



Final report from 30 October 2024

SimOEP'24

International Conference on Simulation of Organic Electronics and Photovoltaics



SimOEP'24

International Conference on
Simulation of Organic Electronics
and Photovoltaics 2024



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SimOEP Conference 2024

The seventh International Conference on Simulation of Organic Electronics and Photovoltaics (SimOEP 2024) was held from the 2nd to the 4th of September 2024 (in-person event) in Winterthur as the continuation of a conference series (2012 in Oliva, 2014 in Palma de Mallorca, 2016 in Winterthur, 2018 in Winterthur, 2020 online, 2022 in Winterthur, 2024 in Winterthur).

The conference hosted 70 participants, primarily from Switzerland and Europe, and featured a three-day program, details of which can be found in the annex.

The first day was dedicated to perovskite solar cells and photovoltaics, the second day focused on novel devices and methods such as batteries and machine-learning and the last day was devoted to OLEDs and related topics.

In total, there were 18 invited talks out of 46 contributions including one remote talk from the U.S. A total of 16 contributions from Swiss research institutions or companies was reached allowing for a knowledge transfer within the country. Breaks and the conference dinner offered further engagement and exchange of ideas.

In the Appendix the scientific program shows the high-quality scientific presentations of this years' SimOEP edition.

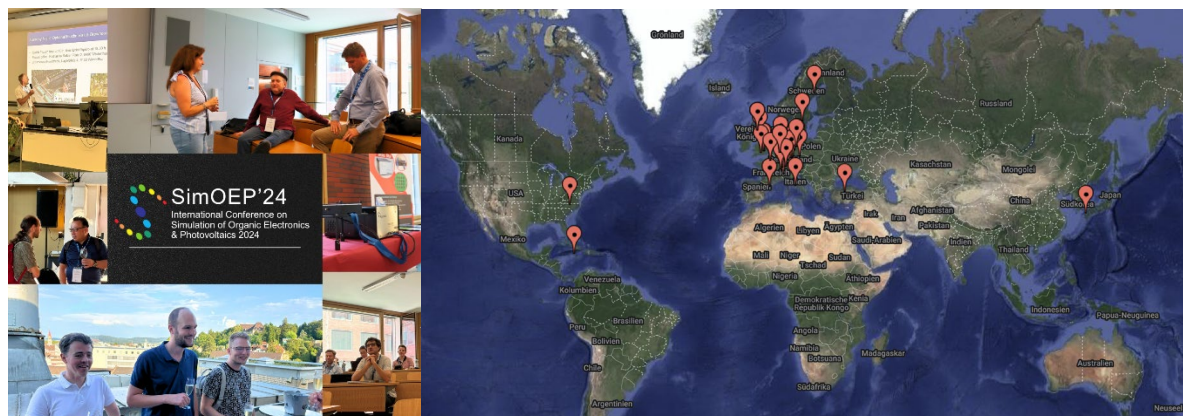


Figure 1: Left: Impressions of the SimOEP'24 conference in Winterthur. Right: Map of origin of participants.



Appendix



School of
Engineering

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International Conference on Simulation of Organic Electronics and Photovoltaics 2024



Zurich University of Applied Sciences

2.-4. September 2024

Version August 30, 2024

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SWISS PHOTONICS

Scientific Program

	Monday, 02.09.24	Tuesday, 03.09.24	Wednesday, 04.09.24	
	PV	PV/Novel Devices/ML	OLED	
09.00-09.15	Registration	Urs Aeberhard	Ludvig Edman	09.00-09.15
09.15-09.30		Yasin Ameslon	Anna Köhler	09.15-09.30
09.30-09.45		George Koutsourakis		09.30-09.45
09.45-10.00	Welcome	Antonio Cabas Vidani	Edoardo Stanzani	09.45-10.00
10.00-10.15			Rifat Kaçar	10.00-10.15
10.15-10.30	Christian Wolff	break	break	10.15-10.30
10.30-10.45	James Connolly	Larry Lüer	Franky So	10.30-10.45
10.45-11.00				10.45-11.00
11.00-11.15	Gemma Giliberti	Jesper Jacobsson	Ifor Samuel	11.00-11.15
11.15-11.30	Matthias Diethelm			11.15-11.30
11.30-11.45	Pilar Lopez	Oliver Zbinden	Zeina Amer	11.30-11.45
11.45-12.00	break	Mohammed Azzouzi	Savanna Lloyd	11.45-12.00
12.00-12.15		break	break	12.00-12.15
12.15-12.30				12.15-12.30
12.30-12.45	Imaging Prototype Session			12.30-12.45
12.45-13.00	Safa Shoaee	Priscilla Caliendo	Peter Levermore	12.45-13.00
13.00-13.15	Atika Abid	Alex Morata	Eglė Tankelevičiūtė	13.00-13.15
13.15-13.30	Fransien Elhorst		Roland Hany	13.15-13.30
13.30-13.45	Lukas Frommel	Giles Richardson	Vasilis Georgakopoulos	13.30-13.45
13.45-14.00	Peyman Amiri		Markus Regnat	13.45-14.00
14.00-14.15	break / Litos Lite Demo	break	Kurt Pernstich	14.00-14.15
14.15-14.30		Battery Tool Prototype Session	Farewell	14.15-14.30
14.30-14.45	Firouzeh Ebadi	Davide Moia	Display Prototype Session	14.30-14.45
14.45-15.00	Miguel Torre		break	14.45-15.00
15.00-15.15	Andreas Schiller	Wolfgang Tress	Setfos OLED	15.00-15.15
15.15-15.30	Christoph Kirsch	Mahmoud Samadpour		15.15-15.30
15.30-15.45	break	Mojca Jazbinsek		15.30-15.45
15.45-16.00	Setfos PV Workshop	Litos Lite Workshop		15.45-16.00
16.00-16.15				16.00-16.15
16.15-16.30				16.15-16.30
16.30-16.45				16.30-16.45
16.45-17.00				16.45-17.00
17.00-17.15				17.00-17.15
17.15-17.30				17.15-17.30
18.30-21.00	Conference dinner		invited talks contr. talks Prototype Instrument Session Fluxim Workshop	

Monday, 02.09.2024

08.45-10.15	Registration	
10.15-10.30	Welcome/Opening <i>Beat Ruhstaller, ICP ZHAW and Fluxim AG, Switzerland</i>	
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11.45-12.00	Probing Ionic Conductivity and Electric Field Screening in Perovskite Solar Sells: A novel Exploration through Ion Drift Currents <i>Matthias Diethelm, University of Oxford, United Kingdom</i>	10
12.00-12.15	The Hallmark of Ion Migration in Perovskite Solar Cells by Impedance Spectroscopy Measurements and Simulations <i>Pilar López-Varo, IPVF, France</i>	11
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14.15-14.30	Improve Vacuum-Deposited Formamidinium-Based Perovskite Solar Cells by Device Modelling <i>Fransien Elhorst, University of Groningen, Netherlands</i>	15
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15.30-15.45	On the Role of the Photo Physics of Cs ₂ AgBiBr ₆ Double Perovskites on Solar Cell Performance - A Temperature-dependent Study of Urbach Energy and Luminescence <i>Firouzeh Ebadi, ZHAW ICP, Switzerland</i>	19
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18.30-21.00	Conference Dinner <i>Caribbean Pearl, Zürcherstrasse 3, 8400 Winterthur</i>	

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16.15-16.30	Litos Lite Workshop	

Halide Perovskite Multijunction Solar Cells

Mostafa Othman, Hilal Can, Austin Kuba, Jonas Diekmann, Chiara Ongaro, Mohammadreza Golobostanfard, Kerem Artuk, Deniz Turkay, Aïcha Hessler-Wyser, Christophe Ballif, Christian Wolff

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To enhance the efficiency of single-junction solar cells beyond the thermodynamical limits, multijunction devices are currently the only realized method. Among the many different material systems, there are currently few that have matured enough in terms of efficiency, stability, and cost-competitiveness. Among these are CdTe, c-Si and potentially halide perovskites. In the presentation, I will show our latest developments in the field of perovskite-based multijunction devices. In particular, we developed monolithic two-terminal dual- and triple-junction devices based on halide perovskites and c-Si, i.e., perovskite/silicon and perovskite/perovskite/silicon devices. In the quest to enhance the efficiency of said devices, the complexity of the devices scales non-linearly with the number of layers in the devices. As such, the optical and electrical properties of many layers have interactions and are co-dependent, further complicated by the need to have processing compatibility, e.g., to avoid sputter damage or enable conformal deposition of thin films < 1 micrometer on structures such as random pyramids with > 1 micrometer height. As an example, for a dual-junction, we typically have 12-14 layers in the stack, and in a triple-junction, 18-20 layers. This high-dimensional problem is very time-consuming and practically impossible to explore experimentally. Hence, we use experimentally validated optical and electrical models to guide our experimental developments. For example, the optical system can be optimized via a Bayesian optimization methodology to rapidly attain optimal thicknesses within physically meaningful limits. Similarly, we address the electrical properties working towards a full optoelectronic model. This combined simulation-experiment approach allows us to identify individual loss mechanisms, which we reduce to achieve power conversion efficiencies of $> 32\%$ and recently $> 26\%$ in dual- and triple-junction devices, respectively. These numbers are on par with the current world records for these technologies but still allow further gains, Figure 1.

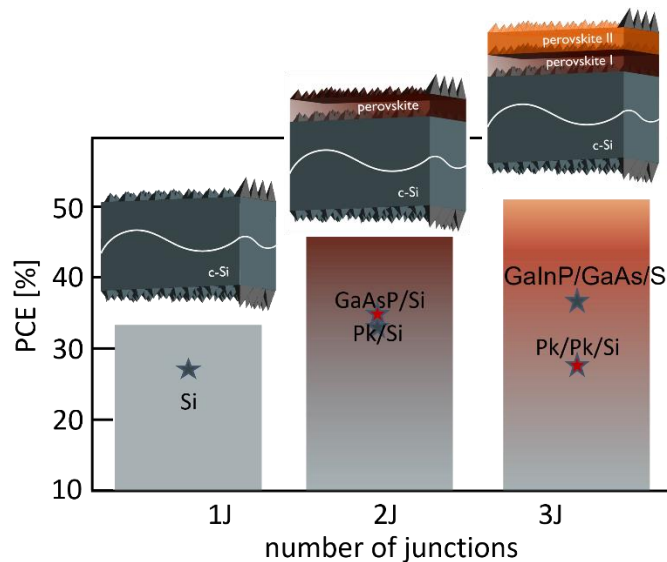


Figure 1 – Efficiency vs. number of junctions in monolithic devices along with the records for Si or III-V/Si (grey stars) and Pk/Si (red stars) and the theoretical limits (bars).

