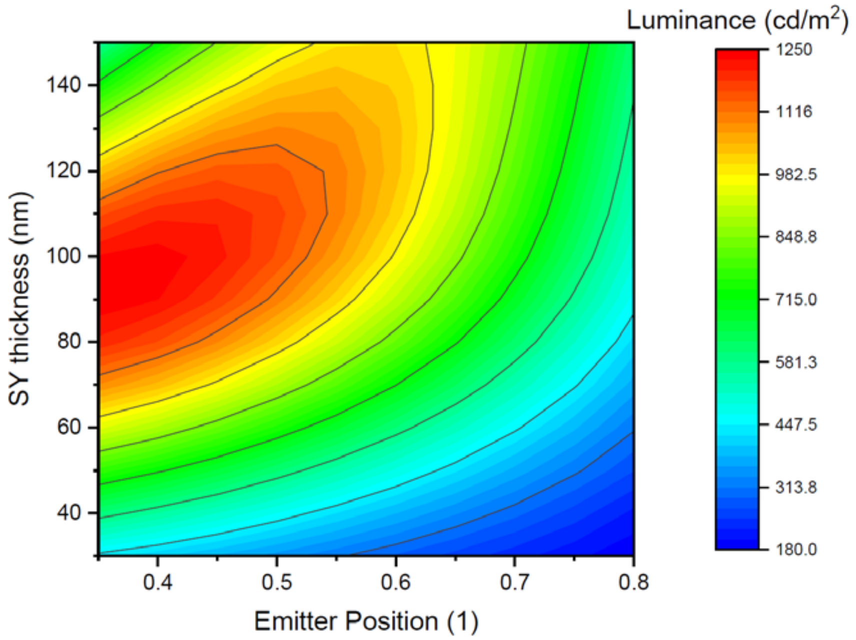

Fig. 1 Out-coupled luminance for different emitter positions and active layer thicknesses. Position 0 is at the ITO, 1 at the aluminium electrode. The current density is 7.7mA/cm^2, an internal quantum efficiency of 68.3%[5] and an exciton conversion efficiency of 25% is assumed. Changing real and imaginary refractive indices of p- and n-doped regions with respect to intrinsic values are included in the model[6].

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[5] S. D. Yambem, M. Ullah, K. Tandy, P. L. Burn, and E. B. Namdas, "ITO-free top emitting organic light emitting diodes with enhanced light out-coupling," Laser Photonics Rev., vol. 8, no. 1, pp. 165–171, 2014.

[6] T. Lanz, E. M. Lindh, and L. Edman, "On the asymmetric evolution of the optical properties of a conjugated polymer during electrochemical p- and n-type doping," J. Mater. Chem. C, vol. 5, no. 19, pp. 4706–4715, 2017.

Time-Dependent p–i–n Structure and Emission Zone in Sandwich-Type Light-Emitting Electrochemical Cells

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Light-emitting electrochemical cells (LECs) can be fabricated as single emissive organic/salt-layer sandwiched between two electrodes, offering cost-effective lighting applications. The ideal device situation during operation is considered to be a p-i-n junction with doped regions at the electrodes which facilitate balanced hole and electron injection. Clearly, the position of the p-i-n junction and the emission zone (EZ) influence the efficiency of LECs. Their investigation over time is therefore crucial to obtain further understanding and improvement of these devices. In planar LECs the active area can be directly imaged. The width of the EZ in sandwich-type LECs, however, remains elusive because it must not correspond to the width of the low-conductive intrinsic region which is estimated by impedance spectroscopy.

We first introduce a method to determine the center of the intrinsic region in sandwich LECs that is based on spectral photocurrent response measurements combined with optical modelling. Together with capacitance measurements, this yields a detailed picture of the evolution of the p-i-n structure.[1] Secondly, the EZ is determined by simulating experimentally determined angle-dependent emission spectra. The comparison between EZ and p-i-n structure reveals sufficient agreement, suggesting that both methods can render independent insights into the device situation of a sandwich-type LEC.[2]

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[1] S. Jenatsch, L. Wang, M. Bulloni, A. C. Véron, B. Ruhstaller, S. Altazin, F. Nüesch, R. Hany, "Doping Evolution and Junction Formation in Stacked Cyanine Dye Light-Emitting Electrochemical Cells", ACS Appl. Mater. Interfaces 8, 6554 (2016).

