International Conference on Simulation of Organic Electronics and Photovoltaics 2020
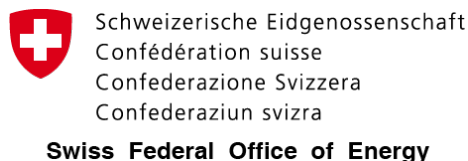
Zurich University of Applied Sciences

31. August -2. September 2020

Final Version (September 2, 2020)

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This year's edition is a virtual event.

Scientific Program

IMPORTANT: Central European Summer Time (CEST)

time	Monday, 31.8.20 *Emerging PV*	Tuesday, 1.9.20 *OLED*	Wednesday, 2.9.20 *Novel Devices/PV*
08.45-09.00	Welcome	Welcome	Welcome
09.00-09.20	**Q. Jeangros** *EPFL PVLab, CH*	**K. Vandewal** *Hasselt Univ., BE*	**T. David** *Bangor Univ., UK*
09.20-09.40	**M. Stolterfoht** *Potsdam Univ., GER*	**M. Liero** *WIAS, GER*	**M. Hess** *Battronics, CH*
09.40-10.00	**T. Kirchartz** *FZ Jülich, GER*	**A. Hofmann** *Augsburg Univ., GER*	**S. O'Kane** *Imperial College, UK*
10.00-10.20	break	break	break
10.20-10.40	**U. Paetzold** *Karlsruhe Inst. Tech., GER*	**G. Wetzelaer** *Max Planck Institute, GER*	**A. Riedinger** *Max Planck Institute, GER*
10.40-11.00	**J. Nelson** *Imperial College, UK*	**S. Zeder**, *Fluxim, CH* **Ch. Hauenstein**, *Simbeyond, NLD*	**P. Paudel**, *KSU , USA* **G. Mourouga**, *ZHAW, CH*
11.00-11.10	**A. Prel**, *ICube, FRA*	**R. Saxena**, *BPS, GER*	**W. Tress**
11.10-11.20	**J. Gorenflot**, *KAUST, SAU*	**St. Sem**, *Fluxim, CH*	*ZHAW, CH*
11.20-11.40	break	break	break
11.40-11.50	**P. Lopez-Varo**, *IPVF , FRA*	**M. Regnat**, *ZHAW, CH*	**U. Aeberhard**, *Fluxim, CH*
11.50-12.00	**M. Azzouzi**, *Imperial College, UK*	**M. Baldoni**, *CNR-ISMN, ITA*	**S. Jenatsch**, *Fluxim, CH*
12.00-12.10	**J. Yan**, *Imperial College, UK*	**J. Bangsund**, *UMN, USA*	**S. Shital**, *BGU, ISR*
12.10-12.20	**V. Bharti**, *UNL, PRT*	**M. Diethelm**, *EMPA, CH*	**D. Ompong**, *CDU, AUS*
12.20-12.30	**K.S. Nithya**, *UOC, IND*		

invited talks

contr. talks

Tuesday, 1.9.2020

08.45-09.00	Welcome/Opening	
	Beat Ruhstaller, ICP ZHAW and Fluxim AG, Switzerland	
09.00-09.20	Emissive and charge-generating donor-acceptor interfaces	
	Koen Vandewal, Hasselt University, Belgium	24
09.20-09.40	Drift-Diffusion Simulation of S-Shaped Current-Voltage Relations	
	for Organic Semiconductor Devices	
	Matthias Liero, WIAS, Germany	25
09.40-10.00	Orientational anisotropy in organic thin films and the impact	
	on electrical properties of organic light emitting diodes	
	Alexander Hofmann, Augsburg University, Germany	27

10.00-10.20	**Coffee Break**	

10.20-10.40	Efficient and stable single-layer organic light-emitting diodes	
	Gert-Jan Wetzelaer, MPI Mainz, Germany	28
10.40-10.50	Coupled 3D master equation and 1D drift-diffusion approach	
	for advanced OLED modeling	
	Simon Zeder, Fluxim AG, Switzerland	30
10.50-11.00	A kinetic Monte Carlo study of deconfinement	
	in transient photoluminescence of TADF host-guest systems	
	Christoph Hauenstein, Simbeyond, Netherlands	32
11.00-11.10	A kinetic Monte Carlo study of triplet-triplet annihilation	
	in conjugated luminescent materials	
	Rishabh Saxena, University of Bayreuth, Germany	34
11.10-11.20	Extraction of TADF OLED parameters using multiple PL transients	
	Stefano Sem, Fluxim AG, Switzerland	36

11.20-11.40	**Coffee Break**	

11.40-11.50	Analysis of degradation phenomena in exciplex TADF OLEDs	
	Markus Regnat, ZHAW ICP, Switzerland	38
11.50-12.00	Multiscale simulations of realistic metal/organic interfaces	
	Matteo Baldoni, CNR-ISMN, Italy	40
12.00-12.10	Sub-Turn-on Exciton Quenching Due to Spontaneous Orientation Polarization	
	in Organic Light-Emitting Devices	
	John S. Bangsund, University of Minnesota, USA	42
12.10-12.20	The Dynamic Emission Zone in Sandwich Polymer Light-Emitting Electrochemical Cells	
	Matthias Diethelm, EMPA, Switzerland	43

Wednesday, 2.9.2020

08.45-09.00	Welcome/Opening	
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09.00-09.20	Lifetime and performance prediction for organic and perovskite solar cells through machine learning	
	Tudur David, Bangor University, United Kingdom	45
09.20-09.40	New Li-ion battery technologies introduced in EV's and their characterization	
	Michael Hess , Battronics AG, Switzerland	47
09.40-10.00	Physics-based modelling of Li-ion batteries	
	Simon O'Kane, Imperial College, United Kingdom	48
10.00-10.20	**Coffee Break**	
10.20-10.40	Kinetically driven self-assembly of semiconductor nanoplatelets	
	Andreas Riedinger, MPI Mainz, Germany	49
10.40-10.50	Modeling Ion Currents in Organic Electrochemical Transistors	
	Pushpa Raj Paudel, Kent State University, USA	50
10.50-11.00	Capacity fade in Redox Flow Batteries: coupled phenomena of transport in concentrated solutions	
	Gaël Mourouga, ZHAW ICP, Switzerland	51
11.00-11.20	Transient photovoltage measurement of perovskite solar cells	
	Wolfgang Tress, ZHAW ICP, Switzerland	52
11.20-11.40	**Coffee Break**	
11.40-11.50	Opto-electronic modeling of organic and hybrid multijunction solar cells	
	Urs Aeberhard, Fluxim AG, Switzerland	53
11.50-12.00	Electro-thermal simulation and optimisation of organic solar cells and modules	
	S. Jenatsch, Fluxim AG, Switzerland	54
12.00-12.10	Spectrum sharing between Perovskite and Silicon solar cells: An alternative to tandem structures	
	Shilpi Shital, Ben-Gurion University, Isreal	55
12.10-12.20	Effective masses of heavy, light, and split-off electrons and effective g-factor of electrons in perovskite materials	
	David Ompong, Charles Darwin University, Australia	57

Perovskite/silicon tandem solar cells: microstructural aspects & efficiency

Quentin Jeangros, Florent Sahli, Xin Yu Chin, Peter Fiala, Quentin Guesnay, Daniel Jacobs, Ricardo Razera, Fan Fu, Vincent Paratte, Mathieu Boccard, Christophe Ballif

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Thanks to impressive industrialization efforts, the cost of mainstream crystalline silicon (c-Si) solar modules is now down to ~0.2-0.4 €/W, only a small share of the total cost of a photovoltaic system. Due to this cost distribution, increasing cell and module efficiencies is and will continue to be the main driver for solar electricity deployment. Yet, the efficiency of c-Si modules will soon reach a plateau as record R&D cells already approach their practical efficiency limit. One approach to keep improving efficiencies and go beyond the 30% mark is to stack different absorbers in a multi-junction solar cell. Such structure enables a better usage of the incoming light energy. Combining a III-V solar cell with c-Si in a tandem device can lead to efficiencies of ~33%, however costs are prohibitive. A lower cost alternative capable of targeting similar efficiencies is to upgrade c-Si cells by stacking a perovskite solar cell on their front side.

This contribution will discuss several microstructural aspects of perovskite/c-Si tandem stacks and draw links to device performance and eventually stability. A first microstructural feature that will be discussed is the pyramidal texture present on the front side of c-Si solar cells to reduce reflection losses and promote light trapping. This pyramidal texture is not compatible with standard perovskite solution-based deposition protocols, requiring a troublesome polishing or downsizing of the pyramid size. To ensure compatibility with any pyramid dimensions, a hybrid perovskite processing route was developed. The method involves thermally evaporating a conformal inorganic template (lead/cesium halides), before spin coating the organic precursors (formamidinium iodide/bromide) to crystallise the perovskite absorber. The impact of the c-Si texture on the morphology of the evaporated template and, as a result, on that of the final perovskite layer will be assessed. In addition, the influence of process parameters and choice of layer stack on the microstructure of the c-Si and perovskite contacts will be detailed. It will be shown how, combined with either an n- or a p-type c-Si bottom cell, a fine control of the perovskite top cell morphology enables to achieve tandem efficiencies >25% on a small active area of 1.42 cm^2 (Fig. 1a).[1,2] Results regarding the upscaling of the perovskite absorber area to

industry-relevant sizes (6 inch c-Si wafers) by replacing the spin coating step with a second vapour-phase deposition will also be discussed (Fig. 1b).

The second part of this contribution will discuss briefly operational stability aspects, notably degradation pathways triggered by i) light soaking,[3] ii) reverse bias voltages which typically appear when a module becomes partially shaded (Fib. 1c),[4] or iii) during long-term operation at maximum power point at various temperatures (Fig. 1d)[5]. The microstructural evolution of the layer stack at the µm to nm scale depending on external stimuli will be correlated to device performance.
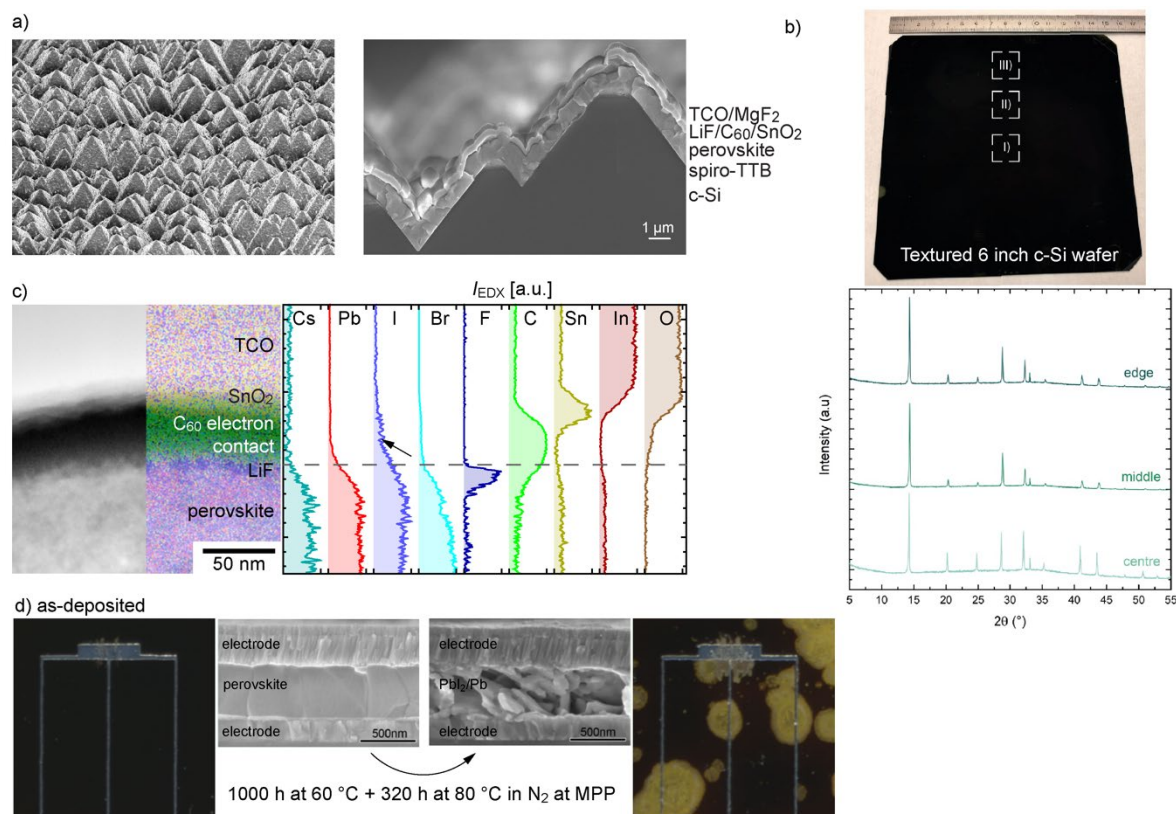

Fig. 1: a) Electron microscopy images of the front side of a textured perovskite/c-Si tandem, a design leading to efficiencies of >25%, b) image of a perovskite-coated 6 inch textured c-Si wafer, with X-ray diffraction patterns highlighting the full conversion to the perovskite phase across the wafer, c) energy-dispersive X-ray (EDX) spectroscopy maps highlighting the migration of halides into the electron transport layer during reverse biasing, d) optical and electron microscopy images of the front side and cross-section of a solar cell in its as-deposited state and after 1000 hours at 60 °C, followed by 320 hours at 80 °C at maximum power point.

1. Sahli, F. *et al.* Fully textured monolithic perovskite/silicon tandem solar cells with 25.2% power conversion efficiency. *Nat. Mater.* **17**, 820–826 (2018).
2. Nogay, G. *et al.* 25.1%-Efficient Monolithic Perovskite/Silicon Tandem Solar Cell Based on a p-type Monocrystalline Textured Silicon Wafer and High-Temperature Passivating Contacts. *ACS Energy Lett.* **4**, 844–845 (2019).
3. Holovský, J. *et al.* Lead Halide Residue as a Source of Light-Induced Reversible Defects in Hybrid Perovskite Layers and Solar Cells. *ACS Energy Lett.* **4**, 3011–3017 (2019).
4. Razera, R. A. Z. *et al.* Instability of p–i–n perovskite solar cells under reverse bias. *J. Mater. Chem. A* **8**, 242–250 (2020).
5. Fu, F. *et al.* I2 vapor-induced degradation of formamidinium lead iodide based perovskite solar cells under heat–light soaking conditions. *Energy Environ. Sci.* **12**, 3074–3088 (2019).