Three Terminal Organic-Silicon Tandem Models

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² Université de Bordeaux, IMS-CNRS, UMR 5218, Bordeaux INP, ENSCBP, F33405 Talence, France

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The search for ever higher efficiency solar cells is at present focussed on multijunction devices. In this field, there is enormous research on tandems consisting of a high bandgap top sub-cell coupled to a Si bottom sub-cell¹. An emerging top cell candidate is the organic solar cell, given recent impressive breakthroughs in efficiency and stability², thanks in part to non-fullerene acceptors. In this context, we report on approaches to modelling organic solar cells for silicon / organic tandems. The device studied is the three-terminal selective band-offset tandem cell³. This innovative design shown in figure 1a is based on the Si interdigitated back contact solar cell⁴, which features a number of fabrication and operating advantages over four terminal and two terminal tandems⁵. The higher gap organic top sub-cell consists of donor and acceptor organic phases in an absorber blend, contacted to hole and electron transport layers, which is in development within the French ANR project ORGANIST. The modelling of the organic sub-cell is the main focus of this presentation, and is investigated with increasing levels model complexity. The modelling of the complete tandem is first described with a simple first approximation which only considers idealised classic drift-diffusion phenomena of inorganic semiconductors, with optical and band structure data from current best estimates of suitable non-fullerene high bandgap organic solar cell materials⁶. It is shown that this approach is sufficient to quantitatively predict tandem efficiencies with suitable approximations for optical and transport parameters. Figure 1b shows the resulting quantum efficiency of a preliminary 26% tandem without device optimisation, and with a non-textured Si IBC. Organic modelling is then developed from standard open access models⁷, by moving from the widespread effective medium approach treating the absorber blend as a homogeneous material, to a bulk heterojunction model where the acceptor and donor organic phases are simulated separately. We conclude with lessons learned on the comparative benefits of the modelling approaches for the design and development of high efficiency organic solar cells.

¹ James P. Connolly *et al.*, “Designing III-V multijunction cells on silicon”, Progress in Photovoltaics, Volume 22, Issue 7, July 2014, Pages 810-820, <https://dx.doi.org/10.1002/pip.2463>

² Y. Cui, Y. Xu, H. Yao, *et al.*, Single-Junction Organic Photovoltaic Cell with 19% Efficiency; Adv. Mater. (2021) 2102420; DOI: <https://dx.doi.org/10.1002/adma.202102420>

³ J.-P. Kleider, *et al.*, “Three-Terminal Tandem Solar Cells Combining Bottom Interdigitated Back Contact and Top Heterojunction Subcells: A New Architecture for High Power Conversion Efficiency”, 35th EU PVSEC, 4 to 28 September 2018, Brussels, <https://doi.org/10.4229/35thEUPVSEC20182018-1AO.2.4>

⁴ Hiroyuki Kanda *et al.*, “Three-terminal perovskite/integrated back contact silicon tandem solar cells under low light intensity conditions”, Interdisciplinary Materials. 2022;1:148–156, <https://doi.org/10.1002/idm2.12006>

⁵ J.P. Connolly *et al.*, “A new design : three terminal band offset barrier organic/si tandem solar cells”, 40th EU PVSEC, 17 - 22 September 2023, <https://dx.doi.org/10.4229/EUPVSEC2023/2CV.2.25>

⁶ Robin Kerremans *et al.*, “The Optical Constants of Solution-Processed Semiconductors—New Challenges with Perovskites and Non-Fullerene Acceptors”, Adv. Optical Mater. 2020, 8, 2000319, <https://doi.org/10.1002/adom.202000319>

⁷ L. J. A. Koster, *et al.*, “Device model for the operation of polymer/fullerene bulk heterojunction solar cells”, Phys. Rev. B 72, 085205, <https://dx.doi.org/10.1103/PhysRevB.72.085205>

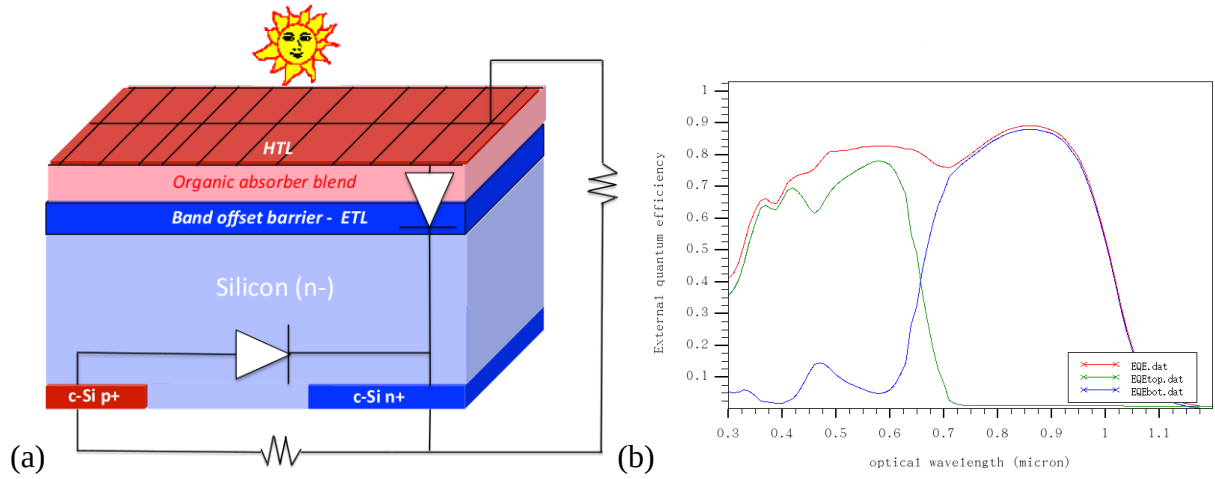


Fig. 11 (a) Schematic of the three terminal band offset barrier tandem here in the organic on silicon embodiment **(b)** external quantum efficiency of the 26% efficiency tandem resulting from independent organic cell efficiency of 15.2% AM1.5 for a effective gap of 1.8eV, and untextured Si IBC efficiency 10.8% under AM1.5G.

Multi-scale modeling of 3-Terminal Perovskite/Silicon Tandems

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Perovskite/silicon (PVS) tandem solar cells have surpassed 30% efficiency, highlighting their potential to significantly boost the terrestrial PV market¹. Two-Terminal (2T) architectures are the most studied solutions due to the simple monolithic device integration and module interconnection, but suffer from matching current constraint under real operating conditions². On the other hand, 3T tandems, while maintaining a monolithic structure, are more resistant to power loss due to shading² and offer the opportunity to exploit perovskites with energy gaps that do not match those of silicon, which is attractive with a view to achieving both high power and stability.

In this work, we study PVS 3T-tandems with a transistor-like structure compatible with silicon cells with both sides contacted instead of the more complex interdigitated back-contact ones. In this architecture the third terminal is realized at the interface between the perovskite and silicon sub-cells and accessed through a top interdigitated contact (Fig.1a). Therefore, design optimization requires a multi-scale modeling approach to minimize: (i) electrical and optical loss of the tandem stack; (ii) shadow and resistive losses caused by the metal grids, which are particularly important in view of realizing large area devices.

To this aim, we have developed a model hierarchy that combines physics-based simulations of the quasi-1D tandem stack,³ with equivalent circuit simulations (see Fig.1) of the 3D large area device. The quasi-1D device is studied by means of drift-diffusion simulations, with photogeneration profile obtained by Monte Carlo ray tracing and transfer matrix method. From the calculated current-voltage characteristics one extracts the tandem equivalent circuit model in Fig. 2(d), that is instrumental to study parasitic losses in large area devices⁴.

¹ Wagner, Lukas, et al. "The resource demands of multi-terawatt-scale perovskite tandem photovoltaics." *Joule* 8.4 (2024): 1142-1160

² Kikelj, Miha, et al. "Do all good things really come in threes? The true potential of 3-terminal perovskite-silicon tandem solar cell strings." *Joule* (2024).

³ Giliberti, Gemma, and Federica Cappelluti. "Physical simulation of perovskite/silicon three-terminal tandems based on bipolar transistor structure." *Physics, Simulation, and Photonic Engineering of Photovoltaic Devices XI*. Vol. 11996. SPIE, 2022.

⁴ Alonso-Álvarez, D., et al. "Solcore: a multi-scale, Python-based library for modelling solar cells and semiconductor materials." *Journal of Computational Electronics* 17 (2018): 1099-1123.

Devices currently under study include tandems based on Formamidinium (FA)-perovskites with iodide (HBT-I, $E_g = 1.5$ eV) and bromide halide (HBT-Br, $E_g = 2.3$ eV) fabricated on a textured heterojunction (HIT) silicon sub-cell. Their EQE is shown in Fig.2(a)-(b). The tandems provide from 8% (high-gap HBT-Br) to 10% (low-gap HBT-I) efficiency gain with respect to the HIT silicon cell, surpassing the Shockley-Queisser efficiency of their 2T counterpart. By exploiting an optimized layout⁵ for the top metal grids and low sheet resistance ($< 300 \Omega/\text{sq}$) transport layers, the gain is reduced by only 3% for devices with area up to $10 \text{ cm} \times 10 \text{ cm}$.

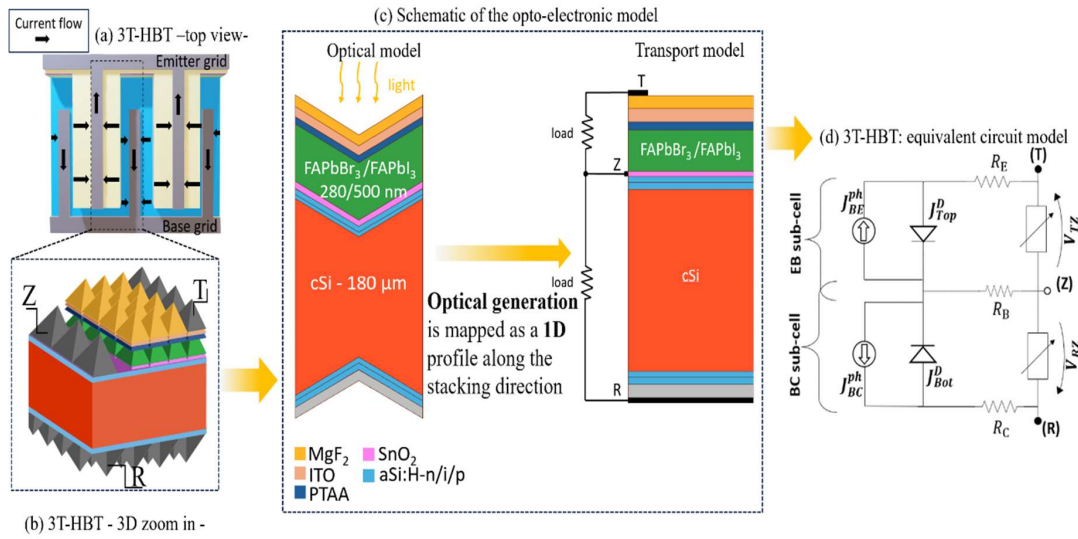


Figure 2 (a) TIC layout of the 3T-HBT: top view (b) 3D view of the fully textured PVS 3T-HBT (c) Schematic description of the opto-electronic model (d) Equivalent circuit of the 3T-HBT tandem. Emitter, base, collector contacts are named T, Z and R, respectively.