[2] S. Jenatsch, M. Regnat, R. Hany, M. Diethelm, F. Nüesch, B. Ruhstaller, "Time-Dependent p–i–n Structure and Emission Zone in Sandwich-Type Light-Emitting Electrochemical Cells", ACS Photonics 5, 4, 1591 (2018)

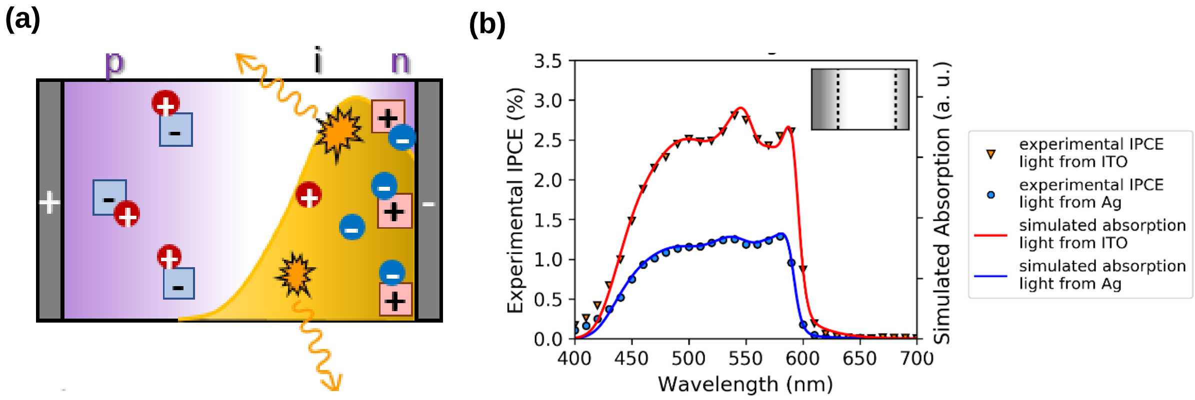

Fig. 1 (a) Sketch of the p-i-n device situation and the emission zone in an operated LEC. (b) Incident photon-to-electron conversion efficiency and simulated absorption of the intrinsic region for a semi-transparent LEC at one point in time. The inset shows a sketch of the determined p-i-n junction formation.

Angular luminescence spectroscopy: measurement and simulation of OLED emitter orientation and QD down-conversion films

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OLEDs and quantum dot (QD) enhanced LCDs are the key technologies for today's best-in-class displays for both mobile and TV applications. Novel high performance long lifetime emitting and light-converting materials are essential to the further success of the OLED and QD on the market. Display scientists and manufacturers have a constant need to characterize light emitting OLED and quantum dot materials in their drive for brighter, more colorful, sharper and more efficient displays. All of these characteristics are strongly influenced by the orientation, position and spectrum of the light emitting species inside the device stack. Tuning these material and device parameters is one of the most promising approaches to enhance the efficiency in state-of-the-art OLEDs.[1]

We have developed an angular luminescent spectrometer that determines the position and orientation of emitters inside a working OLED stack or a single emitter film by measuring the electroluminescence (EL) or photoluminescence (PL) spectrum in all emission- and polarization angles. The angular spectrum and polarization is a fingerprint of the emitter molecules' orientation and of the position inside the emitting layer, where electrons and holes recombine and generate light. In combination with optical simulations, from a single emitting layer up to the full OLED stack, the measured angular characteristics allows for a reliable and accurate extraction of these key quantities.

In this presentation we will review various aspects of angular EL and PL spectroscopy and the data analysis by optical modeling on the basis of selected measurements.

One significant advantage of the angular PL and EL method over traditional approaches to characterize the optical transition dipoles, like variable-angle spectroscopic ellipsometry (VASE), is its capability to precisely analyze the dipole orientation even if the emitters are embedded in a host matrix. We will specifically discuss the characterization of pure emitters films vs. host-guest systems with respect to the emitter orientation.

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[1] D. Schmidt et al., Phys. Rev. Appl. **8**, 037001 (2017)

In a second part, we will focus on the measured angular resolved down-conversion properties of QD films and compare our experimental findings to optical simulations describing the absorption, re-emission and scattering mechanism of the QD particles in a mean-free-path model. Finally, we will discuss the sensitivity of the angular spectroscopy to determine key parameters like particle concentration and QD diameter from measured emission profiles.

On the ionic conductivity in thin-film LLZO solid state electrolyte materials

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The persistent trend to more and more powerful mobile devices as well as the shift towards e-mobility significantly push the requirements for stable and safe storage solutions with even higher energy density. However, if not sacrificing on safety and stability, the Li-ion batteries with liquid electrolyte will soon reach a limit for gravimetric and volumetric energy densities. The commonly suggested workaround is the use of solid-state electrolyte materials instead of the flammable liquid electrolytes currently in use. This technology has the potential to offer higher energy densities and extended lifetime, reduce safety issues, and enable new geometries and form factors.[1]

Solid-state electrolyte materials with wide electrochemical stability window typically suffer from rather low bulk ionic conductivities. Reducing the thickness of such electrolyte materials to a couple of hundred nanometers does facilitate sufficient ionic conductance for battery applications, and reduces the total volume of inactive material, therefore increasing energy density. Garnet-type $Li_7La_3Zr_2O_{12}$ (LLZO) electrolyte is a promising ionic superconductor for the development of all-solid-state thin-film batteries.[2] In bulk, this material has demonstrated high ionic conductivities (~1 mS/cm at RT), as well as a wide electrochemical stability window (against metallic lithium and above 4V vs. Li^+).[3] However, if deposited as a thin film, the ionic conductivities reported so far have lagged behind by some orders of magnitude.[4]

In this contribution, we will discuss how the ionic conductivity of garnet-type $Li_{7-3x}M_xLa_3Zr_2O_{12}$ (LLZO) electrolyte thin films depends on the crystalline structure, the morphology, and the chemical composition. LLZO films are prepared by magnetron co-sputtering from LLZO, Li_2O, and M_2O_3 (or M) targets, where M stands for a three-valent metal (aluminum or gallium) that is added for stabilizing the more conductive cubic phase at room temperature.