Pathways towards 30% efficient single-junction perovskite solar cells: The Role of mobile ions and interfaces

Martin Stolterfoht

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Perovskite semiconductors have demonstrated outstanding power conversion efficiencies (PCEs), however the precise conditions that are required to advance to an efficiency regime above monocrystalline silicon cells are not well understood. Here, we demonstrate a simulation model[1] that well describes efficient *p-i-n* type perovskite solar cells and a range of different experiments using experimental input from transient and steady-state photoluminescence (PL) measurements.[2,3] We discuss the role of important device and material parameters with a particular focus on the carrier mobilities, mobile ions, doping, energy-level alignment and the built-in potential (V_{BI}) across all stack layers. We will also address the important question to what extent the presence of mobile ions influences the built-in field and with that the device performance. By consider only parameters that have been already demonstrated in recent literature, we find that an efficiency regime of 30% can be unlocked by optimizing the built-in potential across the perovskite layer by using either highly doped (10^{19} cm^{-3}) or ultrathin undoped transport layers (TLs), e.g. self-assembled monolayers. The theoretical findings are correlated with intensity dependent quasi-Fermi level splitting QFLS(I) measurements, which allow to assess the efficiency potential of neat perovskite films with and without attached TLs.[4] Experimental results on FAMAPbI₃ double-cation perovskites with low bandgap energy (1.54 eV) and exceptional Shockley-Read-Hall lifetimes of over 18 µs and high PL quantum yields (>20%) are presented. These exceptional opto-electronic qualities enable an implied PCE of 28.4% in the neat perovskite material. We show that this efficiency potential can be realized by a) minimizing non-radiative recombination at the interfaces with respect to bulk recombination, b) improving the carrier mobility in the hole transport layer by a factor of 10 and c) optimizing the average external quantum efficiency to 95%. The numerical and experimental findings lay out a clear path for further advancements of *pin*-type perovskite cells towards the radiative limits.

1. Diekmann, J. *et al.* Pathways towards 30% efficient perovskite solar cells. (2019). Preprint available on ArXiv:1910.07422
2. Stolterfoht, M. *et al.* The impact of energy alignment and interfacial recombination on the internal and external open-circuit voltage of perovskite solar cells. *Energy Environ. Sci.* **12**, 2778–2788 (2019).
3. Caprioglio, P. *et al.* On the Origin of the Ideality Factor in Perovskite Solar Cells. *Adv. Energy Mater.* **10**, 2000502 (2020).
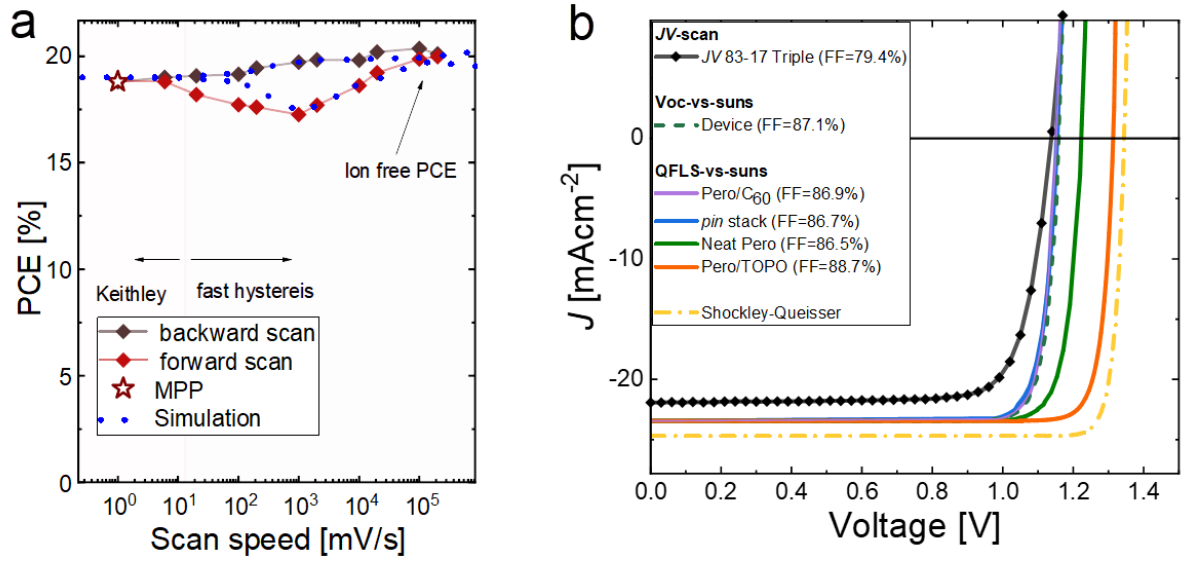4. Stolterfoht, M. *et al.* How To Quantify the Efficiency Potential of Neat Perovskite Films: Perovskite

Fig. 1 a Fast hysteresis *JV*-scans on triple cation perovskites cells and fits using numerical simulations. **b** Experimentally measured pseudo-*JV*-curves of different solar cell stack layers using intensity-dependent photoluminenscence measurements.

Charge carrier lifetimes in lead-halide perovskites

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Both transient and steady state photoluminescence PL have been frequently used to analyze the properties of halide perovskite films[1] and recently also layer stacks, i.e. films with interfaces.[2-4] Here, we present our current level of understanding of how to analyze the data. In the case of films, long decays in transient PL correlate well with strong steady state PL. The shape of the decays allows us to determine bimolecular and monomolecular recombination coefficients, the former of which is clearly affected by photon recycling.[1, 5] In the case of films with one interface, we show that high luminescence is still beneficial for high open-circuit voltages in devices and still correlates with long photoluminescence decays.[2] We show by simulation how the combination of steady state PL with tr-PL can be used to better understand band alignment at interfaces and how it provides an estimate of the surface recombination velocities. Finally, we discuss the case of layer stacks with two contacts and of full devices. Here, additional effects such as the conductivity and capacitance of contact layers become important. In addition, the question arises on how to compare purely optical techniques with techniques that use electrical detection. One example is the comparison between transient PL and transient photovoltage. The difference between the two is that transient PL measures the internal voltage, i.e. the quasi-Fermi level splitting, and transient photovoltage measures the external voltage that builds up at the external terminals of the cell. While both decays are affected by the contact layers, the impact is substantially different. The external voltage first has to be built up by charging up the capacitance of the interfacial layers, the internal voltage peaks immediately after the laser pulse and then decays fairly quickly.

Energy Yield Modelling of Perovskite-Based Tandem Photovoltaics

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We will present our latest work on energy yield modelling of perovskite-based tandem photovoltaics. Considering the possible strong dependence of light absorption in multilayer stacks - such as perovskite/c-Si tandem solar cells - on the angle of incidence and incident sun spectrum, careful optimization of the tandem solar module architectures is required under realistic solar irradiation conditions. Our energy yield modelling considers the varying diffuse and specular irradiation, realistic spectra and the real angle of incidence during the course of the day and the year for various geographic locations[1]. We present specific research studies that investigate (I) energy yield modelling and optical loss analyses of perovskite/silicon tandem solar cells with microscopic as well as nanophotonic light management textures[2,3], (II) energy yield modelling of bifacial perovskite/Si tandem photovoltaics[4], and energy yield modelling of 3-terminal perovskite/Si tandem photovoltaics[5].

References:

1. Schmager, R. *et al.* Methodology of energy yield modelling of perovskite-based multi-junction photovoltaics. *Opt. Express* **27**, A507 (2019).
2. Hossain, I. M. *et al.* Nanostructured front electrodes for perovskite/c-Si tandem photovoltaics. *Opt. Express* **28**, 8878 (2020).
3. Lehr, J. *et al.* Energy yield modelling of perovskite/silicon two-terminal tandem PV modules with flat and textured interfaces. *Sustain. Energy Fuels* **2**, 2754–2761 (2018).
4. Lehr, J. *et al.* Energy yield of bifacial textured perovskite/silicon tandem photovoltaic modules. *Sol. Energy Mater. Sol. Cells* **208**, 110367 (2020).
5. Gota, F., Langenhorst, M., Schmager, R., Lehr, J. & Paetzold, U. W. W. Energy yield advantages of three-terminal perovskite/silicon tandem photovoltaics. *under Rev.* (2020).

Molecular scale models of key processes in organic photovoltaic devices

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In organic heterojunction devices, current generation results from the sequence of photon absorption, charge separation, and charge collection in competition with recombination. To understand and design organic PV devices, we need models of these processes that incoporate both the device architecture and the molecular nature of the materials. Device models work fairly well in describing charge collection and recombination, and resulting curent-voltage curves, but usually with some empirical form for the charge generation efficiency and recombination coefficients. A full description of microscopic processes such as interfacial charge transfer requires molecular scale models. For design purposes, we would like to be able to predict device behaviour from the properties of the molecular components, but it is challenging to combine these aspects in a single model. In this talk we will discuss the degree to which molecular level models and time-resolved device models can explain measurements both of charge carrier dynamics, and of overall device behaviour. We will then address the challenges in bringing the two approaches together into a single framework.

Can 1D models really capture bulk-heterojunction geometry as effective parameters?

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To explicitely express the dominant geometry features of bulk-heterojunction (BHJ) devices, 2D or 3D models are needed. This comes at a high computational cost when simulating opto-electronic measurements.

Substituting a 0D or 1D model for characterization data analysis means compressing the relevant geometry information into effective parameters. For instance, effective mobilities are not only intrinsic materials properties, but also encode how tortuous the conduction pathways are[1]. Compacting the model in this manner allows for realistic computation times for model-intensive applications such as parameter estimation[2] or machine-learning training[3].

I will outline a methodology to compact BHJ geometry information into effective parameters, when possible. It is intuitive that effective mobilities should be a function of intrinsic mobilities and some quantity representing tortuosity. Is this true? If yes, what is this function? Does it have other dependencies?

To reach this goal, I combine two approaches. First, I use theoretical arguments to quantify geometry features. Second, I simulate systematic variations of a realistic (but slow) 2D model[4] and fit its response using a fast (but effective) 1D model. The effective parameters obtained can be empirically related to the input BHJ geometry. I will select some of these relationships, in the context of the analysis of a real device, and demonstrate the added value in terms of effective parameters interpretability.
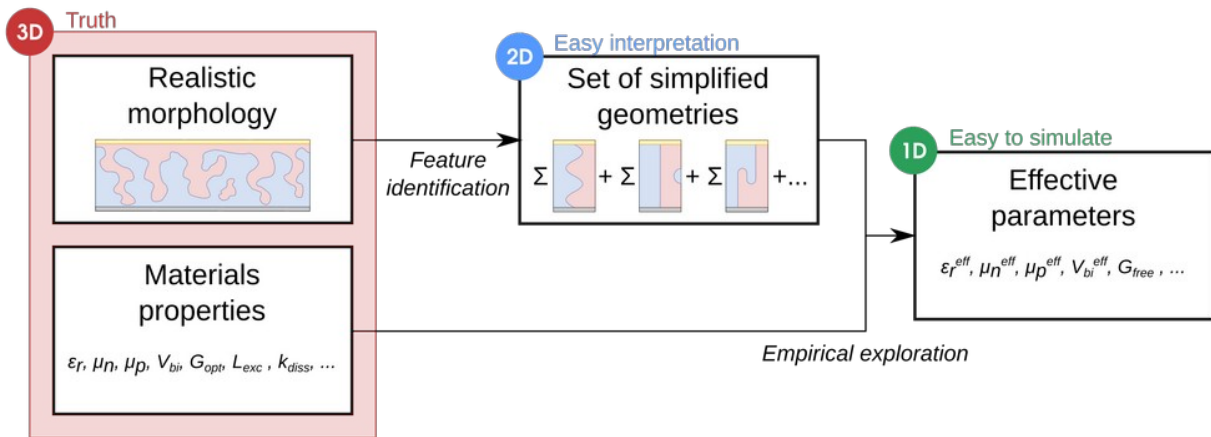

Fig. 1 This work combines theory and 2D simulations to relate 1D effective description of bulk-heterojunction geometries to their explicit 2D/3D counterparts.

[1]M. C. Heiber, K. Kister, A. Baumann, V. Dyakonov, C. Deibel, and T.-Q. Nguyen. "Impact of Tortuosity on Charge-Carrier Transport in Organic Bulk Heterojunction Blends". *Physical Review Applied* 8, 5 (2017)

[2]M. Neukom, S. Züfle, S. Jenatsch, and B. Ruhstaller. "Opto-Electronic Characterization of Third-Generation Solar Cells." *Science and Technology of Advanced Materials* 19, PV1 (2018)

[3]N. Majeed, M. Saladina, M. Krompiec, S. Greedy, C. Deibel, and R. C. I. MacKenzie. "Using Deep Machine Learning to Understand the Physical Performance Bottlenecks in Novel Thin-Film Solar Cells." *Advanced Functional Materials* 30, 7 (2020)

[4]A. Raba, Y. Leroy, and A.-S. Cordan. "Organic Solar Cells: A Rigorous Model of the Donor-Acceptor Interface for Various Bulk Heterojunction Morphologies." *Journal of Applied Physics* 115, 5 (2014)

From Transient Spectroscopy on Films to Steady-state Solar Cell Device Performance

Julien Gorenflot,[1] Safakath Karuthedath,[1] Armantas Melianas,[2] Zhipeng Kan,[1] Martijn Kemerink,[2] Frederic Laquai[1]

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[2] Complex Materials and Devices, Department of Physics, Chemistry and Biology, Linköping University, Linköping, Sweden

Time-resolved spectroscopy is an unrivalled tool to study photophysical phenomena, involving both neutral and charged excited species, for instance, the processes involved in photocurrent generation and those limiting the device efficiency. However, it is not straightforward to extrapolate (transient) spectroscopy results acquired after pulsed laser excitation with high photon density to devices operating under steady-state one sun illumination conditions. In order to bridge that gap, we quantified the rates of the different photophysical processes, which we identified by transient absorption spectroscopy, and used them to simulate operating solar cell devices. The simulations indeed reproduce the experimentally-measured performances and thus explain the losses during photocurrent generation. Finally, our simulations enable us to gain information, which are experimentally not accessible, such as the density of triplet excitons, in an operating organic solar cell. This paves the way to a better understanding of the impact of those states on the device performance.[1]
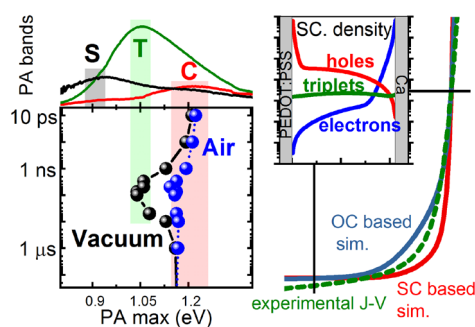
Fig. 1 (left) Transient shift of the photoinduced absorption signal on a TQ1:PC$_{71}$BM film indicating the transient buildup and decay of a triplet state density. **(right)** Corresponding device simulation: *J-V* characteristics and excited states density in short circuit conditions. Reprinted with permission from J. Phys. Chem. Lett. 2020, 11, 8, 2838–2845. Copyright 2020 American Chemical Society.