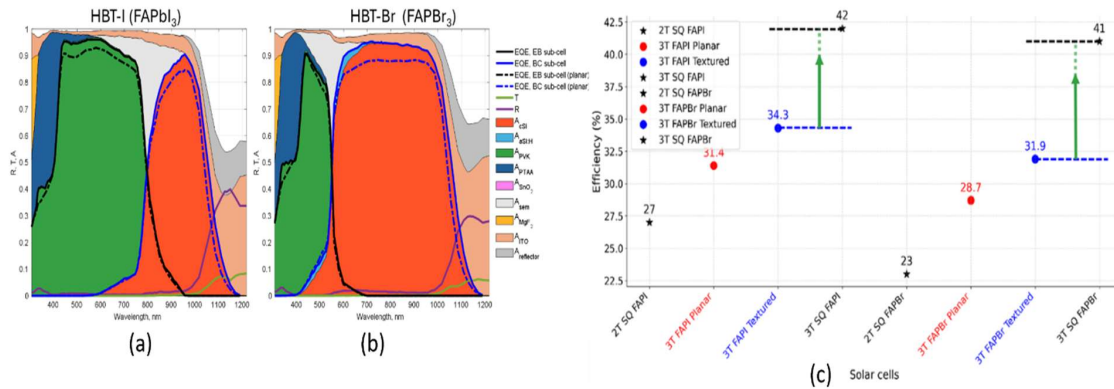


Figure 2 Absorbance, reflectance, and transmittance spectra of textured HBT-I (a) and HBT-Br (b), and corresponding EQE of the two sub-cells (blue and black solid lines). For reference, the EQE of a planar device is also shown (dashed lines). (c) Summary of the power conversion efficiency for the tandem devices under study compared to the Shockley-Queisser limit for 2T and 3T configurations.

⁵ Giliberti, Gemma, Matteo Cagnoni, and Federica Cappelluti. "Monolithic 3-terminal perovskite/silicon HBT-based tandem compatible with both-side contact silicon cells: a theoretical study." EPJ Photovoltaics 14 (2023): 37.

Probing ionic conductivity and electric field screening in perovskite solar cells: A novel exploration through ion drift currents

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It is widely accepted that mobile ions are responsible for the slow electronic responses observed in metal halide perovskite-based optoelectronic devices, and strongly influence long-term operational stability¹. Electrical characterisation methods mostly observe complex indirect effects of ions on bulk/interface recombination, struggle to quantify the ion density and mobility, and are typically not able to fully quantify the influence of the ions upon the bulk and interfacial electric fields. We analyse the bias-assisted charge extraction (BACE) method for the case of a screened bulk electric field, and introduce a new characterisation method based on BACE, termed ion drift BACE. We reveal that the initial current density and current decay dynamics depend on the ion conductivity, which is the product of ion density and mobility. This means that for an unknown high ion density, typical in perovskite solar absorber layers, the mobility cannot be directly obtained from BACE measurements. We derive an analytical model, to illustrate the relation between current density, conductivity and bulk field screening, supported by drift-diffusion simulations. By measuring the ion density independently with impedance spectroscopy, we show how the ion mobility can be derived from the BACE ion conductivity. We highlight important differences between the low- and high-ion density cases, which reveal whether the bulk electric field is fully screened or not. Our work clarifies the complex ion-related processes occurring within perovskite solar cells and gives new insight into the operational principles of halide perovskite devices as mixed ionic-electronic conductors.

¹ J. Thiesbrummel, et al., “Ion-induced field screening as a dominant factor in perovskite solar cell operational stability”, Nat Energy, (2024)

The Hallmark of Ion Migration in Perovskite Solar Cells by Impedance Spectroscopy Measurements and Simulations

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Ion migration lies at the heart of perovskite solar cell (PSC) performance and stability. Different experimental techniques have been used to better understand the puzzling performance of ion migration in PSCs. In this work, we focus on the characterization of ion migration by impedance spectroscopy (IS) measurements interpreted by drift-diffusion simulations¹. We present the results of numerical drift-diffusion simulations¹ in relation to the study case of NiOx-based PSCs with various interface passivation treatments². Our simulations approach several experimental measurements of IS under short-circuit conditions at different illumination intensities, along with bias-stress accelerated operational stability tests under constant illumination. Drift-diffusion simulations suggest that interface modification with the hole transport material may reduce electron mobility within the NiOx layer and ion mobility within the perovskite layer. Notably, capacitance and resistance exhibit maximum and minimum values, respectively, within specific ranges of mobile ion concentration. Our findings provide a systematic approach for characterizing instability mechanisms in PSCs using IS under short-circuit conditions. Lastly, we analyze the effect of ion migration in PSCs using IS under open-circuit condition by experimental measurements and drift-diffusion simulations. We present the challenges to interpret IS measured under open-circuit voltages since the device is close to flat-band condition and different mechanisms are competing at similar time scales.

¹ O. Almora, P. López-Varo, R. Escalante, J. Mohanraj, Ll. F. Marsal, S. Olthof, J. A. Anta, "Instability Analysis of Perovskite Solar Cells via Short-Circuit Impedance Spectroscopy: A case study on NiOx passivation", <https://doi.org/10.48550/arXiv.2402.00439>

² J. Mohanraj, B. Samanta, O. Almora, R. Escalante, Ll. Marsal, S. Jenatsch, A. Gadola, B. Ruhstaller, J. Anta, M. C. Toroker, S. Olthof, "NiOx Passivation in Perovskite Solar Cells: From Surface Reactivity to Device Performance", <https://doi.org/10.48550/arXiv.2402.10286>

Illuminating The Dark Side Of Triplet State And Its Role On VOC In PM6:o-IDTBR Solar Cells

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The top-performing organic solar cells (OSCs) currently achieve similar peak external quantum efficiencies and fill factors as traditional photovoltaic devices. Nevertheless, they experience significantly elevated voltage losses, primarily stemming from nonradiative recombination, imposing a significant constraint on their performance. To explore the potential influence of triplet states within the donor or acceptor materials on this phenomenon, we investigate the PM6 and o-IDTBR system. While we suspect that the open-circuit voltage (VOC) is constrained by the energy of the triplet state, the measured non-radiative voltage loss is surprisingly minimal. This study delves into a crucial aspect of OSC design: effectively managing the population of triplet excitons generated after non-geminate charge recombination. By comparing as-prepared and thermally annealed blends, we demonstrate that triplet-triplet annihilation may potentially offset the detrimental effects of triplet-induced dark losses.

Design of a Simple Bifunctional System as a Self-Assembled Monolayer (SAM) for Inverted Tin-Based Perovskite Solar Cells

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In this work, we functionalized the ITO substrates with a series of self-assembled monolayer (SAM) molecules to improve the hole extraction ability of the electrodes and retard the charge recombination with the devices in an inverted planar p-i-n configuration. Organic molecules with simple structures, namely 4-aminobenzoic acid (AB), 4-(2-aminomethyl)benzoic acid (AM), 4-(2-aminoethyl)benzoic acid (AE), and 4-nitrobenzoic acid (NB) were chosen to functionalize the ITO substrates via simple immersion method to form hole-selective SAM on ITO¹.

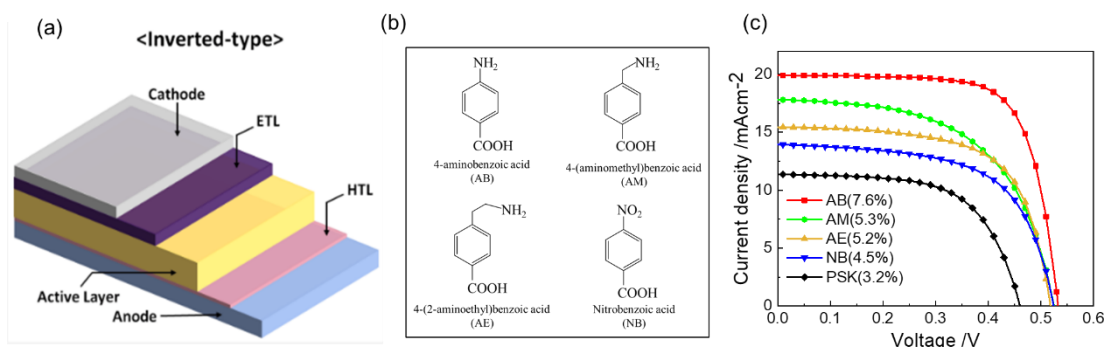


Fig. 1 (a) Inverted architecture of device (b) Chemical structures of SAM molecules (c) JV characteristics.

The TPSCs were fabricated according to a two-step sequential deposition approach using a co-solvent system², and the AB device was found to exhibit an attractive efficiency of power conversion (PCE) of 7.6 % while the other SAMbased devices showed poorer performance. The AB device also displayed impressive long-term storage stability by maintaining about 80 % of its initial efficiency for over 3500 h without encapsulation, in addition to a longterm (6 h) light-soaking stability, which is superior to the PEDOT: PSS-based device in ambient conditions. The SAM/perovskite interfacial characteristics were studied using UPS, EIS, and TCSPC to understand the energy levels, charge recombination, and hole-extraction nature, respectively, and to support the outstanding performance and stability of the AB device.