Crystalline phases have been investigated using grazing-incidence X-ray diffractometry. Scanning electron microscopy and time-of-flight secondary ion mass spectrometry have been used to assess the density and the distribution of substitutional element in the film. The ionic conductivity has been measured by in-plane impedance spectroscopy and equivalent circuit fitting.

Our results reveal that the key factor for improving ionic conductivity in LLZO thin films consists not only in obtaining the right cubic phase, but also in increasing the density of the film and improving its stability.

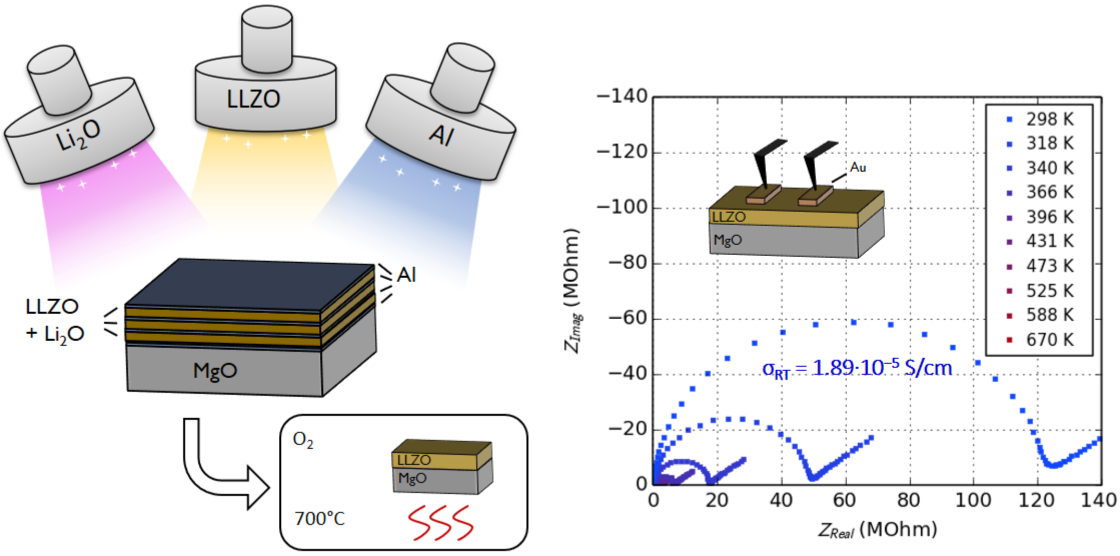

Fig. 1 Schematic of the fabrication process and temperature-dependent impedance spectroscopy measurement of an Al:LLZO thin film.

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2. Murugan, R., Thangadurai, V. & Weppner, W. Fast Lithium Ion Conduction in Garnet-Type $Li_7La_3Zr_2O_{12}$. *Angew. Chem. Int. Ed.* **46,** 7778–7781 (2007).
3. Matsuda, Y. *et al.* Sintering behavior and electrochemical properties of garnet-like lithium conductor $Li_{6.25}M_{0.25}La_3Zr_2O_{12}$ (M: Al^{3+} and Ga^{3+}). *Solid State Ion.* **311,** 69–74 (2017).
4. Rawlence, M. *et al.* Effect of Gallium Substitution on Lithium-Ion Conductivity and Phase Evolution in Sputtered $Li_{7-3x}Ga_x La_3Zr_2O_{12}$ Thin Films. *ACS Appl. Mater. Interfaces* **10,** 13720–13728 (2018).

Charge transport in organic semiconductor materials: a numerical simulation perspective

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In this talk a generalized kinetic Monte Carlo (kMC) framework for the simulation of organic semiconductors and electronic devices will be presented [1,2]. This includes devices such as solar cells (OSCs) [3] and light-emitting diodes (OLEDs). The model generalizes the representation of the multifaceted properties of the organic material from atomistic details up to morphology features. This is achieved by the implementation of a multiscale model to describe the organic semiconductor. The atomistic part, which is generally computationally very demanding, has been powered by using an advanced machine learning methodology. Applications of the model to predict charge carrier mobility will be presented.

[1] W. Kaiser et al., *Algorithms* **2018**, *11*(4), 37
[2] W. Kaiser et al., *Phys. Chem. Chem. Phys.*, **2018**, *20*, 8897-8908
[3] T. Albes and A. Gagliardi, *Phys. Chem. Chem. Phys.*, **2017**, 19, 20974-20983