[1] S. Karuthedath, J. Gorenflot, A. Melianas, Z. Kan, M. Kemerink, F. Laquai. *J. Phys. Chem. Lett*. 2020, 11, 8, 2838–2845, DOI: 10.1021/acs.jpclett.0c0075

How Temperature influences on the Perovskite Solar Cells

Arthur Julien[1,2], Pilar Lopez-Varo[1], Mohamed Amara[3], Stefania Cacovich[2], Philip Schulz[2], Armelle Yaïche[4], Mohamed Jouhari[1], Jean Rousset[4], Jean-François Guillemoles[2], Jean-Baptiste Puel[4,1]

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[4] EDF R&D, Palaiseau, 91120, France.

Insight into how temperature influences the performance of perovskite solar cells (PSCs) is essential to improve the stability of these devices[1, 2]. Recently, outstanding works on the characterization of PSCs under different temperatures have been performed by W. Tress et al.[1] and M. Jošt et al.[2]. From the characterization, M. Jošt et al.[2] estimated the power temperature coefficients of their cells and proposed to evaluate the cell temperature by using a linear relation with the Nominal Operating Cell Temperature (NOCT). Including these temperatures dependent parameters into the energy model makes it possible to predict the generated energy of the devices. However, the NOCT is strongly dependent on operating conditions such as irradiation, wind velocity, etc. R. Gehlhaar et al.[3] proposed a simple transient thermal model to calculate the cell temperature based on global irradiance and ambient temperature, that does not depend on device parameters. From all of that, in this work, we propose a more advanced self-consistent thermal model which is a function of device parameters, environmental variables and is strongly linked with the experimental optical-electrical-thermal performance (Schematic in Fig. 1). The optical-electrical-thermal performance is defined by an experimental matrix of the output power as a function of temperature and light intensity. The thermal model considers the absorption, convection, conduction, and radiation exchanges. We validate the transient our model by comparison between the output power simulated with the output power obtained from laboratory measurements. Linking the experimental results and our model, we conclude that the increment of the temperature in non-inverted solar cells is mainly controlled by absorption losses in the front glass (18.9 %), electron transport layer

[1] W. Tress, K. Domanski, B. Carlsen, A. Agarwalla, E. A. Alharbi, M. Graetzel, A. Hagfeldt "Performance of perovskite solar cells under simulated temperature-illumination real-world operating conditions" Nat. Energy, 4, 568-574, (2019).

[2] M. Jošt, B. Lipovšek, B. Glažar, A. Al-Ashouri, K. Brecl, G. Matič, A. Magomedov, V. Getautis, M. Topič, S. Albrecht. "Perovskite Solar Cells go Outdoors: Field Testing and Temperature Effects on Energy Yield" Adv. Energy Mater. 2000454, (2020).

(19.2 %) and the perovskite layer (61.9 %). Finally, we also analyse the annual energy yield of PSC modules working on different geographical location and we show the importance of thermal modelling for such estimations as it can change the results by 10 %.
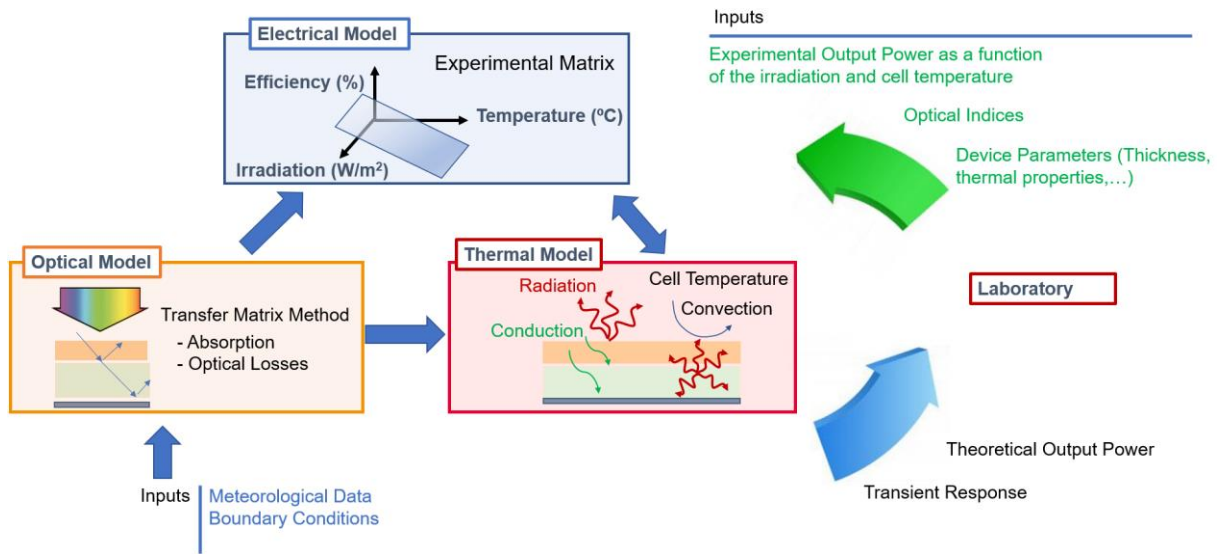

Fig. 1 Schematic of the electrical-optical-thermal model and the feedback with experimental measurements.

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[3] R. Gehlhaar, T. Merckx, W. Qiu, and T. Aernouts, "Outdoor Measurement and Modeling of Perovskite Module Temperatures," Glob. Challenges, 1800008, (2018).

What Limits the Fill Factor of Organic Solar Cells with Marginal Exciton–Charge-Transfer State Offset?

Mohammed Azzouzi[1#], Nathaniel P. Gallop [2], Flurin Eisner [1], Artem Bakulin[2] and Jenny Nelson[1]

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The performance of solar cells based on molecular electronic materials has historically been limited by relatively high non-radiative voltage losses. With the advent of non-fullerene acceptors, non-radiative voltage losses as low as 0.2V have been achieved by reducing the energetic offset between the initial photo-excited singlet state and charge-transfer state in the bulk-heterojunction. However, the devices with the lowest voltage losses appear to be limited instead by a low Fill Factor (FF), for reasons which are not yet fully understood.

In this work we consider devices based on the high performing C8-ITIC acceptor blended with PBDB-T donors with different level of fluorination that modulate the energy offset. We have previously reported a low non-radiative voltage loss of 0.23V in the blend device based on the lowest offset polymer:C8-ITIC combination. However, the FF of those devices was limited to 55% whereas devices based on the largest offset system had FF around 70%[1].

To understand the relation between the reduced voltage losses and the limited FF, we first use time-resolved spectroscopy to study the impact of the energy offset on the early time processes of charge transfer (CT) state dissociation and charge recombination. We find that the CT state dissociation into free charges is slower for the low offset system. We then

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[1] Eisner, Flurin D., Mohammed Azzouzi, Zhuping Fei, Xueyan Hou, Thomas D. Anthopoulos, T. John S. Dennis, Martin Heeney, and Jenny Nelson. "Hybridization of local exciton and charge-transfer states reduces nonradiative voltage losses in organic solar cells." Journal of the American Chemical Society 141, no. 15 (2019): 6362-6374.

measured the free charge carrier lifetime using a newly developed optoelectronic technique [2], and show that the device with lowest offset also has the shortest free charge carrier lifetime.

Using a drift diffusion device model that accounts for both the reformation of the CT state from the free charge carriers and the CT state dissociation, we were able to explain the experimental observations. We found in this model that the relatively high rate constant of CT state reformation reduces the power conversion efficiency of the marginal offset blend. This observation explains why the marginal offset blend shows the lowest efficiency in spite of showing the slowest rate of recombination from the CT state. Our findings offer a better understanding of what limits fill factor and power conversion efficiency in marginal offset bulk heterojunction solar cells.

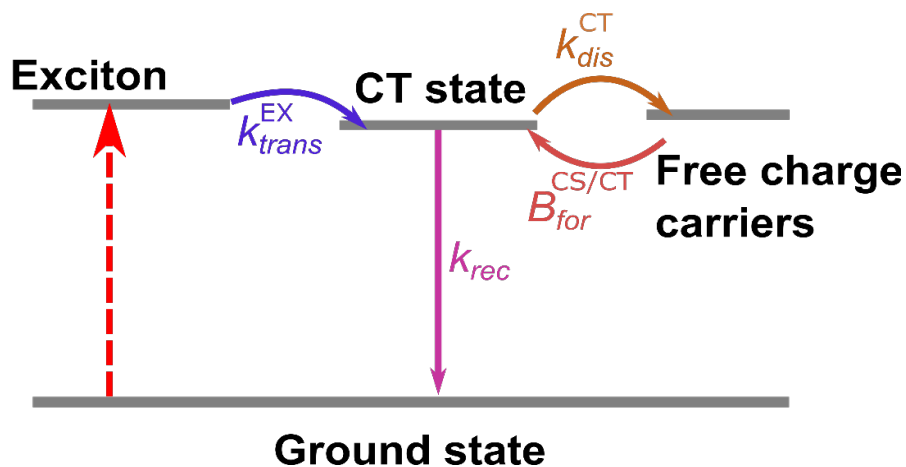**Fig. 1** Kinetic model for charge generation and recombination following photoexcitation of the exciton.

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Relationship between fill factor and light intensity in solar cells based on organic disordered semiconductors: The role of tail states

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The origin of the relationship between fill factor and light intensity (*FF-I*) in organic disordered-semiconductor based solar cells is studied. An analytical model describing the balance between transport and recombination of charge carriers, parameterized with a factor, Γ_m, is introduced to understand the *FF-I* relation where higher values of Γ_m correlate to larger *FF*. Comparing the effects of direct and tail state mediated recombination on the *FF-I* plot, we find that for low mobility systems direct recombination with constant transport mobility can only deliver a negative dependence of $\Gamma_{m,dir}$ on light intensity. By contrast, tail state mediated recombination with trapping and de-trapping processes can produce a positive $\Gamma_{m,t}$ vs. Sun dependency. The analytical model is validated by numerical drift-diffusion simulations. To further validate our model, two material systems that show opposite *FF-I* behaviour are studied: PTB7-Th:PC71BM devices show a negative *FF-I* relation while PTB7-Th:O-IDTBR devices show a positive correlation. Optoelectronic measurements show that the O-IDTBR device presents a higher ideality factor, stronger trapping and de-trapping behaviour, and a higher density of trap states, relative to the $PC_{71}BM$ device, supporting the theoretical model. This work provides a comprehensive understanding of the correlation between *FF* and light intensity for disordered semiconductor based solar cells.

Elucidation of Förster Resonance Energy Transfer in Optically Resonant Dual Donor Based Organic Solar Cell

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The Solution-processed bulk heterojunction (BHJ) organic solar cells (OSCs) are one of the emerging photovoltaic technology among third-generation solar cells in which organic materials (conjugated polymers or small organic molecules) are used to harvest the light energy (outdoor as well as indoor). The OSCs are comprised of several layers (electron transport layer and hole transport layer) including a photoactive layer (blend of donor and acceptor materials) and two electrode layers. Over the past two decades, OSCs have garnered much attention due to its unique properties such as ecofriendly materials, solution processibility, an ultra-lightweight, flexibility, ultra-thin (< 1 mm), tunable electronic properties, radiation stability, low-temperature fabrication, minimum material consumption and large scale mass production (roll to roll processing). Recent developments such as new low bandgap materials, non-fullerene acceptors (NFAs), interface engineering and novel device fabrication techniques in OSCs have led to tremendous advances in power conversion efficiency (PCE), with current leading NREL certified efficiencies of over 16% for single-junction solar cell devices.[1] However, expanding the absorption spectrum and efficiently harvesting photogenerated excitons are crucial tasks to realize high-efficiency polymer solar cells (PSCs).