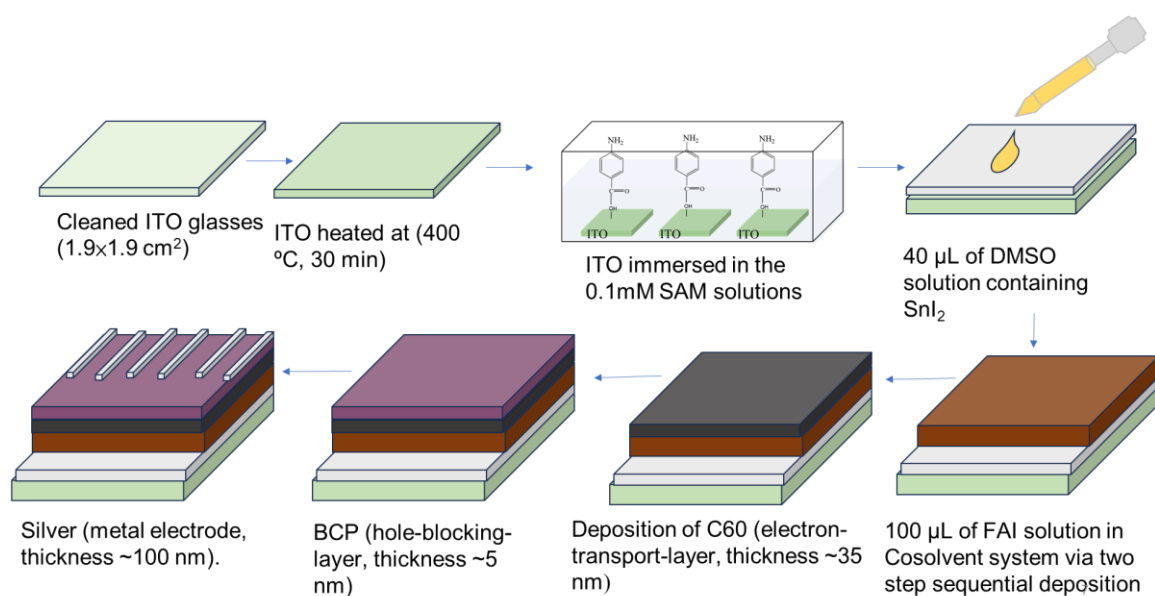


Fig. 2 The TPSCs were fabricated according to a two-step sequential deposition approach using a co-solvent system.

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² S. Shahbazi, M.Y. Li, A. Fathi, and E.W.G. Diau, "Realizing a Cosolvent System for Stable Tin-Based Perovskite Solar Cells Using a Two-Step Deposition Approach," *ACS Energy Lett.* **5**(8), 2508–2511 (2020).

Improve Vacuum-Deposited Formamidinium-Based Perovskite Solar Cells by Device Modelling

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Perovskite solar cells have captured significant attention owing to their exceptional power conversion efficiencies. Recently, formamidinium-based perovskites are of greater interest than their methylammonium counterparts because of their better thermal stability and smaller band gap.

We demonstrate how the dominant recombination losses in vacuum-deposited formamidinium-based perovskite solar cells can be determined. The morphology of these perovskite films can be varied by varying the processing conditions. Consequently, notable variations emerge in the solar cell performance parameters.

The role played by mobile ions, bulk and interface traps as well as other factors such as charge carrier mobility, and illumination intensity are investigated with our drift-diffusion modelling tool SIMsalabim¹. The device parameters that primarily contribute to recombination losses are found to be electron mobility, bulk and interface traps. Similarly, ion mobility is found to have the most influence on the hysteresis.

Ultimately, this approach enables us to characterize the material parameters of the measured solar cells and propose strategies for enhancing their overall performance.

¹ M. Koopmans, V.M. Le Corre, and L.J.A. Koster, "SIMsalabim: An open-source drift-diffusion simulator for semiconductor devices", J. Open Source Softw. 7, 3727, (2022)

Correlation of Defect Densities and Carrier Lifetimes in Perovskite Solar Cells

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Perovskite solar cells have a high efficiency despite a high number of electronic defects in the perovskite.¹ The defect density N_d can be obtained by drive-level capacitance profiling (DLCP). The inherent assumption for this method to work is that the measured capacitance is dominated by the capacitance of the space charge region, which depends on the defect density for an intrinsic semiconductor. Previous work has shown that the geometric capacitance of the contacts should also be considered, because it can dominate the measured capacitance². This leads to a resolution limit of the DLCP method for small thicknesses and low defect densities, as shown in figure 1.

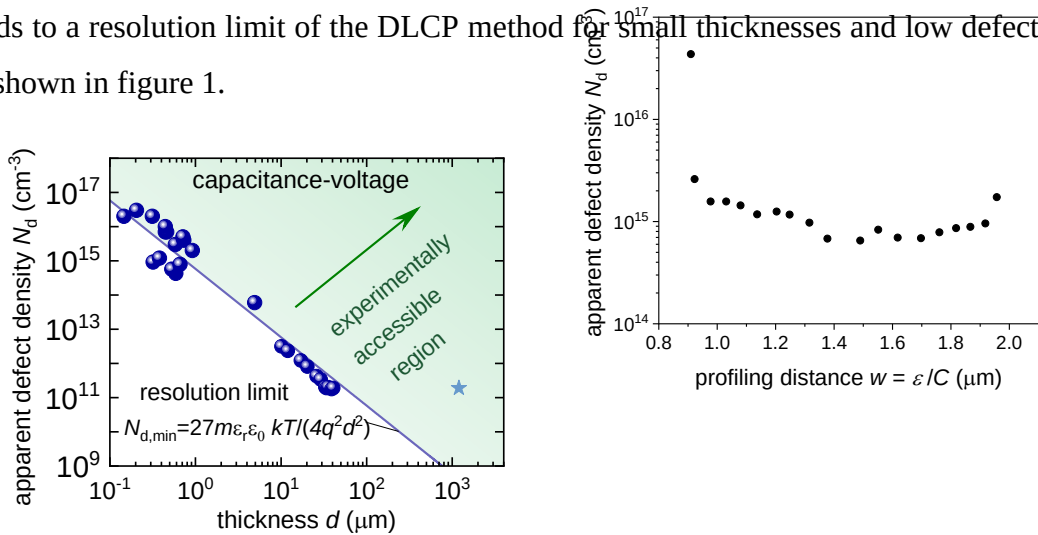


Fig. 1 (a) Reported values for defect densities for PSC¹ with the derived resolution limit².
(b) Measured defect densities of a 25 μm perovskite single crystal.

In our project we could achieve measurements of the defects densities in the experimentally accessible region by using single crystal devices with a thickness of 25-50 μm, like shown in figure 1b. Further, we can obtain information about the lifetime of the charge carriers in the single crystals from transient photoluminescence measurements. The correlation of the measured defect densities with the efficiency of the device and lifetime of charge carriers combined with drift-diffusion simulations of the devices with SETFOS help us to better understand the influence of the defects on the solar cell performance.

¹ Z. Ni et al. "Resolving spatial and energetic distributions of trap states in metal halide perovskites", *Science* 367, 1352-1358 (2020)

² S. Ravishankar et al., *Science* 10.1126/science.abd8014 (2021).

Solar cell Thickness and Photon Recycling: A Simulation Study

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We present a comprehensive, self-consistent model designed to simulate the photon recycling effects observed in solar cells. This model integrates the drift-diffusion (DD) framework for charge transport with a Transfer-Matrix Method (TMM) to account for the optical effects. This model uses TMM with external source and internal source for modelling sun irradiance and internal radiation in solar cells, respectively. Radiative recombination will be simulated by dipole model as described by Cho¹. By considering both internal and external light sources, this approach allows for an accurate evaluation of the impact of photon recycling on the overall efficiency of the solar cell. As shown in Fig.1, the process begins with solving TMM with only the external source; the generation rate will be calculated and provided as an input to the DD model. In the next iterations, TMM for internal source will be also solved using radiative recombination profile from DD module. The loop will continue until the results converge. The entire model has been implemented in TiberCAD². The proposed model facilitates a detailed examination of internal emissions from the solar cell, intricately coupled with the charge transport mechanisms. This integration ensures that the interplay between optical and electrical processes is thoroughly captured, providing deeper insights into the fundamental workings of solar cells. Our model has been successfully applied to a perovskite solar cell, demonstrating its capability in accurately predicting variations in open-circuit voltage (VOC) and power conversion efficiency (PCE) with respect to the active layer thickness. The results in Fig.2 highlight the critical role of photon recycling in enhancing PCE, particularly for thicker active layers, where increased photon re-absorption significantly boosts performance metrics. This underscores the importance of including photon recycling effects in the design and optimization of high-efficiency perovskite solar cells.

Acknowledgments: This work has received funding from the European Union's Horizon Europe research and innovation program under grant agreement No 101084422 "SUNREY". A. Di Carlo gratefully acknowledges the support of the Horizon Europe Project SOLMATES (No. 101122288).

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² <http://www.tibercad.org/>

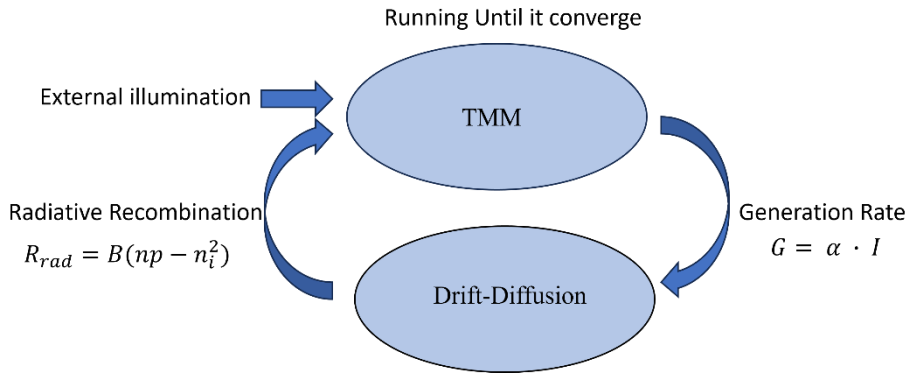


Fig. 1 Self-consistent simulation of the photon recycling in solar cells using TMM and DD models.

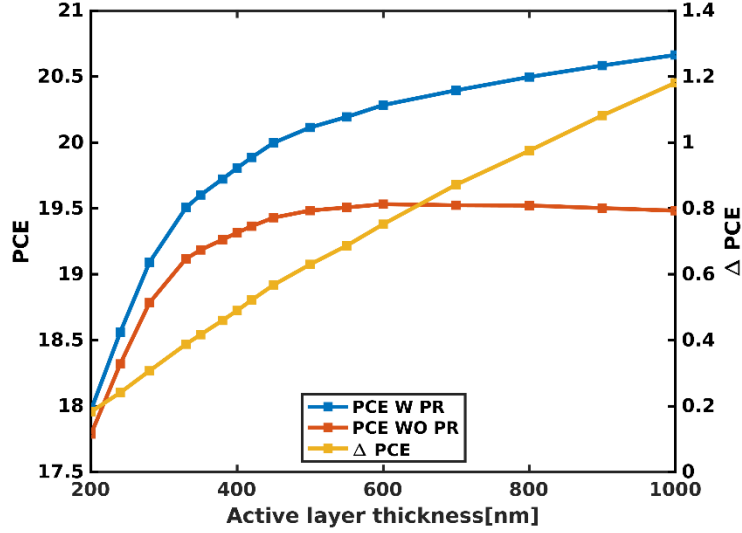


Fig. 2 PCE vs active layer thickness for two models, with and without photon recycling effects corresponding to SRH limit.