In the last few years, ternary blend PSCs with complementary absorptions into a single junction device has been emerging as a promising strategy to enhance the absorption of binary PSCs.[2] Förster resonance energy transfer (FRET) in the ternary blend system significantly improves the PCE in bulk heterojunction polymer solar cells.[3-5] In this work we have comprehended the FRET mechanism in PTB7-Th:PCDTBT based dual donor ternary blend polymer solar cells and shows how significantly FRET mechanism is responsible for boosting the efficiency from 8.6% to more than 10%. The ultrafast energy transfer from energy donor to energy acceptor has been established by steady-state absorbance and photoluminescence emission spectrum photoluminescence decay. Our results reveal that optically resonant donor polymers can exploit a broader range of the solar spectrum effectively without incurring excessive processing costs.
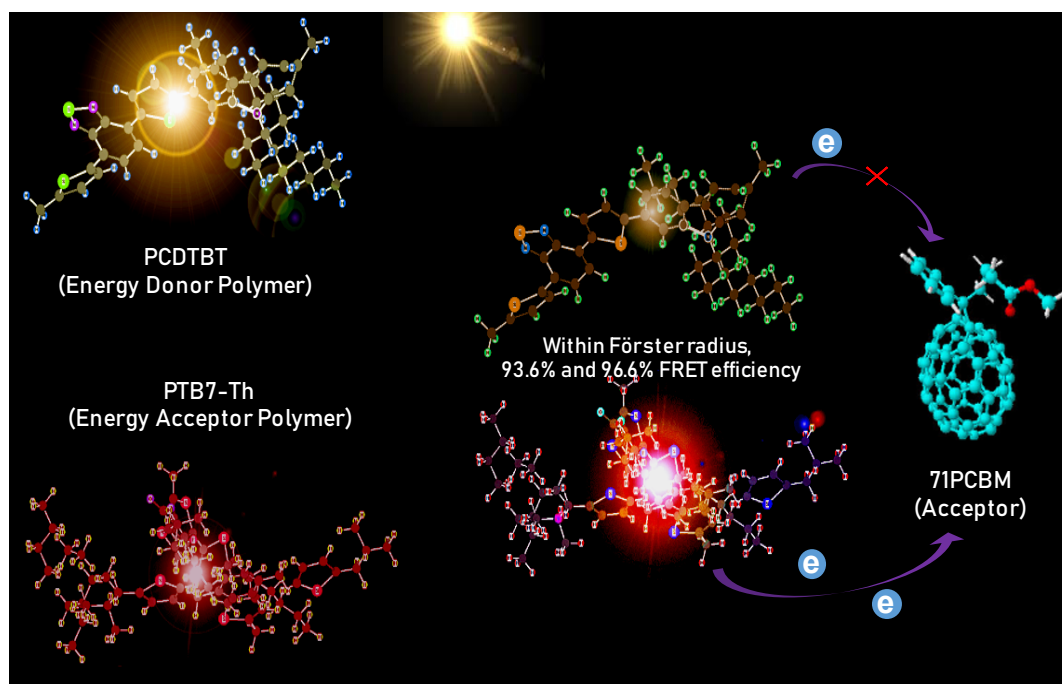
Fig. 1 Schematic diagram of FRET in a dual donor (PTB7:PCDTBT) based polymer solar cells.

Reference:
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Simulation studies on the effect of inorganic CuI hole transport layer on PBDB-T/ITIC-OE organic solar cell

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ITIC-OE(3,9-bis(2-methylene-3-(1,1-dicyanomethylene)-indanone)-5,5,11,11-tetraki(4-hexylphenyl)-dithieno[2,3-7d:2,3-d]-s-indaceno [1,2-b:5,6-b]dithiophene) with oligo-ethylene sidechain is a high di-electric constant non-fullerene acceptor. Its combination with PBDB-T (poly[(2,6-(4,8-bis(5-(2-ethylhexyl)thiophen-2-yl)benzo[1,2-b:4,5-9b]dithiophene)-co-(1,3 di(5-thiophene-2-yl)-5,7-bis(2-ethylhexyl)benzo[1,2-c:4,5-c]dithiophene-4,8-dione)]) polymer provides a suitable active layer for highly efficient Non-fullerene acceptor bulk heterojunction (NFA-BHJ) organic solar cells[1]. Hole transport layer(HTL) plays an important role in the smooth working of OSC. The conventional HTL of PEDOT:PSS degrades the cell due to its acidic nature[2-3]. Introduction of an alternate HTL material can enhance the output of NFA-BHJ along with providing better stability. This work presents a comprehensive device model-ling of PBDB-T/ITIC-OE NFA-BHJ with inorganic CuI hole transport layer. SCAPS 1-D is used to numerically study the efficiency enhancement of the solar cell by optimising the tech-nological parameters[4]. The simulated results are validated by comparing with the experi-mental reference from literature. Upon optimization of the cell parameters, the device output shows an improved result with an Open Circuit Voltage (Voc) of 0.9393 V ,Short Circuit cur-rent density(Jsc) of 16.625 mA/cm^2 ,Fill Factor(FF) of 69.96% and Power Conversion Efficiency (PCE) of 10.93% . The results promises a new direction in organic solar cell re-search to fabricate highly efficient photovoltaic devices.
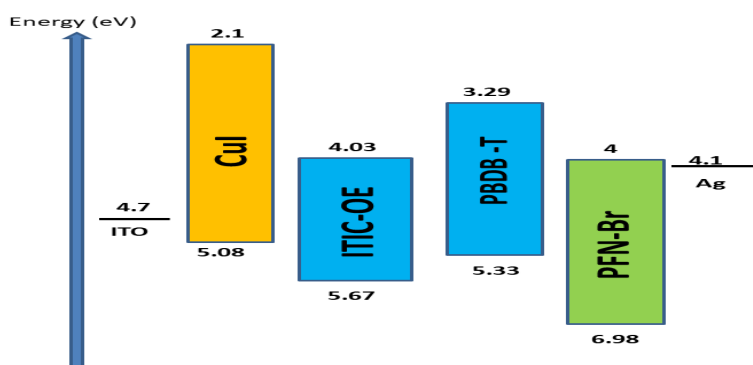

Fig. 1 Energy band alignment of simulated solar cell

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Emissive and charge-generating donor-acceptor interfaces

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Charge transfer (CT) states at the interface between electron-donating (D) and electron-accepting (A) materials in organic thin films are characterized by absorption and emission bands within the optical gap of the interfacing materials.[1] Depending on the used donor and acceptor materials, CT states can be very emissive, or generate free carriers at high yield. The former can result in rather efficient organic light emitting diodes (OLED), via thermally activated delayed fluorescence, while the latter property is exploited in organic photovoltaic (OPV) devices. In this talk, I will show that proper understanding and control of CT state properties allows simultaneous occurrence of a high photovoltaic and emission quantum yield within a single, visible-light-emitting D–A system.[2] This leads to ultralow-emission turn-on voltages in OLEDs as well as significantly reduced voltage losses in OPV devices.

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Drift-Diffusion Simulation of S-Shaped Current-Voltage Relations for Organic Semiconductor Devices

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In inorganic high power transistors and lasers, thermal effects resulting from strong electric and optical fields and from strong recombination processes are of significant importance and have to be included into mathematical models. However, electrothermal effects are even more potent in organic semiconductors where the temperature activated hopping transport of charge carriers leads to a strong interplay between electric current and heat flow. They result in interesting phenomena like S-shaped current-voltage relations with regions of negative differential resistance in resistors and Organic Light Emitting Diodes (OLEDs) [1] [2] and lead to inhomogeneous luminance in large-area OLEDs. Moreover, electrothermal effects have a strong impact on the performance of organic solar cells and transistors [3] [4] [5].

In this talk, we discuss an electrothermal drift-diffusion model for organic semiconductor devices with Gauss-Fermi statistics and positive temperature feedback for the charge carrier mobilities [6]. We apply temperature dependent Ohmic contact boundary conditions for the electrostatic potential and discretize the system by a finite volume based generalized Scharfetter-Gummel scheme. Using path-following techniques we demonstrate that the model exhibits

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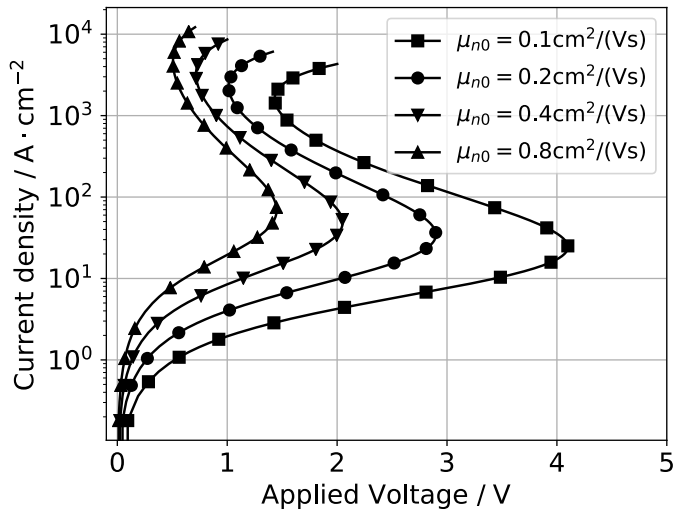
S-shaped current-voltage curves with regions of negative differential resistance, which were only recently observed experimentally.

Fig. 1 Simulated current-voltage characteristics using the electro-thermal drift-diffusion model for different reference mobilities

Orientational anisotropy in organic thin films and the impact on electrical properties of organic light emitting diodes

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The orientational anisotropy in organic thin films and the resulting preferential alignment of emitter molecules has already been identified a key parameter in controlling the quantum efficiency of organic light emitting diodes (OLEDs). Hereby, the orientation of the emissive transition dipoles relative to the surface is crucial for high light outcoupling efficiencies[1]. Additionally, oriented molecules comprising a permanent dipole moment will lead to a macroscopic film polarization commonly identified with the giant surface potential (GSP)[2]. The GSP can be controlled by dipolar doping, allows to draw conclusions on molecular alignment[3,4,5] and can affect OLED device performance by influencing carrier injection into the electron transport layer[6,7]. Just recently, we could show that this applies to the hole injection layer as well[8].

However, with many aspects of the optical influences of molecular anisotropy already known, the exact mechanisms behind molecular orientation as well as its impact on electrical performance are still under investigation.

In this talk, a short introduction on molecular anisotropy and the determination of molecular alignment with a focus on electrical measurements is given. The alignment of polar molecules is demonstrated in dependence of their concentration in a matrix material. Furthermore, the impact of different functional groups of an Iridium complex is discussed. Finally, the influence of molecular orientation on electrical device performance is then shown with various examples, comprising neat films of different polarity and doped organic layers.

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Efficient and stable single-layer organic light-emitting diodes

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Organic light-emitting diodes (OLEDs) serve as the active component in high-end displays and have received a considerable amount of interest because of their potential in lighting applications. However, for a more widespread application, production costs need to be lowered and the energy efficiency and lifetime need to be improved. Over the past two to three decades, OLEDs were designed with increasing complexity, using a multilayer structure consisting of typically five layers. Here, we have developed an efficient and stable single-layer OLED[1], stepping aside from the conventional multilayer device concept that has been commonplace in the OLED field for more than two decades. This could be achieved based on some of our recent discoveries. A major problem of organic semiconductors is that charge transport is not balanced due to trapping of charges by defects, limiting the efficiency of single-layer OLEDs. Recently, we have found that when the ionization energy of an organic semiconductor surpasses 6.0 eV, hole trapping will occur, whereas an electron affinity lower than 3.6 eV will give rise to electron trapping. Therefore, to design organic semiconductors with trap-free electron and hole transport, their electron affinity and ionization energy should be situated between 3.6 eV and 6.0 eV, respectively, resulting in an energy window spanning 2.4 eV [2]. Combining efficient charge injection[3] with the energy window for trap-free charge transport enabled the design of a highly efficient single-layer OLED based on thermally activated delayed fluorescence. The balanced charge transport and efficient charge injection resulted in record-low operating voltages and high efficiencies, as well as a 20-fold increase in lifetime compared to a conventional multilayer OLED. As a result, this single-layer concept combines a high power efficiency with a long lifetime in a simplified architecture, rivalling and even exceeding the performance of complex multilayer devices. Combined charge-transport and optical simulations are used to explain the high performance of such single-layer devices.

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Coupled 3D Master Equation and 1D Drift-Diffusion Approach for Advanced OLED Modeling

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Two main approaches for modeling and simulation of organic light emitting diodes (OLEDs) and organic photovoltaics (OPV) are computationally efficient drift-diffusion (DD) models which partly lack precise description of the underlying physics, and sophisticated yet computationally demanding atomistic models based on kinetic Monte Carlo and Master Equation (ME) approaches[1,2].

In the present talk we show a hybrid model combining the best of both worlds by using a 1D DD model for the charge carrier dynamics and electrostatics and a 3D Master Equation approach[3] describing the exciton dynamics, as long range interactions play a significant role in exciton transport and interaction which has to be resolved on a discrete atomistic domain. Such phenomena are mostly absent for free charge carriers, making a continuous 1D description appropriate. The resulting hybrid model is applied and compared to various experiments and simulations in literature.

The equations to be solved are given by

$$\Delta \psi = \frac{q}{\varepsilon}(n - p + C),$$

$$\frac{\partial n}{\partial t} - \nabla \cdot J_n = G - R(n,p),$$

$$\frac{\partial p}{\partial t} + \nabla \cdot J_p = G - R(n,p),$$

$$J_n := n\mu_n \nabla\psi - D_n \nabla n,$$

$$J_p := -p\mu_p \nabla\psi - D_p \nabla p,$$

$$\frac{d\chi_i}{dt} = \sum_{j\neq i}\left[\chi_j \omega_{ji}^{\mathrm{F}} - \chi_i \omega_{ij}^{\mathrm{F}}\right] + \sum_{j\neq i}\left[\chi_j \omega_{ji}^{\mathrm{D}} - \chi_i \omega_{ij}^{\mathrm{D}}\right]$$

$$- \left(\frac{1}{\tau_{\mathrm{r},i}} + \frac{1}{\tau_{\mathrm{nr},i}}\right)\left(\chi_i - \exp\left(\frac{E_{\mathrm{b},i} - E_{\mathrm{g},i}}{k_B T}\right)\right)$$

$$\pm \frac{\chi_i^{\mathrm{t}}}{\tau_{\mathrm{RISC},i}} \mp \frac{\chi_i^{s}}{\tau_{\mathrm{ISC},i}}$$

$$- \frac{\chi_i a_0^3 (n+p)}{\tau_{\mathrm{PQ},i}} \pm \frac{(\chi_i^{\mathrm{t}})^2}{(2)\tau_{\mathrm{TTA},i}}$$

$$+ a_0^3\left(g_{\mathrm{rec},i} R + g_{\mathrm{opt},i} G\right)$$

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The left equations describe the drift-diffusion model for charge carrier densities n and p as well as for the potential ψ. The equation on the right describes the change in excitonic occupation number χ for a single state (molecule) over time, where the terms describe Förster and Dexter energy transfer, (non-) radiative decay, (reverse) inter-system crossing, polaron quenching and triplet-triplet annihilation and exciton generation through carrier recombination and optical excitation. The two models are directly coupled through the carrier densities as of polaron quenching, as well as through the recombination rate.