On the role of the photo physics of $\text{Cs}_2\text{AgBiBr}_6$ double perovskites on solar cell performance – A temperature-dependent study of Urbach energy and luminescence

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All inorganic $\text{Cs}_2\text{AgBiBr}_6$ perovskite is one of the alternatives to poorly stable organic/inorganic perovskites. However, due to its high bandgap, the photocurrent remains limited. Therefore, most research on solar cells focused on modifying the material to shift the absorption onset towards the red^{1,2}. In parallel, various studies on the photophysics have been conducted to understand the origins of the absorption and the photoluminescence^{3–5}. These studies aimed to find reasons for performance limiting factors in solar cells, amongst them high defect densities causing non-radiative recombination, ultra-fast transition to self-trapped excitons hampering charge transport, high exciton binding energies, and low electron diffusion lengths. However, in-depth studies directly on solar cells are rare. In this study, we investigate the temperature-dependent optoelectronic response of the full solar cell. We determine the Urbach energy, discuss the evolution of the PL as a function of applied voltage, which can be described by three peaks, deduce information regarding the bandgap from the V_{oc} , and determine the dielectric constant from capacitance measurements.

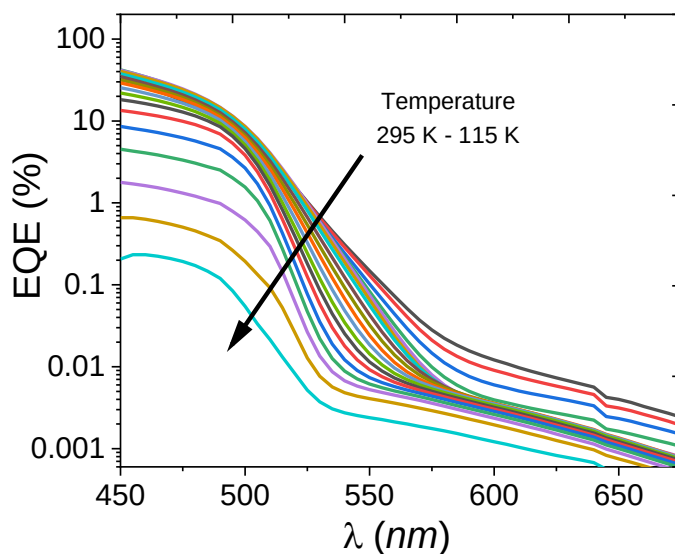


Fig. 1 Temperature dependent EQE of the $\text{Cs}_2\text{AgBiBr}_6$ double perovskites versus energy.

Fig. 1 shows the EQE of the $\text{Cs}_2\text{AgBiBr}_6$ solar cell devices as a function of temperature. We infer that the main absorption happens below 500 nm and identify an exponentially decreasing IPCE up to 530 or 570 nm dependent on the temperature. Assuming that $\text{Cs}_2\text{AgBiBr}_6$ can be described as a semiconductor with a defined band gap, such exponentially decreasing signal is characteristic of sub-gap states. This means the band gap would be around 500 nm and the tail would originate from disorder and could be described by Urbach theory. We showed that the deduced Urbach energy values are strongly temperature dependent and reduce from 55 meV to 25 meV.

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Ion Migration and Its Impact on Recombination in Perovskite Solar Cells

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Perovskite solar cells (PSCs) have shown great promise to enter the photovoltaic market, thanks to the outstanding performance of metal halide perovskite materials as the light absorber in thin film solar cell stacks, their simple solution-processing and low-cost fabrication process. To further optimize the power conversion efficiency (PCE), stability, and reliability of PSCs, detailed characterization and understanding of performance losses over time is required. This includes examining the recombination pathways of photogenerated charge carriers, which can suppose a major limiting factor for achieving (and maintaining) the highest possible PCE.

Solution-processed perovskite semiconductors show mixed ionic-electronic conductivity and an intrinsically high density of defects. The redistribution of mobile ionic defects can significantly affect device performance in multiple timescales. In this work, the effect of ionic redistribution on charge collection and recombination properties is explored through an approach combining experimental data and drift-diffusion simulations. The simulations are carried out including mobile ionic charges and comparing the effect of their redistribution under different competing non-radiative recombination mechanisms; either recombination at the interfaces with the charge transport layers (CTLs), or via traps in the bulk perovskite. Different device architectures are compared, highlighting the importance of the choice of CTLs to achieve a high and stable radiative yield.

Assessing the Influence of Illumination on Ion Conductivity in Perovskite Solar Cells

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Electrochemical impedance spectroscopy measurements of perovskite solar cells (PSCs) show characteristic features at low frequencies, such as a large illumination-dependent capacitance^{1,2}. While this effect is well known, the debate on its origin persists^{3,4,5}. An illumination-dependent increase in the conductivity of ionic charge carriers was suggested early on². However, experiments to elucidate the presence of such a photo-conductive effect require special devices or measurement techniques² and are not beyond all doubt^{3,4}. Thus, only a few studies investigated this effect in detail.

Using drift-diffusion simulations, we show how the illumination-dependent part of the capacitance originates from electron and hole charge carrier currents caused by the ions screening the alternating electric field⁶. This is inherently caused by the mixed electronic-ionic interaction as the simulation results in Figure 1 (a) demonstrate. Counter-intuitively, an illumination-dependent ion conductivity even reduces the magnitude of the capacitance increase as shown in Figure 1 (b).

¹ E.J. Juarez-Perez, R.S. Sanchez, L. Badia, G. Garcia-Belmonte, Y.S. Kang, I. Mora-Sero, J. Bisquert, "Photoinduced Giant Dielectric Constant in Lead Halide Perovskite Solar Cells", J. Phys. Chem. Lett. 5, 13, 2390-2394 (2014)

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⁶ A. Schiller et al., *manuscript in preparation*

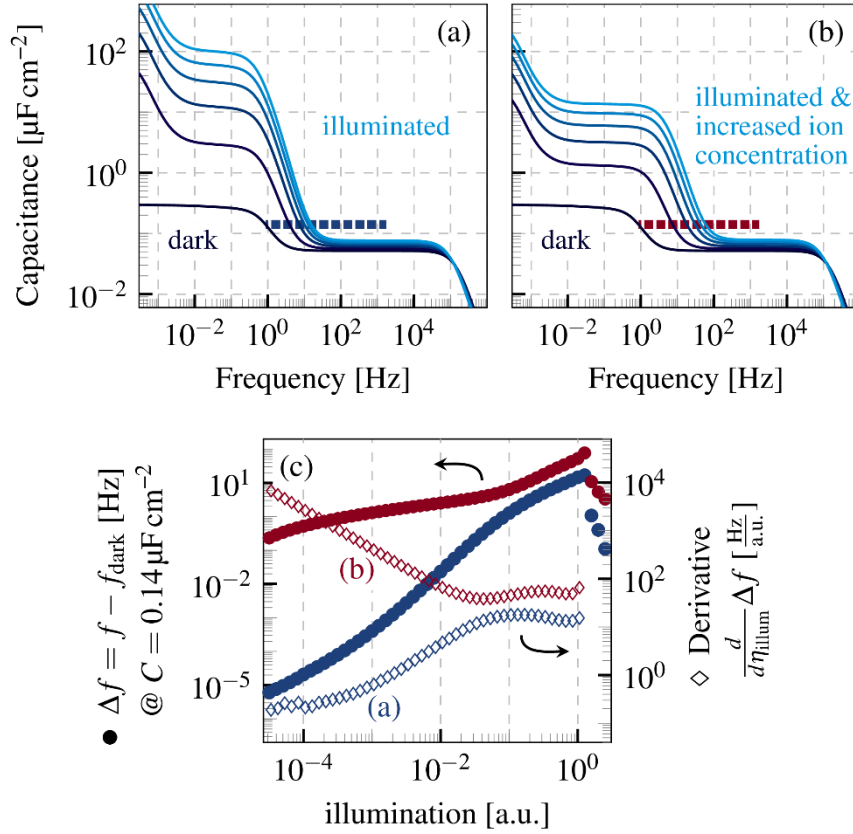


Fig. 1 Simulated capacitance results for (a) varying illumination intensity and (b) varying illumination intensity and ion concentration in parallel. (c) Frequency shift of the onset in capacitance and its derivative w.r.t. illumination for both cases.

As the presence and magnitude of a low-frequency capacitance increase by itself are unsuited to assess the presence of illumination-dependent ion conductivity, we propose a novel characterization technique based solely on capacitance measurements at short-circuit on fully integrated devices⁶. The frequency shift of the onset in capacitance is extracted at varying illumination intensity. As shown in Figure 1 (c), this quantity shows a distinct qualitative difference depending on whether the ion conductivity depends on illumination or is constant.

As these measurements can be performed on unaltered, fully integrated devices and with standard equipment, the method is well suited for widespread investigation of a photoconductive effect in different materials and devices or in response to degradation. We demonstrate the method's practicality by applying it to measurements of various PSCs.

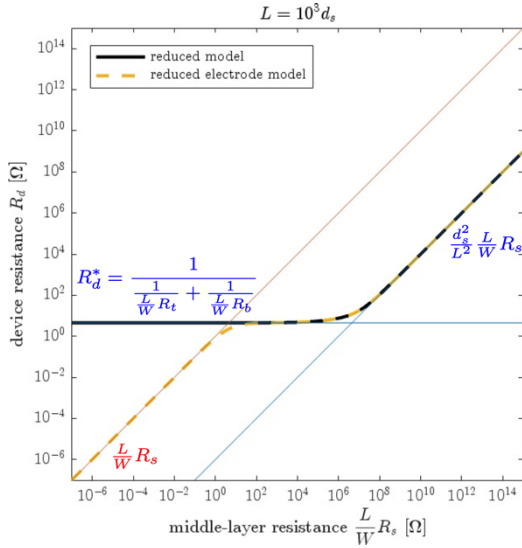
Simulation Study of a Model Reduction Approach for Large-Area Devices

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Winterthur, Switzerland

A thin-film device such as an organic solar cell or organic light-emitting diode typically consists of a stack of semiconducting layers sandwiched between two electrodes. In a large-area device, the sheet resistance of the electrodes has a significant influence on the device performance¹, as the contacting scheme implies both vertical and lateral current flow. Reduced mathematical models are often used for the numerical simulation of such devices, where two-dimensional domains are used for the electrodes together with a zero-dimensional coupling law for the semiconductor stack^{2,3}.

While such reduced mathematical models have the advantage of a much lower computational cost than a full three-dimensional device model⁴, their validity for large-area devices also needs to be investigated.



We present an electrical simulation study of a simple linear three-layer large-area device to illustrate the influence of model reduction on the calculated device characteristics. We find that the 2D-0D model-reduction approach fails in the case of a low middle-layer resistance (cf. Fig. 1), because then the electric current mainly flows laterally in the middle layer, which contradicts the assumption of vertical current flow.

Fig. 1 Influence of model reduction on calculated device resistance

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Multi-Scale Simulation of Reverse-Bias Breakdown in All-Perovskite Tandem Photovoltaic Modules under Partial Shading Conditions

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As single junction solar cell efficiencies of metal halide perovskites approach those of crystalline silicon, and as the stability of the perovskite absorbers increases, the focus of research shifts to the up-scaling from small-area lab cells to large area industrial modules and from single junction to tandem architectures. However, the perovskite films produced using commercially viable large-area deposition methods such as, e.g., slot-die or blade coating, do not show the same high quality in terms of uniformity and defect density as those produced by the standard spin-coating process used for the high-efficiency small-area cells. Also, the monolithic interconnection of the thin-film modules requires special considerations to prevent material damage in the case of partial shading that forces the affected cell into reverse bias. In fact, reverse-bias breakdown in perovskite solar cells is receiving increased attention due to the peculiar role of the mobile ions present in these materials, as the rearrangement of ions increases the strength of the field in the device region where reverse-bias breakdown occurs.

In our contribution, we study the reverse-bias breakdown in all-perovskite tandem solar cells and its impact on the photovoltaic characteristics of partially shaded monolithically interconnected large-area modules with a multi-scale simulation approach. Using the electrostatic potential and the quasi-Fermi levels of electrons under reverse-bias conditions (Fig. 1a) as obtained from a cell-level drift-diffusion simulation with the SETFOS tool that includes mobile ions, we perform a microscopic calculation of the tunneling breakdown current in top and bottom sub-cells by means of a quantum transport formalism (Fig. 1b). The divergence of the spectral current provides non-local generation rates for holes in the valence band and electrons in the conduction band, respectively, which are then fed back to SETFOS to obtain the cell-level current-voltage characteristics including the tunneling contribution. To account for the extreme sensitivity of tunneling to the local field, these JV curves are computed for a range of mobile ion concentrations (Fig. 1c) - resulting in a significant spread of reverse breakdown voltages (inset). The reverse-bias JV curves are subsequently used as local 1D coupling laws

connecting the 2D electrodes in a quasi-3D finite-element module simulation approach as implemented in the LAOSS tool. This provides the module characteristics under full consideration of spatial variation in active area quality (mobile ion concentration, defect density), resistive electrode losses, and module interconnection details. In the case of a fully shaded cell stripe, a spatially fluctuating density of mobile ions leads the appearance of local hot spots with massively increased current density (Fig. 1d).

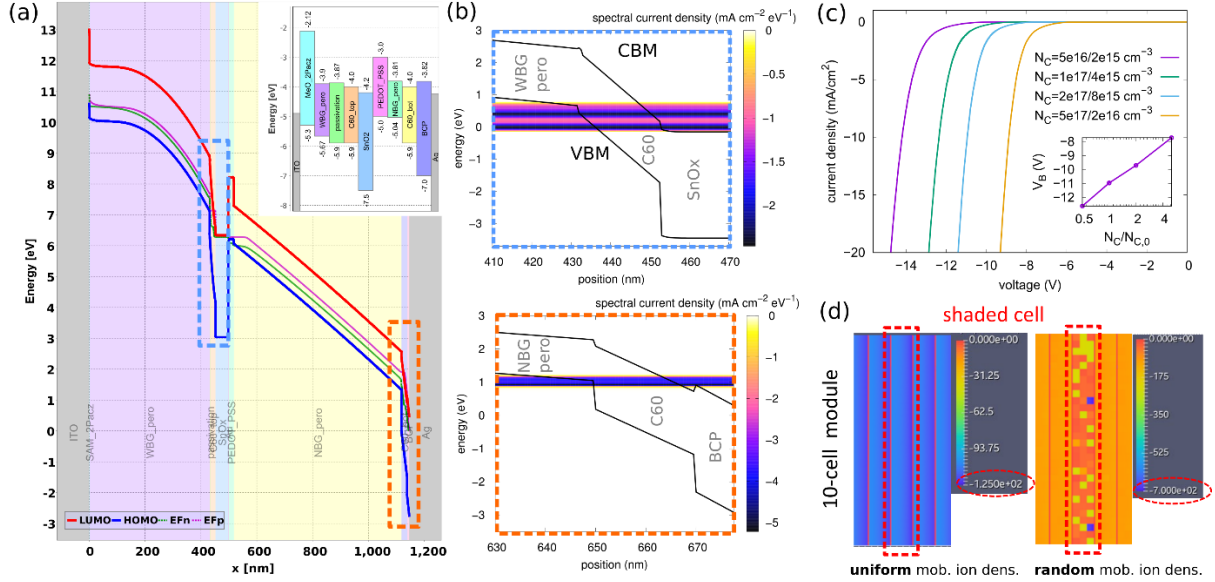


Fig. 1.: Simulation of reverse-bias breakdown characteristics in all-perovskite tandem solar cells & modules: (a) Band profile at reverse breakdown voltage of ~ -11 V. (b) Microscopic simulation of tunnel currents in the sub-cells at reverse-bias breakdown. (c) Dark reverse-bias breakdown characteristics for different concentration of mobile ions. (d) Impact of mobile ion concentration on the vertical current density maps in shaded cell stripes of an all-perovskite tandem module: uniform vs. random distribution with local current hot spots.

Phase-Field Simulations of Thermal Annealing For All-Small Molecule Organic Solar Cells

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For printed organic solar cells (OSC), the device performance depends on the bulk heterojunction (BHJ) nanomorphology, which forms during solution processing and additional post-treatment. In this work, the effect of thermal annealing (TA) on an all-small molecule DRCN5T:PC71BM blend is studied by means of phase field simulations¹. The objective is to identify the physical phenomena driving the evolution of the BHJ morphology for a better understanding of the posttreatment/morphology relationship. Simulation results are used to determine the impact of the DRCN5T crystallization-related mechanisms (nucleation, growth, crystal stability, impingement, grain boundary coarsening, and Ostwald ripening), of the amorphous-amorphous phase separation (AAPS), and diffusion limitations on the final BHJ morphology. A comparison between the simulations and the experimental data from the literature results in the following findings: the BHJ morphology evolution under TA is mainly due to dissolution of the smallest, unstable DRCN5T crystals and anisotropic growth of the largest crystals. Moreover, the morphology can be analyzed in terms of simple descriptors related to charge generation, transport and recombination². This provides insights into the relationship between BHJ morphology and solar cell properties. Such an approach will improve the understanding of the impact of such a posttreatment on the final device efficiency.

¹ Ronsin, Olivier J. J., and Jens Harting. 'Formation of Crystalline Bulk Heterojunctions in Organic Solar Cells: Insights from Phase-Field Simulations'. ACS Applied Materials & Interfaces 14, no. 44 (2022): 49785–49800. <https://doi.org/10.1021/acsami.2c14319>.

² Wodo, Olga, Srikanta Tiruthapara, Sumit Chaudhary, and Baskar Ganapathysubramanian. 'A Graph-Based Formulation for Computational Characterization of Bulk Heterojunction Morphology'. Organic Electronics 13, no. 6 (June 2012): 1105–13. <https://doi.org/10.1016/j.orgel.2012.03.007>.

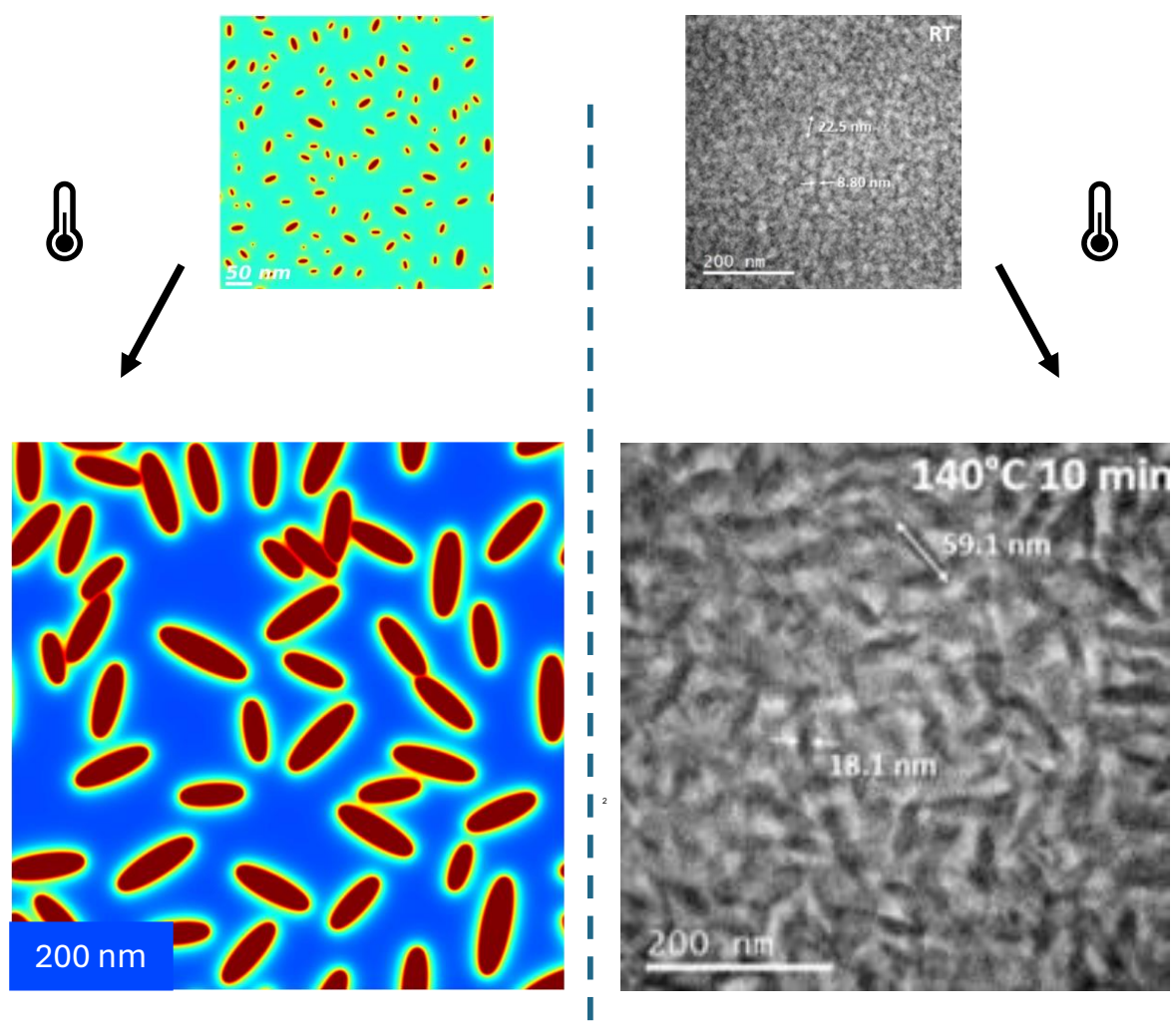


Fig. 1 Simulated (left) versus experimentally measured (right) morphologies of as cast (top) and thermally annealed (bottom) DRCN5T:PC71BM bulk heterojunction.