An example result of the hybrid model for a simple OLED turn on – turn off simulation is shown in Fig. 1, showing the transient capabilities of the approach. In Fig. 1 a) the energetic disorder is visible as variations in exciton density, which can be easily modeled in the ME approach.
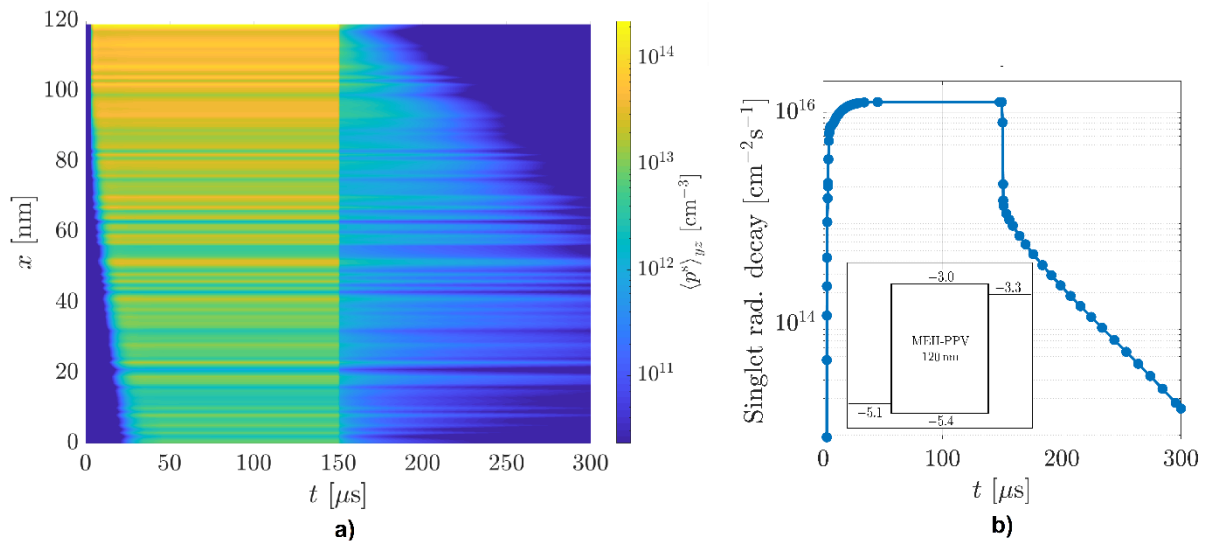

Fig. 1 Single layer OLED turn on at 10V and turn off at t=150\mu s. a): Laterally averaged singlet density over time. b) Total radiative decay over time (inset: energetic structure of the OLED)

In conclusion, the 1D DD model can be solved very efficiently and fast. At the same time, the 3D ME model allows for physically sound transport models using Förster and Dexter transfer rates taking long range interaction into account. Furthermore, the discrete nature of the model allows for very easy treatment interspersed host-guest complexes. Despite the lower dimensionality of the DD model the subsequent ME simulation for the exciton dynamics yields physically accurate results with the benefit of lower computation times compared to a fully coupled 3D ME approach for both the charge carrier and the exciton dynamics.

A kinetic Monte Carlo study of deconfinement in transient photoluminescence of TADF host-guest systems

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For the development of more efficient organic light-emitting diodes (OLED), different device and material concepts can be employed to utilize the usually non-emissive triplet excitons. Among them, thermally activated delayed fluorescence (TADF), relies on fluorescent emitters with an exceptionally small energy gap between singlet S_1 and triplet T_1 excited states. This results in fast thermally activated reverse intersystem crossing (RISC) from the triplet to the singlet state, even at room temperature. The relevant processes are shown in Fig. 1.

Fig. 1 Relevant states and processes for excitons in a TADF host-guest system. Radiative decay (fluorescence), and (reverse) intersystem crossing rates are among the most important characteristics of any TADF emitter. The Dexter transfer rate between guest and host $k_{D,gh}$ is affected by the triplet confinement energy ΔE_T and the transfer rate among host sites $k_{D,gh}$ can be expressed as a host diffusion coefficient D_h.
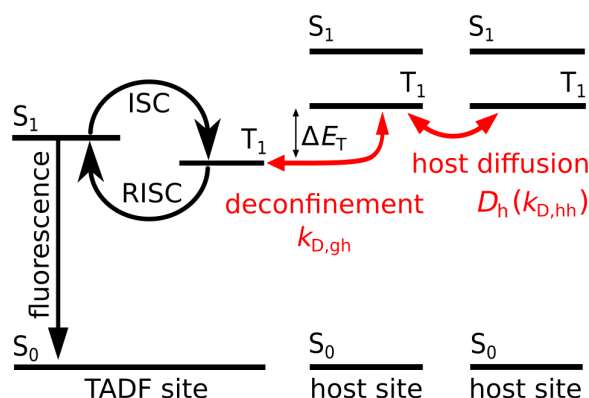
Transient photoluminescence (PL) experiments of such emitters in different host materials are crucial to determine their photophysical rates, which are used as key figures of merit for material development and are fundamental input parameters in many modelling and device simulation tools. Various methods have been developed for the extraction of rates from the characteristic PL transients[1,2]. At the current state however, not all decay features sometimes observed in literature are unambiguously identifiable and can be adequately included in the analysis. This can present problems with the comparability of material characteristics (rates) and interfere with optimal choices for material and device design.

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We extend the known analytical models to include triplet exciton transfer to the host material ("deconfinement") and assuming fast subsequent host diffusion ("fast diffusion limit"), as shown schematically on the right side of Fig. 1.[1,2] The decreased triplet density on the guest $P_{T,g}$ is shown in Fig. 2(a) with dependencies on the confinement energy ΔE_T and the guest concentration c_g. Fig. 2(b) shows the impact of such deconfinement on the measured PL signal, which is expected to be proportional to the singlet population, and also showing the corresponding increased triplet population. Notably, the signal maintains its bi-exponential shape typical for TADF emitters, potentially obscuring the presence of deconfinement.
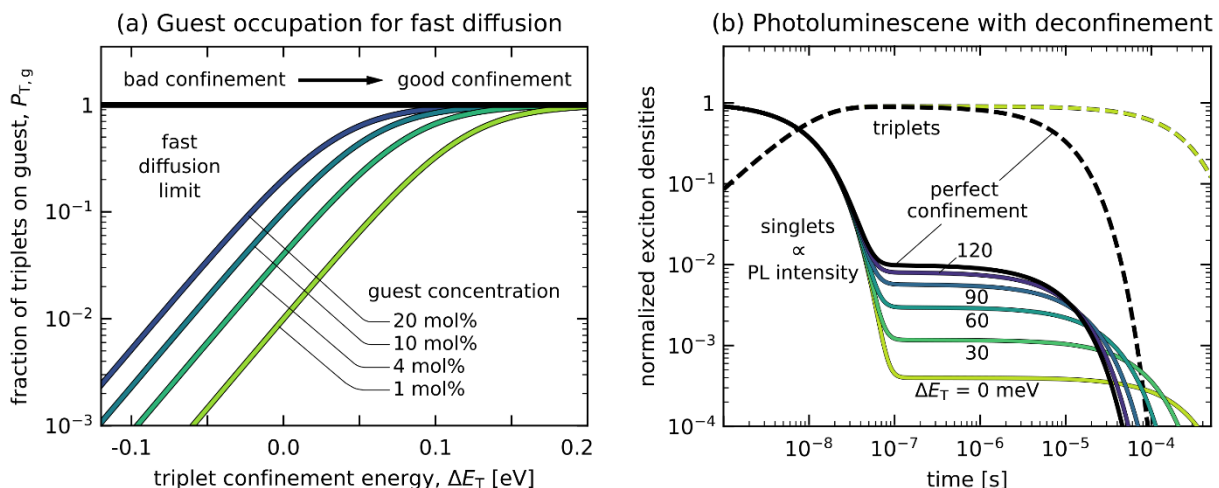

Fig. 2 Predictions of an analytical model for (a) the probability $P_{T,g}$ for a triplet to be occupying a guest site in the fast diffusion limit, in dependence of the confinement energy ΔE_T and for different guest concentrations and for (b) the transient singlet ($\propto$ PL) and triplet populations affected by deconfinement in the fast diffusion limit. For the TADF material typical state-of-the-art parameters of k_{prompt} = 10 ns, $k_{delayed}$ = 10 µs and integrated intensity ratio $\Phi_{delayed}$ / Φ_{prompt} = 10 are assumed with c_g = 4 mol%.

Due to the delicate interaction between the involved processes, the PL practically cannot be modeled analytically if the deconfinement and diffusion are occurring on the same time scale as the delayed fluorescence. We therefore use more powerful 3D kinetic Monte Carlo simulations to comprehensively study the role of ΔE_T and c_g in combination with a wide range of typical guest-host (k_{gh}) and host-host transfer rates (k_{hh}).[3]

Disentangling these parameters allows us to identify several deconfinement regimes with significant effects on the transient PL but different decay dynamics. The results will help to unambiguously identify deconfinement in TADF host-guest systems and thereby establish comparability and precision in parameter determination and facilitate optimal design choices.

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A kinetic Monte Carlo study of triplet-triplet annihilation in conjugated luminescent materials

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It is well known that in organic solids the collision of two excitons can give rise to delayed fluorescence (DF). Revived interest in this topic is stimulated by the current endeavor towards the development of efficient organic opto-electronic devices such as OLEDs and solar cells, or sensitizers used in photodynamic therapy. In such devices, triplet excitations are ubiquitously present but their annihilations can be either detrimental, e.g. giving rise to a roll-off of intensity in an OLED, or mandatory, e.g. if the sensitizer relies on up-conversion of long-lived low energy triplet excitations. Since the employed materials are usually non-crystalline, optical excitations migrate via non-coherent hopping. The method of choice to unravel the complex pattern of individual elements in the hopping process is kinetic Monte Carlo simulation (kMC). In the current work we employ kMC to study the interplay of triplet-triplet annihilation (TTA) and quenching of the triplet excitations by impurities in a single component system featuring a Gaussian energy landscape. Our simulation results are in agreement with the experimental observations of Hoffmann *et. al.* for oligomers and polymers with different conjugation length.[1] By examining the material parameters, we find that enhanced room temperature DF requires:

(i) a transport morphology that allows for isotropic hopping

(ii) materials with a long conjugation length

(iii) materials that are well purified so that they have a defect concentration $\leq 10^{17}$ cm^{-3}, and

(iv) materials that show a high degree of energetic disorder ($\sigma \geq 70$ meV).

The role of energetic disorder is twofold. First, an increased disorder (and dispersive transport) reduces the triplet diffusivity. A high diffusivity enables triplet motion to impurity sites where their concentration is reduced. Since TTA depends quadratically on the triplet concentration, the fraction of TTA events eventually reduces. Thus, a moderately low triplet diffusivity is desirable. The second role of energetic disorder, however, is that it causes filamentary transport, thus enhancing the probability of two triplets to encounter each other rather than an impurity. This is related to disorder induced filamentary currents and thus locally enhanced triplet densities. A key conclusion is that the DF features a maximum at a temperature

that scales with σ/K_BT as shown in Fig.1; observing a maximum at $\sigma/K_BT \approx 3$ and thus, the energetic disorder is crucial for obtaining a high yield of TTA events at room temperature.

We also explore the effect of polaronic contributions to the hopping rates. We found that the choice of hopping rate is not critical when considering the yield of TTA events, and that analytical studies need to include the intensity and time-dependence of quenching and annihilation constants to come to a description that reflects experiments.
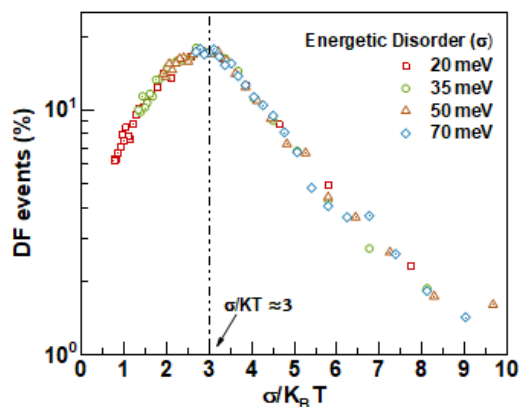

Fig. 1. Delayed fluorescence peaks at $\sigma/K_BT \approx 3$ for all the disorder values.

[1] Hoffmann, S. T.; Koenen, J. M.; Scherf, U.; Bauer, I.; Strohriegl, P.; Bassler, H.; Kohler, A.., *J. Phys. Chem. B* 2011, **115**(26), 8417-23.

Extraction of TADF OLED parameters using multiple PL transients

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A common characterization technique performed on TADF thin film emitter materials is transient photoluminescence (TrPL) which allows the extraction of fundamental parameters such as radiative decay rate k_{RAD} (S) and the intersystem crossing rates, k_{ISC} (S→T) and k_{RISC} (T→S)[1]. A general approximation applied when fitting a TrPL experiment is to neglect some phenomena such as non-radiative decays (S,T) and annihilation (TTA, SSA and STA), such that the rate equations can be simplified enough to have a small number of parameters to fit. Going beyond these approximations the complexity of the rate equations of singlet and triplet excitons increases and the fit results can become highly correlated and thus less reliable.

In this work we show how the increased complexity of the model could be counterbalanced by employing a global fit applied to a larger dataset of TrPL experiments performed at different temperatures and with multiple laser fluencies.

In order to evaluate the performance of this approach, the entire methodology has been applied to TrPL reference simulations[2] performed with Setfos instead of real experiments. This procedure allows for a direct comparison between the resulting values from the fit and the parameters with which the simulations were generated. This check for consistency is exemplified in (Fig. 1) and demonstrates the beneficial concept of incorporating datasets with multiple temperatures and laser fluences.

The fitting was conducted with Setfos using the "Optimization" feature, where two optimization methods have been run in series: Bayesian (global search) and Levenberg-Marquardt (local search).