Indoor Standard Testing Conditions (ISTC) for Indoor Photovoltaic Device Testing

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Indoor photovoltaic (IPV) devices have the potential to power Internet of Things (IoT) applications, low power communications and indoor environmental sensing. Until recently, the lack of standardised indoor conditions for IPV device testing resulted in a lack of established independent measurements offered by test labs in this area, limiting IPV market penetration and integration. Indoor Standard Testing Conditions (ISTC) have now been defined in the recently published IEC TS 62607-7-2:2023. This will allow the measurements and evaluation of different technology IPV devices under the same ISTC conditions. The first reported system for performance measurements of IPV devices under ISTC conditions has been developed at NPL, compliant with IEC TS 62607-7-2:2023. We demonstrate the measurements and procedure to define the classification status (spectral coincidence, uniformity, stability) of the system based on IEC TS 62607-7-2:2023. We have initiated national and international intercomparison activities to investigate the challenges and practicality of the IEC TS 62607-7-2:2023 document and determine common issues and future improvements, with initial results and findings presented. This work will define the future standards and procedures in IPV device testing, supporting a new global industry and leading to sustainable solutions for powering IoT and low power sensing applications.

Distortion of parallel efficiency and stability measurements due to sample layout design

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As for efficiency, also estimating solar cell stability requires protocols to ensure results comparability. ISOS protocols provide a framework for documenting the stressing conditions (atmosphere, temperature, bias, light). However, the electrodes' layout and quality can falsify the measurement results.

Small-area samples are often based on substrates with pre-deposited transparent conducting electrodes (TCEs). It is popular that the TCE is shared with multiple solar cell devices deposited on the substrate. In this case, it becomes a common electrode. In some cases, the TCEs are not metalized.

A non-metalized common electrode presents two problems: a high contact resistance and reciprocal electrical influence among the devices sharing the common electrode.

We analyzed the deviation of the PV parameters caused by a common electrode with SPICE simulations. The measuring device is simulated with an ideal voltage source and a measurement resistor, which determines the current flowing through a single pixel. To understand the impact of the common electrode we considered two measuring methods, parallel and sequential. The first entails simultaneous application of the same ramped voltage to all pixels. The latter applies the voltage to one pixel at a time, while the others are at ground potential.

We simulated the JV of devices with increasing contact resistance and with a shunted neighboring device. The estimated maximum power point (MPP) from the JV curve is comparable to the one obtained from continuous MPP tracking, which is the most common stability measurement.

The contact resistance varied from 0.001 to 100Ω. A contact resistance of 1Ω is sufficient to introduce a significant error in the MPP estimation. If a neighboring pixel shunts, it increases the deviation and causes a Voc overestimation. Such deviations falsify any result obtained from stability tests and JV measurements.

Experimental measurements confirmed the conclusions from the simulations. We used a test PCB with a variable contact and shunt resistance to mimic the conditions studied with the simulations.

In conclusion, for reliable parallel stability testing, a common electrode should be avoided. Metallization of the electrode is necessary to minimize the contact resistance.

Identifying crucial device parameters in emerging photovoltaics: towards a digital twin

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Emerging photovoltaic materials such as organic photovoltaics (OPV) have seen a steep performance increase over the last years. Still, for commercialization significant challenges remain, namely reducing voltage losses and increasing operational stability. Discovering new structure-property relationships requires analysis of the detailed device physics, which usually entails slow, discontinuous investigations.

In this presentation, we show that combining high-throughput and knowledge-based approaches enables us to quickly infer hard to measure material properties, such as the interfacial disorder, the effective bandgap and the Langevin reduction factor, critical quantities limiting the electrical performance in OPV devices. On one hand, we use fast proxy experiments which can be trained on the fly to predict the outcome of slower high-fidelity experiments. This is possible because the fast proxy experiments (e.g. optical spectra) convey the essential information about microstructure and energetics needed to predict device performance. On the other hand, we model the outcome of different experimental probes by the same model and the same set of model parameters. We demonstrate an integrated, database driven optimization workflow for real-time parameter extraction from available evidence. In OPV devices of the state of the art blend PM6:Y12, the method gives insight into the relation between the Langevin reduction factor and the microstructure as function of the donor:acceptor mixing ratio. We outline our perspective on how the knowledge - and data driven worlds can be fully integrated to build a digital twin for PV material science, allowing to learn more from less and simpler experiments, and enabling a community driven approach towards overcoming the challenges of emerging PV materials.¹

¹ L. Lüer, I. M. Peters, A. Suncana Smith, E. Dorschky et al., "A digital twin to overcome long-time challenges in photovoltaics", *Joule* 8(2), 295-311 (2024)

The Quest for Interoperable Perovskite Solar Cell Data: Challenges and Opportunities

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The recent development of halide perovskite solar cells has been impressive, both in terms of increased performance and in the number of published papers. The sheer number of papers does, however, make it increasingly difficult to get a good overview of the field. It is also difficult to truly take advantage of all device data generated when it is inconsistently formatted and scattered over thousands of papers. During the last few years, I have been working with different strategies for how we can collect past, present, and future perovskite data in a way that make it useful beyond its appearance in initial publications. Among those efforts we find the Perovskite Database, which contain formatted device data for over 45000 perovskite devices, and a system for unambiguous communication of perovskite compositions. In this talk, I will demonstrate those initiatives as well as present a few stories showcasing insights enabled by this type of interoperable data.

Machine Learning for Surpassing Limits in Perovskite Solar Cells

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We show how Machine Learning (ML) methods can be used to predict the physical parameter that limits a perovskite solar-cell performance most significantly¹, based on the current-voltage (J-V) curve under one Sun illumination. The used data set is based on device simulation, where 20 different physical parameters, that are related to charge transport and recombination, are varied individually. The presented approach allows to cover a wide range of effects that possibly occur when fabrication conditions are varied, or during degradation of a device. Short circuit current density, open circuit voltage, maximum power conversion efficiency, and fill factor are sufficient as an input for a Random Forest to exceed 80% in prediction accuracies. To show the practical relevance of this work, The ML algorithms are applied to reported devices, and our results are analyzed from a physics perspective. It is discussed what conditions have to be met for satisfying performance, advantages and limitations of these models, and possible applications of the described workflow. It will also be shown how this approach can be improved, and what could be done in the future, in order to contribute to increase the efficiency of perovskite solar cells by guiding device fabrication and extraction of information from experiments.

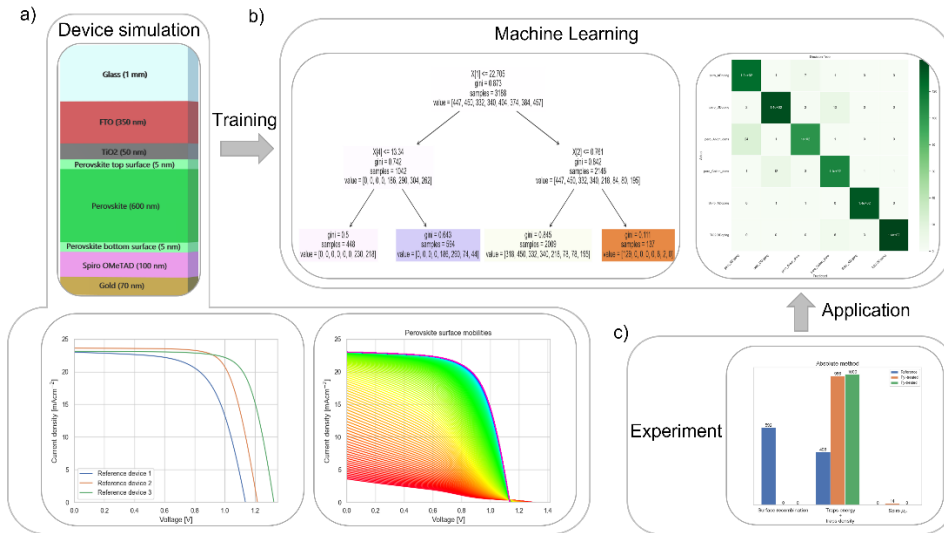


Fig. 1 Used framework to identify limiting parameters in perovskite solar cells.

¹ Zbinden, O., Knapp, E. and Tress, W. (2024), Identifying Performance Limiting Parameters in Perovskite Solar Cells Using Machine Learning. Sol. RRL, 8: 2300999.

Bayesian Inference of Organic Semiconductor Properties Using Temperature Dependent Photoluminescence Spectra.

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Extracting relevant material properties from experimental measurement is challenging, especially in the field of organic semiconductors. The models used to fit and reproduce experimental results are complex with multiple correlated parameters, which render the use of such model to extract relevant material properties very complicated. To overcome such limitations, we consider in this work the use of Bayesian inference for parameter estimation. Bayesian inference is a powerful tool to extract parameters distribution considering the experimental observations and the models considered [1].

In this study, we apply Bayesian inference techniques to analyze temperature-dependent photoluminescence spectra obtained from organic solar cells. We model the photoluminescence spectra of organic semiconductor films using a semi-classical marcus-levich-jortner expression [2, 3]. We model the spectra under different temperature and reproduce the change in spectral shape and relative intensity. Using the model and a Bayesian inference approach, we extract distributions for the different relevant properties of interest such as: Energy of the first excited state, the static disorder in energy, the reorganization energies (low and high frequency) as well as the dominant frequency mode. Our approach provides robust parameter estimation and quantifies uncertainties, enabling more accurate characterization of organic semiconductor materials. The results demonstrate the effectiveness of Bayesian inference in unraveling complex material properties and guiding future research in renewable energy applications.