[1] Nils Haase, Andrew Danos, Christof Pflumm, Antonia Morherr, Patrycja Stachelek, Amel Mekic, Wolfgang Bruetting and Andrew P. Monkman, J. Phys. Chem. C 1 https://doi.org/10.1021/acs.jpcc.8b11020 (2018)
[2] M. Regnat, K.P. Pernstich, K.-H. Kim, J.-J. Kim, F. Nüesch, B. Ruhstaller, Adv. El. Mat. https://doi.org/10.1002/aelm.201900804 (2019)
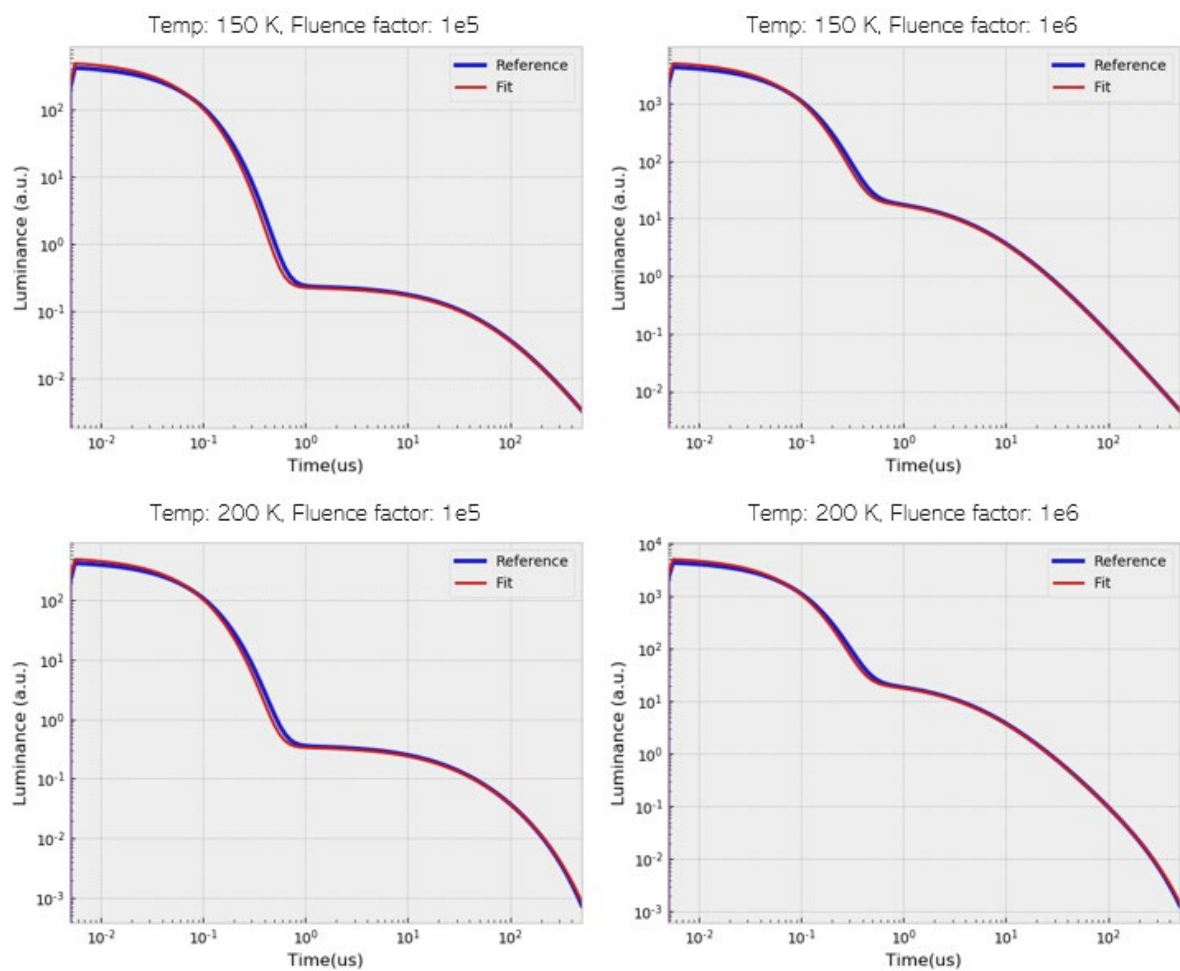
Fig. 1 TrPL reference simulations and fit results at different temperature (200-300 K) and different laser fluence (1e5-1e6 multiplication factor)

Analysis of degradation phenomena in exciplex TADF OLEDs

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Thermally activated delayed fluorescence (TADF) OLEDs are of great interest for industry and research because they achieve high efficiencies without expensive metal complexes as in phosphorescent OLEDs. In an exciplex TADF OLED the emission layer consists of two co-evaporated materials for the host allowing TADF and thus standard fluorescent or phosphorescent emitting dyes can be used instead of TADF emitters.

In this study we investigate the driving voltage increase during prolonged operation at constant current of an exciplex TADF OLED with an orange phosphorescent emitter[1]. With basic and advanced characterization[2] such as current-voltage, impedance, capacitance-voltage and charge extraction by linear increasing voltage (CELIV) measurements a quantitative electrical drift-diffusion model[3] of the exciplex TADF OLED was established. The model can quantitatively reproduce several key features of the data obtained with different measurement methods during degradation and thus enabled us to identify where in the multilayer OLED stack the degradation phenomena occur. The model suggests that an increased hole trap density in the hole transporting and exciplex host layers is the main cause for the driving voltage increase of 25% during the investigated period of nearly 2000 h of stressing.

Figure 1a shows the measured increase of the driving voltage. The measured luminous flux during this period did not change significantly and thus the power conversion efficiency reduction at constant current is caused by the increase in driving voltage. **Figure 1b** shows the measured and simulated J-V characteristics for the different degradation states, where the current density decreases by more than 65%. **Figure 1c** shows the extracted trap densities from the model for the different layers in the exciplex TADF OLED for the different degradation states. The hole trap densities in the hole transporting layers HTL1 and HTL2, as well as in the hole transporting material in the co-evaporated emission layer (EML h) increase, especial-

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ly in the HTL1, whereas no significant increase for electron trap densities in the electron transporting materials EML e and ETL e were necessary to explain the driving voltage increase.
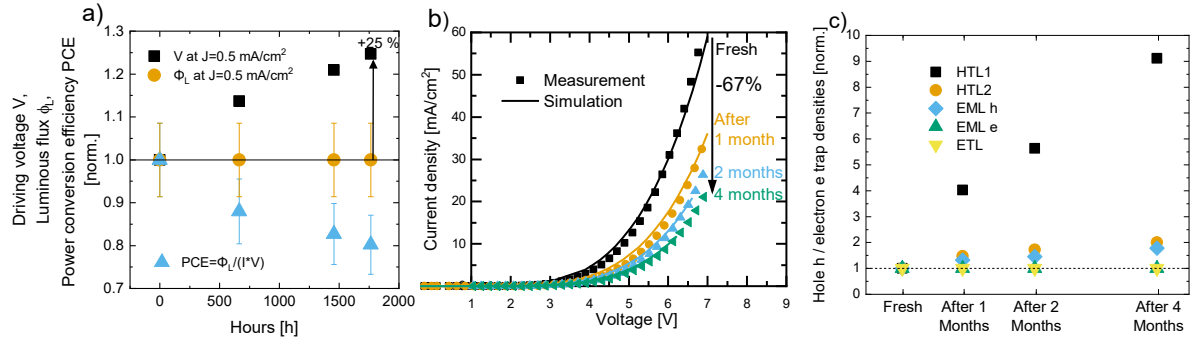

Figure 1: Measured driving voltage, luminous flux and power conversion efficiency at constant current during prolonged operation (a). Measured and simulated J-V curves for different degradation states of the exciplex TADF OLED (b). Extracted trap densities from the model for the different layers for the investigated period.

In our presentation we present the details of the electrical OLED model and discuss the influence of the trap stats on the mobility and other model parameters.

Multiscale simulations of realistic metal/organic interfaces

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Despite the central role played by metal/organic interfaces in light-emitting devices (OLED), organic thin film transistors (OTFT) and organic photovoltaic cells (OPV) their theoretical investigation still lacks a systematic modelling framework. In this work we describe an effort to bridge this gap by the development of a general simulation tool that we call MIRTO (Modeller of Interfaces and charge injection Rates calculaTOr).

The tool offers an atomistic multiscale platform in which interfacial aggregates of small molecules can be grown on top of an inorganic surface by means of classical molecular dynamics (MD) simulations obtaining realistic samples resembling different fabrication conditions. Constrained density functional (C-DFT)[1,2] is then used in order to simulate an electron transfer process between the organic molecules and the metal surface. It is shown that C-DFT gives an accurate value for the energy difference between the initial and final states known as the level alignment problem. The approach allows a first principle calculation of the charge transfer rates at metal/organic interfaces.

As a case study, we did simulate the deposition of the organic semiconductor N,N′-Di(1-naphthyl)-N,N′-diphenyl-(1,1′-biphenyl)-4,4′-diamine (NPB, NPD) on top of a metallic electrode. The electrodes analyzed are either Au or transparent $In_{2-x}Sn_xO_3$ (ITO).

It is found that the first layer of NPB has a natural tendency of electron-transfer to ITO leading to a strongly polarized interface which also leads to a large energy disorder.

[1] N. Holmberg, and K. Laasonen, "Efficient Constrained Density Functional Theory Implementation for Simulation of Condensed Phase Electron Transfer Reactions". JCTC, 13(2), 587–601, (2017).

[2] M. Baldoni, A. Lorenzoni, A. Pecchia, and F. Mercuri, "Spatial and orientational dependence of electron transfer parameters in aggregates of iridium-containing host materials for OLEDs: Coupling constrained density functional theory with molecular dynamics", PCCP, 20(45), 28393–28399, (2018).
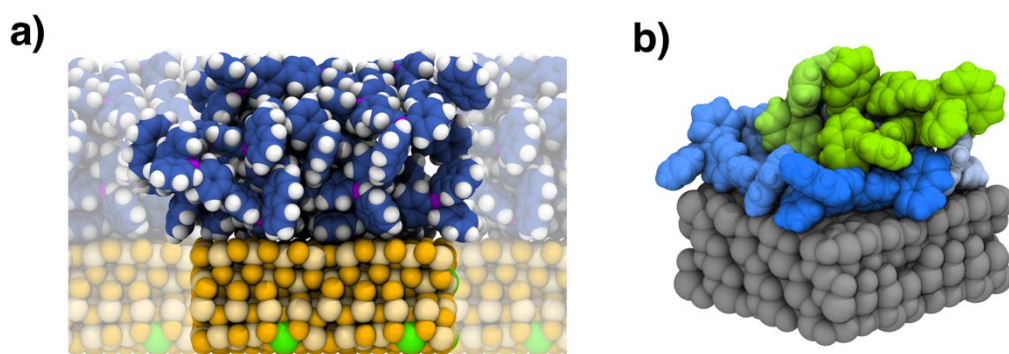
Fig. 1 a) Example of an NPB aggregate grown on top of the ITO surface. b) The shaded area represents periodic images of the simulation box. First and second NPB molecular layers. Colours highlight the spontaneous charge transfer.

Sub-Turn-on Exciton Quenching Due to Spontaneous Orientation Polarization in Organic Light-Emitting Devices

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Many common materials used in organic light-emitting devices (OLEDs) show preferred molecular orientation in thin films[1]. In molecules with a permanent dipole moment, this can lead to spontaneous orientation polarization (SOP) of the film and can generate a large interface charge. This polarization charge is compensated in a device by the accumulation of charge carriers, typically holes, in the adjacent layer. While it has been speculated that these accumulated charges can quench excitons and accelerate degradation[2], no direct demonstration of these effects has been made. Here, we show that electron transport layers exhibiting SOP induce substantial exciton quenching prior to device turn-on, reducing the peak internal quantum efficiency by ~20% relative to layers without SOP (Fig. 1)[3]. We further show that SOP can be eliminated by substrate heating during deposition, thereby improving device efficiency. Using spatial exciton quenching and drift-diffusion modeling, we demonstrate that the magnitude of quenching is consistent with the measured SOP-induced charge accumulation. These findings highlight that 1) SOP is an important material parameter that must be considered when optimizing the efficiency of OLEDs, and 2) exciton quenching can occur at biases below device turn-on, which must be explicitly accounted for to accurately quantify the components of OLED efficiency loss.
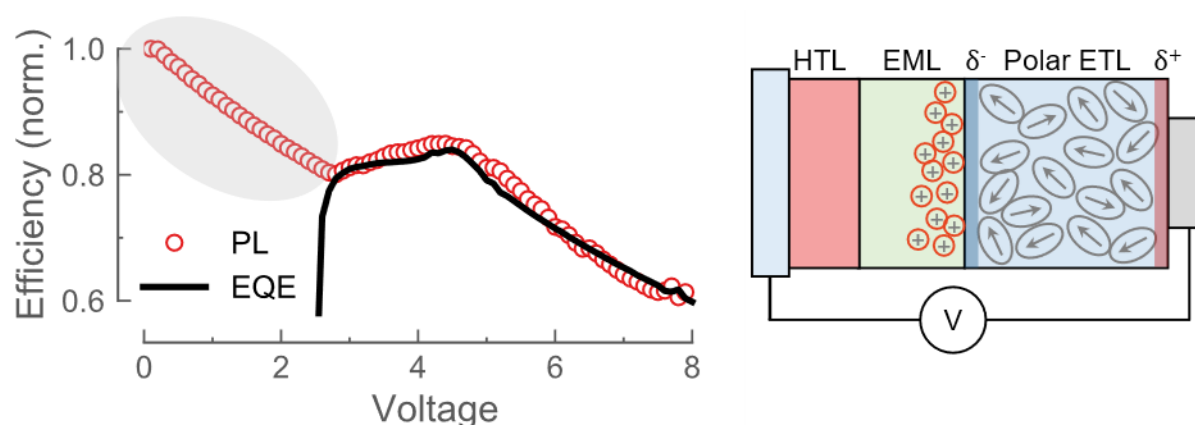

Fig. 1 (Left) Comparison of photoluminescence (PL) intensity and external quantum efficiency (EQE) as a function of applied bias, showing substantial luminescence quenching prior to device turn-on. (Right) Schematic of hole accumulation in the emissive layer (EML) due to spontaneous orientation polarization of the electron transport layer (ETL).

[1] K Osada et al. Organic Electronics 2018, 58, 313–317. DOI: 10.1016/j.orgel.2018.04.026.
[2] Y Noguchi et al. Jpn. J. Appl. Phys. 2019, 58 (SF), SF0801. DOI: 10.7567/1347-4065/ab0de8.
[3] JS Bangsund et al. Sci. Adv. 2020 (*In press, online Aug. 7, 2020*), 6. DOI: 10.1126/sciadv.abb2659.

The Dynamic Emission Zone in Sandwich Polymer Light-Emitting Electrochemical Cells

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After 25 years of research involving experiments and modelling studies, the basic operation principles of light-emitting electrochemical cells (LECs) seems to have been firmly established. Contrary to that claim, we demonstrate here that the analysis of a moving emission zone (EZ) over 20 hours and across more than 30% of the active layer of sandwich (400 nm thick) super yellow polymer LECs affords surprises and far-reaching insights into the functioning of LECs.

We support this view first with results from low frequency capacitance measurement that are commonly related to the dynamics of the intrinsic zone width, or more precisely to the dynamics of the low-conductivity part of the device. The transient capacitance increases first, passes a maximum and decreases to a lower steady state value. This indicates that the intrinsic zone initially gets smaller but increases again during de-vice operation. This capacitance trend has been reported already in literature; however, we observe here that the intrinsic zone width starts to increase again well before the electrical device optimum is reached, i.e. before the voltage minimum in a constant current experiment, and also before the current maximum when using a constant voltage driving mode. Such a behavior is contradicting the common believe that the optimal electrical performance is reached when the doped regions are fully established.

We explain our observations of a moving EZ and a transient capacitance peak with results from electrical simulation and find that the sole pre-condition for these events to occur is that the mobilities of the anions and cations are not equal. From the direction of the emission zone

shift, we can further deduce that the mobility of the cation in our case must be larger than the mobility of the anion. A further surprising result is that the current – and consequently the luminance – decreases by about 40% in constant voltage experiments after passing a maximum. This trend is intrinsic to the LEC operation when the ionic mobilities are different and does not result from degradation, as commonly believed. Device degradation mechanisms (unspecified) prevail only after the ionic movement has stopped. Quantitative Tof-SIMS profiles at different times during operation show that the displacement of anions stops at the same time when the capacitance levels off, confirming the relation between ion movement and the observed EZ shift and capacitance dynamics. Our results provide a simple explanation for the often observed EZ shift in LECs.

For thin devices below 150 nm, we recently optimized the active layer thickness, surpassing comparable literature current efficiency to 11.6 cd/A and introduced an optical model to explain the thickness-dependency.[1] Here, we couple the optical to the electric model to reproduce voltage, capacitance and irradiance transients, and confirm that the same dynamic processes govern the functioning of application-relevant thin devices.[2]
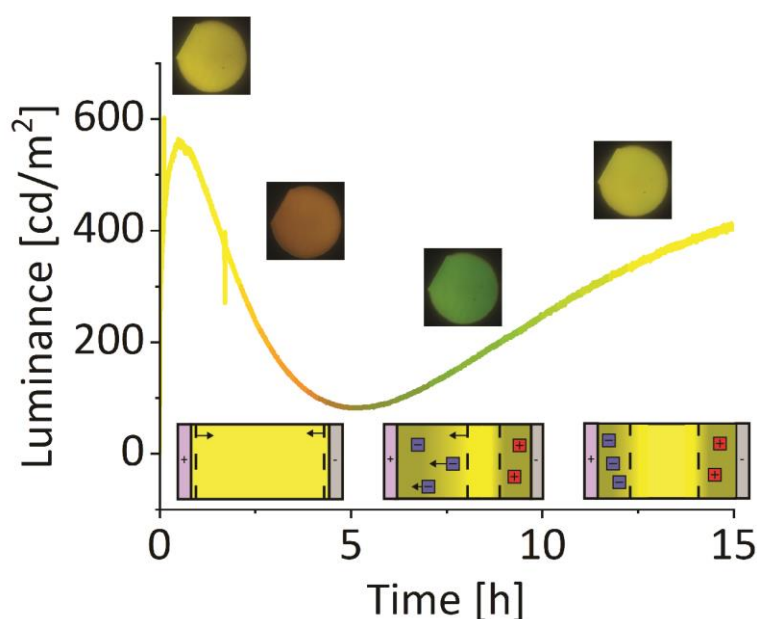

Fig. 1 Color change in a 400nm thick super yellow LEC for a constant current of 7.7 mA/cm². The underlying process is the dynamic of the intrinsic region resulting from ions with different mobilities.

[1] Diethelm, M., Grossmann, Q., Schiller, A., Knapp, E., Jenatsch, S., Kawecki, M., Nüesch, F., and Hany, R. (2019). Optimized Electrolyte Loading and Active Film Thickness for Sandwich Polymer Light-Emitting Electrochemical Cells. Adv. Opt. Mater. 7, 13–15

[2] Diethelm, M., Schiller, A., Kawecki, M., Devižis, A., Blülle, B., Jenatsch, S., Knapp, E., Grossmann, Q., Ruhstaller, B., Nüesch, F, and Hany, R.. (2019). The Dynamic Emission Zone in Sandwich Polymer Light-Emitting Electrochemical Cells. Adv. Funct. Mater. 1906803, 1906803.

Lifetime and performance prediction for organic solar cells through machine learning

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Energy demand is an ever-increasing problem and the requirement to develop cost – effective and renewable energy sources is of key interest for consumers and industries alike. Organic photovoltaic (OPV) solar cells are one emerging technology which could potentially provide a means of clean and renewable energy. However, OPV solar cells suffer from instability when exposed to various environmental stress factors and enhancing their lifetime is at the forefront of scientific research [1] [2]. However, due to the infancy of OPV and other emerging solar cell technologies, their long – term stability is not yet fully understood and understanding how each of the different environmental stress factors govern the stability is a costly and time con-suming task in laboratory conditions. Outdoor monitoring provides an ideal platform to test OPV solar cells under several simultaneous environmental conditions, as well as providing researchers with knowledge of the real – world operation of the technology. Data analytics and machine learning additionally provides a means of attaining greater insight into the fac-tors governing the OPV stability as well as forecasting the performance and stability of such technologies in a much reduced time – frame, thus minimizing experimental costs. This is key to fully realizing the technology, especially given the demand for renewable energy sources. Herein, a machine learning, data – driven approach to forecasting the diurnal performance of OPV technologies is presented and achieved using a multilayer perceptron (MLP) neural net-work algorithm. From the extracted performance parameters, the energy output can be calcu-lated and subsequently forecast. Fig. 1 illustrates the actual and predicted variation in the OPV energy output over the course of a day. This subsequently allows the daily yield to be calculated by integration. Furthermore, a multivariate linear regression method is employed in order to account for the effects of degradation in the OPV modules over the course of time. Subsequently, this offers long – term forecasting of OPV performance and degradation and allows the most influential factors governing the degradation to be determined; this provides invaluable information, such that OPVs can be made more robust against the principle factors affecting their lifetimes.
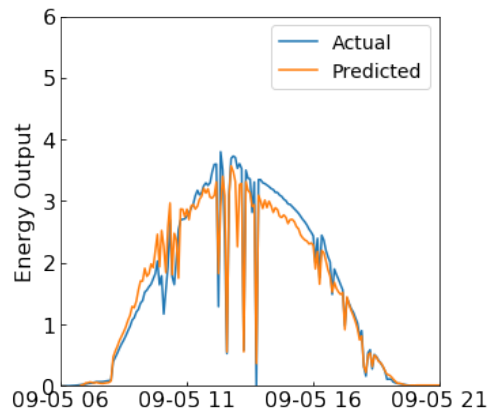
Fig. 1 Actual and predicted diurnal variation in OPV energy output, forecasted using an MLP algorithm.

[1] Zhang, Y., Samuel, I.D., Wang, T. and Lidzey, D.G., 2018. Current status of outdoor lifetime testing of organic photovoltaics. *Advanced Science*, *5*(8), p.1800434.
[2] Stoichkov, V., Kumar, D., Tyagi, P. and Kettle, J., 2018. Multistress Testing of OPV Modules for Accurate Predictive Aging and Reliability Predictions. *IEEE Journal of Photovoltaics*, *8*(4), pp.1058-1065.

New Li-ion battery technologies for EV's and their characterization

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The pace of new technologies entering the electric vehicle market has accelerated considerably. For example, Tesla will use CATL's new Cell-to-pack technology avoid the intermediate step of module assembly before final EV pack assembly. Also BYD and SVolt have introduced new technologies based on Blade battery and Matrix battery which are basically the same with long but very thin prismatic cells packed like very dense domino's next to each other[1].

Additionally, Ni-rich cathodes get introduced in EV's with e.g. SK Innovation introducing NMC 9 ½ ½ into the famous Ford F150 Pick-up in the US in 2023[2].

Here, a small overview of current technology is provided giving the audience a comprehensive overview about the current status of innovation in the field of electric vehicle battery technologies.

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[1] BYD Blade https://insideevs.com/news/427640/byd-shown-blade-battery-factory-chongqing/d, 8.01.2020
[2] SKI's NMC 9 ½ ½ for Ford F-150 http://www.koreaherald.com/view.php?ud=20200810000683, 10.08.2020

Physics-based modelling of Li-ion batteries

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Much like the perovskites used in solar cells, the active materials in Li-ion batteries are mixed ionic-electronic conductors with charged double layers at the interfaces and charge neutrality elsewhere. The mathematical theory behind Li-ion batteries is therefore like that of perovskite solar cells and other devices with mixed conductors.

In this talk, an overview of physics-based models of Li-ion batteries is provided. Three case studies are presented, in the fields of battery optimization,[i] degradation[ii] and safety.[iii]
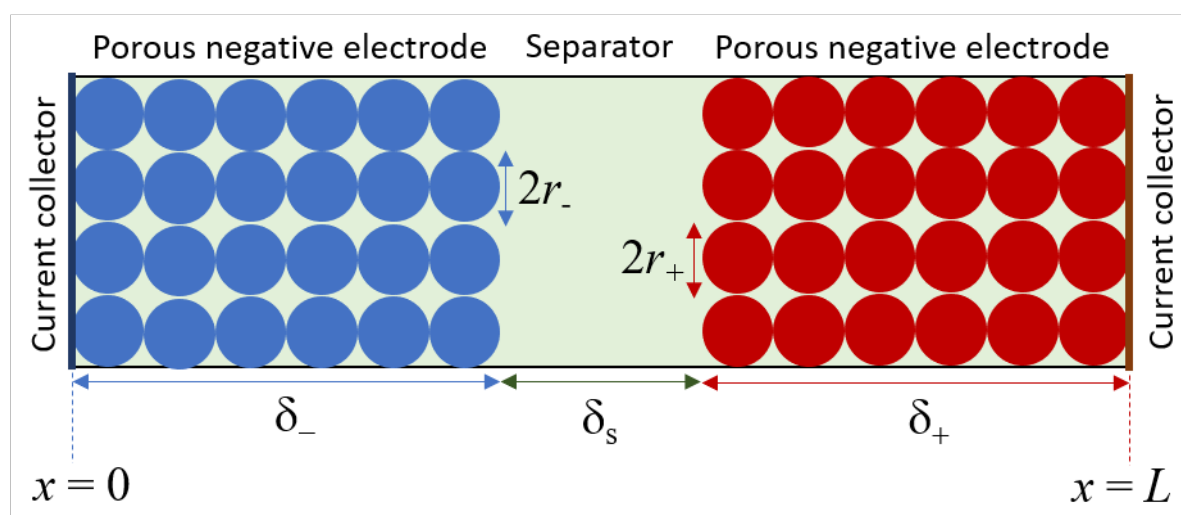

Fig. 1 Geometry of a standard pseudo-2D physics-based battery model.[iv] The electrode particles and electrolyte occupy different volume fractions of the same point in the x dimension. The Li⁺ concentration also varies between the surface and centre of the spherical particles in a second r dimension.

[i] Ian D. Campbell, Krishnakumar Gopalakrishnan, Monica Marinescu, Marcello Torchio, Gregory J. Offer and Davide Raimondo, «Optimising lithium-ion cell design for plug-in hybrid and battery electric vehicles», *J. Energy Storage* vol. 22 pp. 228-238, 2019. https://doi.org/10.1016/j.est.2019.01.006

[ii] Xinhua Liu, Weilong Ai, Max Naylor Marlow, Yatish Patel and Billy Wu, «The effect of cell-to-cell variations and thermal gradients ont he performance of lithium-ion battery packs», *Applied Energy* vol. 248, pp. 489-499, 2019. https://doi.org/10.1016/j.apenergy.2019.04.108

[iii] Simon E. J. O'Kane, Ian D. Campbell, Mohamed W. J. Marzook, Gregory J. Offer and Monica Marinescu, «Physical Origin of the Differential Voltage Minimum Associated with Lithium Plating in Li-Ion Batteries» *J. Electrochem. Soc.* vol. 167, pp. 090540, 2020. https://doi.org/10.1149/1945-7111/ab90ac

[iv] Thomas F. Fuller, Marc Doyle and John Newman, «Simulation of Optimization of the Dual Lithium Ion Insertion Cell», *J. Electrochem. Soc.* vol. 141 pp. 1-10, 1994. https://doi.org/10.1149/1.2054684/

Kinetically driven self-assembly of semiconductor nanoplatelets

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Quasi-two-dimensional semiconductor nanoplatelets exhibit spectrally pure, directional fluorescence due to their highly anisotropic shape. In order to make directional light emission accessible in applications, nanoplatelets have to be collectively oriented in the solid state. Existing methods use excess surfactants to control their self-assembly into ordered films at liquid interfaces. The usage of such additives could be detrimental for optoelectronic applications. Here we report the effective control over the collective orientation of nanoplatelets in self-assembled films by exploiting exclusively the solvent evaporation rate.[1] This kinetically driven self-assembly method yields well-defined monolayer films with controlled nanoplatelet orientation (either all oriented "edge-up" or "face-down") without depositing additives. The absence of additives enables strong electronic coupling between the nanoplatelets making these films suited for optoelectronic applications. The strong coupling is apparent from contact-free photoconductivity measurements on monolayers that demonstrate a clear orientation dependent conductivity in self-assembled NPLs, as opposed to the purely excitonic response of isolated nanoplatelets in a dispersion. The orientation dependence originates from the orientation-dependent inter-nanoplatelet coupling strengths. The ability to assemble nanoplatelets in highly ordered monolayers with varying electronic properties paves the way for new applications in electro-optic devices.
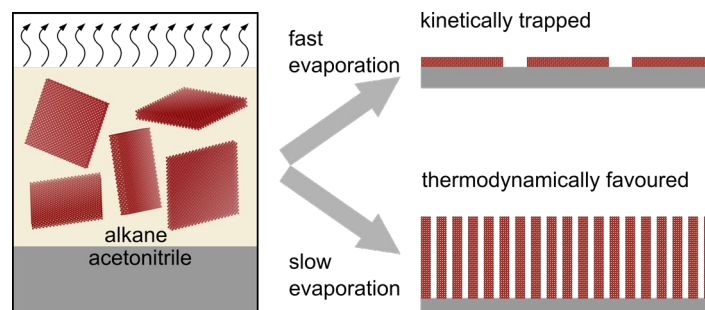
Fig. 1: The collective orientation of semiconductor nanoplatelets at liquid interfaces can be achieved by evaporation kinetics.

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[1] Momper et al, Nano Lett. 2020, 20, 6, 4102–4110

Modeling Ion Currents in Organic Electrochemical Transistors

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Its ability to operate at low voltages in aqueous media makes Organic Electrochemical Transistors (OECTs) highly promising for bio-electronic applications. Its transconductance is highest amongst competing thin film transistor technologies, which facilitates effective transduction of ionic signals into electronic signals essential for efficient bio-sensing. However, despite its outstanding performance, a convincing model describing its working mechanism is still lacking. Here, we study the working mechanisms of OECTs by a two-dimensional drift-diffusion model[1] that self-consistently solves the continuity of holes and ions and by that correctly describes lateral drift and diffusion of ions inside the channel. It will be shown that the ion concentration inside the transistor channel in equilibrium cannot satisfactorily be described by a simple capacitive gate coupling as commonly proposed. Furthermore, the influence of the polymer/electrolyte and polymer/drain interface in equilibrium on device performance will be discussed. Overall, the 2D model will result in the better understanding of OECTs in general and more specifically a better understanding of the scaling laws of this new technology.

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[1] V. Kaphle, P. R. Paudel, D. Dahal, R. K. Radha Krishnan, and B. Lüssem, "Finding the Equilibrium of Organic Electrochemical Transistors", Nat. Commun. **11,** 2515, (2020)

Capacity fade in Redox Flow Batteries: coupled phenomena of transport in concentrated solutions

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The all-organic TEMPO/Paraquat redox-flow battery [1] shows promise as a low-cost, sustainable energy storage device. As in most flow batteries, membranes play a critical role in the performance and cycling stability of the device. In this work, we aim to characterize the transfer of ionic species and solvent in ion exchange membranes through a thermodynamically consistent model in order to predict crossover rates, and estimate trade-offs between performance and stability.

Transport experiments on the membranes allow to measure permeability coefficients and transport numbers for ionic species. Coupled transport experiments allow to measure solvent transfer via osmosis and electro-osmosis, and characterization experiments allow to measure ion-exchange capacity, water content and thickness of the membrane. We use these parameters to model crossover of ionic species and solvent transfer, and predict capacity fade with different membranes and different cycling conditions.

Characterisation experiments are conducted at LEPMI, Grenoble, France. Validation through cell cycling is conducted at JenaBatteries, Jena, Germany under the scope of the FlowCamp project*.
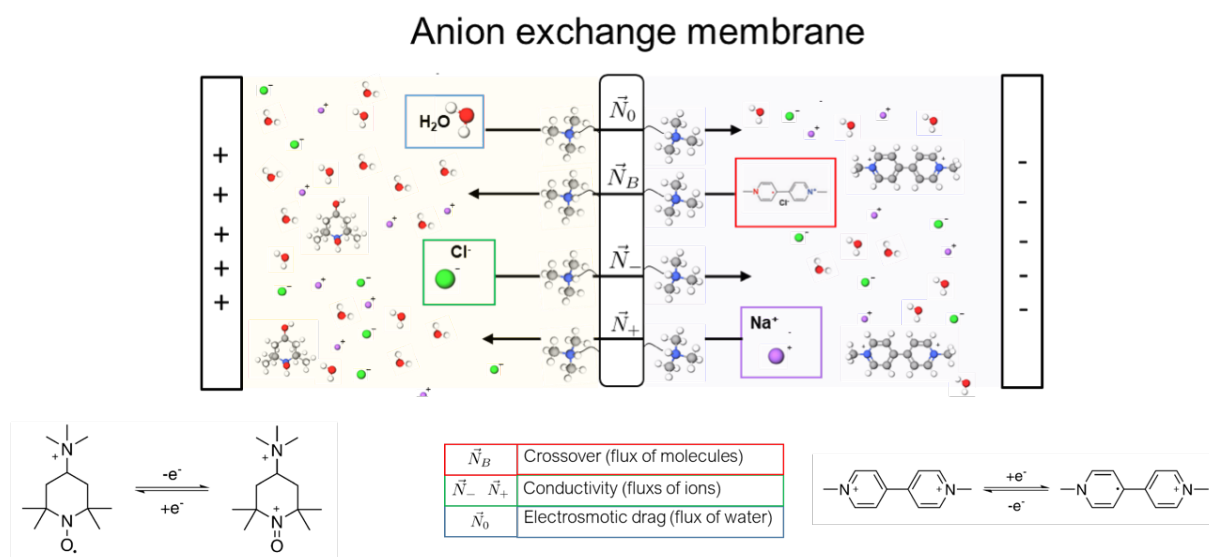

Figure 1: Representation of a TEMPO/Paraquat flow cell, with flux of different molecules through the anion-exchange membrane

[1] T. Janoschka *et al.*, "An aqueous, polymer-based redox-flow battery using non-corrosive, safe, and low-cost materials," *Nature*, vol. 527, no. 7576, pp. 78–81, Oct. 2015, doi: 10.1038/nature15746.

Transient photovoltage measurement of perovskite solar cells

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In all kinds of solar cells, transient photovoltage (TPV) decay measurements have been used to determine charge carrier lifetimes and to quantify recombination processes and orders. However, in particular for thin-film devices with a high capacitance, the time constants observed in common TPV measurements do not describe recombination dynamics but RC times for charging the electrodes. This issue has been revisited for organic and perovskite solar cells in the recent literature. In this contribution, we extend these discussions by analyzing a perovskite model system (Bi defects in $Cs_{0.1}FA_{0.9}Pb(Br_{0.2}I_{0.8})_3$), where we can tune defect recombination. We find that TPV, intensity-modulated photovoltage spectroscopy, and impedance spectroscopy yield the same time constants that do not describe recombination dynamics but are limited by the differential resistance of the diode and the geometric capacitance in common light intensity ranges (<1 sun). Employing numerical device simulations, we find that low charge carrier mobility can furthermore limit the TPV time constants. In samples with spatially non-uniform recombination dynamics, we measure two time constants, which depend on the charge carrier generation profile that can be tuned by the wavelength of the incident light. In that case, numerical simulation provides insights into recombination and charge transport processes in the device.[1]

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Opto-electronic modeling of organic and hybrid multijunction solar cells

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With single junction solar cell efficiencies approaching their fundamental physical limits, multijunction device architectures are shifting into the focus of photovoltaic research, especially the ones based on potentially low cost and abundant materials, such as organic semiconductors[1] and the combination of crystalline silicon with metal-halide perovskites[2]. While optical simulation of the complex multilayer stacks was shown to be instrumental to achieve efficiencies over 17% for organic[3] and over 29% for perovskite-silicon[4] tandems, further improvement requires consideration of electrical losses via full opto-electronic device simulation. Here, we discuss the assessment of the electrical performance of organic and hybrid tandem solar cells based on simulations with the 1D device simulation tool SETFOS[5], which combines multiscale optical simulation with a drift-diffusion-Poisson solver for charge transport, including an interface model to describe charge transfer across the recombination layers that form an integral part of the multijunction device architecture. Special attention is given to the impact of the electrical interconnection on the overall device characteristics.
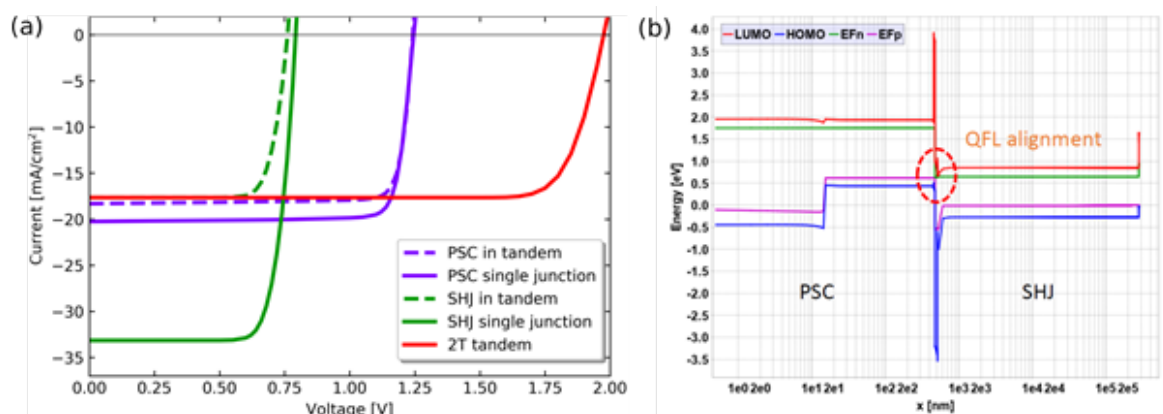

Fig. 1 . (a) Current-voltage characteristics from full opto-electronic simulations of perovskite (PSC) top- and silicon heterojunction (SHJ) bottom cells in single junction and tandem configuration. (b) Band profile at MPP exhibiting the absence of a voltage drop at the recombination junction, which is reflected in the perfect alignment of electron and hole quasi-Fermi levels (QFL).

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[5] Semiconducting Thin Film Optics Simulator (SETFOS), Fluxim AG, Switzerland; www.fluxim.com/setfos-intro.

Electro-thermal simulation and optimisation of organic solar cells and modules

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In this contribution, we present a FEM modelling approach allowing to efficiently optimise the design of solar cells and modules in order to maximize the power output and reduce the lateral electrical losses. In a first example, we compare the IV simulation of a complex-shaped module with experimental data which allows us to understand the limitations of different device parameters. This experimentally validated model is then used to optimise the number of cells connected in series for a module with predefined dimensions. Besides optimising cell and module layout, the modelling approach also lends itself to extract electrode conductivity parameters as we demonstrate with the analysis of electroluminescence (EL) images of organic solar cells having a metal grid. The measured EL image intensity is compared to the simulated current distribution. The position-dependent EL intensity is well reproduced by the simulation and the conductivities of PEDOT:PSS and aluminium electrode materials are thereby extracted.

In the further case study, we investigate shunts and layer non-uniformities that occur in an ink-jet printed OPV mini-module. Using steady-state IR as well as dark lock-in IR image thermography (DLIT) image, non-uniformities due to electrical shunts are observed in addition to Joule heating of the active cell area. The large local current density through a shunt leads to high power dissipation and thus local heating. To study this in more detail, we developed an electro-thermal FEM model for DC and AC operation and compare simulation results with the measured IR images and IV curves. We can thus estimate the conductivity of the shunts. Moreover, the AC model allows us to simulate the impedance spectroscopy response of large cells and modules, which also show interesting features linked to electrode conductivities and cell non-uniformities.

Spectrum sharing between Perovskite and Silicon solar cells: An alternative to tandem structures

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Silicon solar cells have most of the market share, while perovskite solar cells offer cheap and efficient photovoltaic electricity conversion. Hence it is not a surprise to find ~150 research papers on using Silicon solar cells in tandem configurations with Perovskite solar cells. The monolithic structure of the tandem cell has some obvious limitations: It subjects the silicon cell to the limited size and lifetime of the perovskite one. Therefore, we are motivated to construct modules where the two cells are physically separate.

Here we explore the possibility of sharing the solar spectrum between these two types of cells by inserting them into a light trap made of diffuse reflecting walls. The trap is a cost-effective device, unencumbered by the limitations of tandem configuration. Using solar cell simulations, flux-balance analysis, ray tracings, and cost analysis, we show that the solar trap system with a planer standered silicon hetrojunction solar cell and a perovskite cell[1] produces more electricity at only slightly higher module cost compared to its alternatives, at one sun concentration.
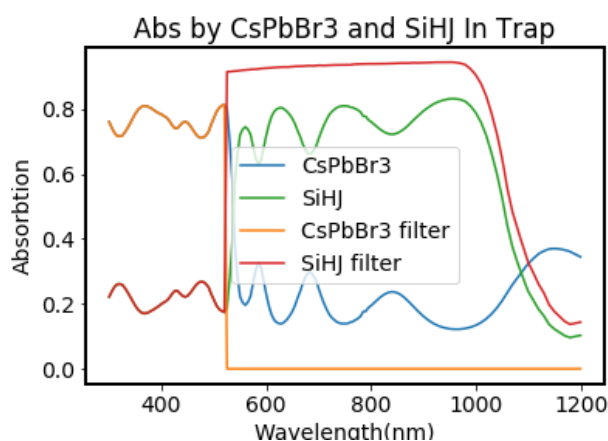

Fig. 1 Absorption by $CsPbBr_3$ and Si Heterojunction solar cell in a solar light trap. We take the cell area as 10% of the light trap area for both the cells (it was verified optimum by simulation). The solar trap wall reflection was 95%, which can be easily achieved by low-cost paint[2].

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Table 1: Comparison of solar cell performance in the solar light trap to flat module performances with 1 sun concentration.

		% η	Module Cost ($/Wp)
1	CsPbBr$_3$/Silicon (HJ)in trap with Filter over CsPbBr$_3$ cell	27.4	0.55
2	CsPbBr$_3$/Silicon in trap	25.9	0.58
3	Perovskite/Silicon tandem	27 [3]	0.48 [4]
4	Silicon (HJ-IBC)	24.4 [5] (Highest η Module)	0.50 [6] (Typical not best)
5	Perovskite	17.9 [4] (Highest η Module)	0.49 [7] (Typical not best)

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Effective masses of heavy, light, and split-off electrons and effective g-factor of electrons in perovskite materials

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The k•p method is very useful for providing analytical expressions to help gain insight into the band structure and physical phenomena occurring near the center of the Brillouin zone of semiconductor materials[1]. Analytical expressions for the effective g-factor and effective masses of heavy, light, and split-off electrons are obtained by diagonalising the 8x8 k•p matrix Hamiltonian[2]. It is found that Cl- and Pb-based perovskite materials have relatively larger heavy, light, and split-off electron effective masses because they have smaller Luttinger parameters compared to Br-, I- and Sn-based perovskite materials. The metal and halide atoms influence the electron effective mass in perovskite materials, which in turn influence the charge carrier mobility in perovskite devices such as perovskite solar cells. The results of our work may be useful for calculating properties of perovskite materials to provide a guide for experimental determination of effective masses and g-factor in these materials.

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