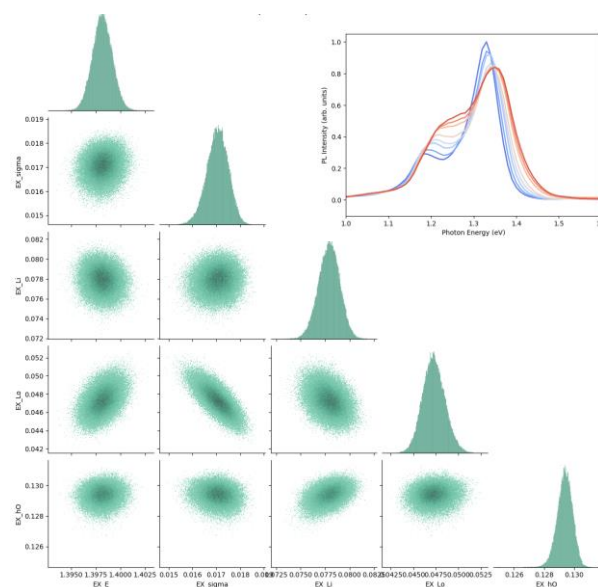


Figure 1 Pair plot distribution of the parameter of the model estimated using Bayesian inference, the inset shows the experimental results.

1. Todorović, M., et al., *Bayesian inference of atomistic structure in functional materials*. npj Computational Materials 2019 5:1, 2019-03-18. **5**(1).
2. Yan, J., et al., *Influence of static disorder of charge transfer state on voltage loss in organic photovoltaics*. Nat Commun, 2021. **12**(1): p. 3642.
3. Azzouzi, M., et al., *Nonradiative Energy Losses in Bulk-Heterojunction Organic Photovoltaics*. Phys. Rev. X, 2018. **8**: p. 031055.

Li ion battery from electrochemical characterization to advance modeling

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Li-ion batteries represent a complex system where degradation mechanisms are intricately linked. Understanding these degradation sources and their responses to various operating conditions requires extensive testing. Such testing typically involves long-term cycling under specific conditions designed to activate different degradation pathways. These mechanisms can be continuously monitored using Electrochemical Impedance Spectroscopy (EIS) throughout the battery's lifetime.

The experimental data gathered from these tests are crucial for parameterizing State of Health (SOH) models, which range from simple semi-empirical models like Open Sesame ([link](#)) to more complex variants.

Recently, a collaborative effort between SUPSI and BFH has been exploring a multiscale modeling framework. This innovative approach aims to derive parameters directly from molecular dynamics models through scaling laws that can capture the degradation effects at a nanoscopic level, under various operating conditions.

This coupling of experimental data with advanced modeling techniques is demonstrated using the open-source, physics-based model PyBaMM as both a benchmark and a modeling platform. The results of this approach are validated against experimental testing, highlighting the potential for improved accuracy and efficiency in predicting battery health and performance.

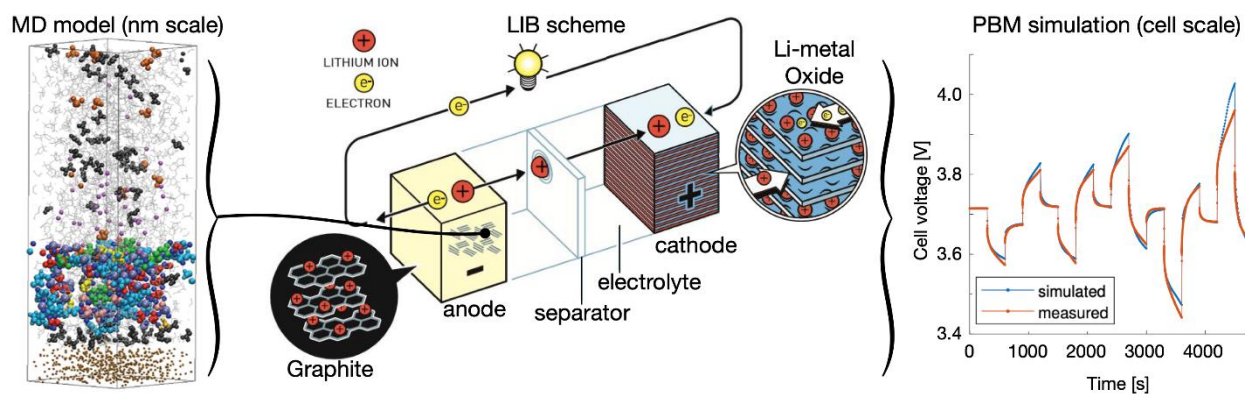


Fig. 1 LIB modeling - Center: scheme of a LIB (adapted from ¹) with graphite anode and Li-metal oxide cathode. Left: the interface between the anode and the electrolyte can be simulated at the nm scale via an MD model (adapted from ²). Right: the time operation of the LIB over its lifespan can be simulated at the cell-scale via a PBM (adapted from ³).

¹ The Nobel Prize in Chemistry 2019. NobelPrizeOrg n.d. <https://link.springer.com/article/10.1557/mrs.2020.81>

² Alzate-Vargas L, Blau SM, Spotte-Smith EWC, Allu S, Persson KA, Fattbert J-L. Insight into SEI Growth in Li-Ion Batteries using Molecular Dynamics and Accelerated Chemical Reactions. J Phys Chem C 2021;125:18588–96. <https://doi.org/10.1021/acs.jpcc.1c04149>.

³ Daniel Luder. Enhanced Physics-Based Models for State Estimation of Li-Ion Batteries. Bern University of Applied Sciences, 2020.

Study of diffusion in Li-ion electrodes by operando spectroscopic ellipsometry

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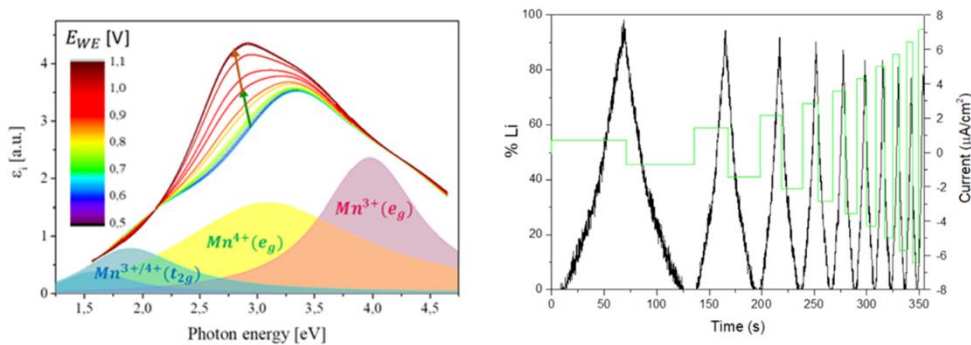
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Ionic diffusion and chemical reactions occurring during operation at the different interfaces of Li-ion batteries govern their overall performance of these devices. For this reason, efforts are devoted to developing non-destructive techniques capable to give information of these phenomena while they take place.

In this talk, we will show the implementation of spectroscopic ellipsometry to perform operando experiments on battery electrodes and interfaces taking advantage of its high spatial accuracy, fast response, and the strong effect of the Li content on the material's optical properties. Despite the well-known capabilities of spectroscopic ellipsometry to infer the properties of thin films, interfaces, and multilayers such as thickness, crystallinity, materials ratio in mixtures, electronic band structure etc., the use of this affordable, non-destructive technique for the study of ion-transport under operation is very limited.

We demonstrate the potential of SE to monitor Li^+ transport properties and degradation phenomena through real-time (sub-second) tracking of the oxidation-state and volume changes associated with lithium insertion and extraction along electrodes such as LiFePO_4 , LiMn_2O_4 and $\text{Li}_4\text{Ti}_5\text{O}_{12}$ ^{1,2,3}. Chambers were developed to perform the operando measurements that can host liquid electrolytes (e.g. LiSO_4 , LiPF_6).



Evolution of complex permittivity with the potential of the LiMn_2O_4 electrode (left). Determination of Li content in a $\text{Li}_x\text{Mn}_2\text{O}_4$ cathode submitted to increasing currents using spectroscopic ellipsometry (right).

1. A. Morata, V. Siller, F. Chiabrera, M. Nuñez, R. Trocoli, M. Stchakovsky and A. Tarancón, *J. Mater. Chem. A*, **8** (2020) 11538–11544.
2. J.C. Gonzalez-Rosillo, V. Siller, M. Nuñez, M. Stchakovsky, R. Arenal, A. Morata and A. Tarancón, *Materials Today Energy* **25** (2022) 100979
3. V. Siller, JC Gonzalez-Rosillo, MN Eroles, F Baiutti, M.O. Liedke, M. Butterling, A. G. Attallah, E. Hirschmann, A. Wagner, A. Morata, A. Tarancón, *ACS Applied Materials & Interfaces* **14** (2022) 33438-33446

Solution of multiscale physics-based models of Li-ion battery performance

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The Li-ion battery market is worth around \$60bn per annum and is growing rapidly. This is in large part because Li-ion batteries have high energy density, are relatively inexpensive and so are widely used in automotive applications in an effort to decarbonize the transport sector. Despite having reached a high level of technological readiness there is a constant drive toward new innovations driven by the necessity of improving performance, reducing costs and eliminating the requirement for rare and expensive materials (such as cobalt or nickel). This has led to the need for adaptable physics-based models that are capable of modelling Li-ion battery performance, that can be solved in real time and that can be adapted to new battery designs. From an engineering perspective the most useful such physics-based models are based on a framework¹ set out by John Newman and colleagues in the 1990's.

Li-ion cells are typically fabricated with a layered structure in which a porous spacer is sandwiched between a porous layer of anode particles and another of cathode particles (see

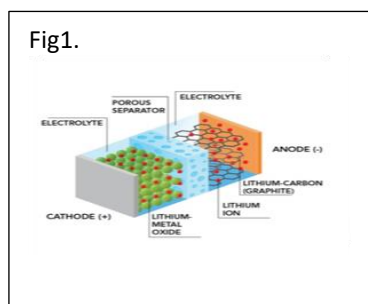


Fig.s 1 & 2). Furthermore, the pores throughout the layered structure are filled with a Li electrolyte which can transport Li-ions (and charge) between the two electrodes. In practice Li-ions in the anode particles have a greater chemical potential than Li-ions in the cathode particles, and thus (when the cell is charged) Li-ions in the anode undergo a de-intercalation reaction in which they move out of an anode particle into the surrounding electrolyte before migrating across the spacer and into the cathode where they undergo an intercalation reaction in which they insert themselves into a cathode particle.

The resulting charge transport, from anode to cathode, leads to a potential difference across the cell that can be used to drive an electric current through a circuit.

Fig2. A 2D schematic diagram of a Li-ion battery cell structure. It shows a central 'Spacer' (width ~150 μm) between an 'Anode' (left) and a 'Cathode' (right). The anode is represented by orange spheres and the cathode by green spheres. 'Li+' ions are shown moving from the anode through the spacer to the cathode. 'heat' is indicated at the interfaces. A coordinate system with 'x' and 'y' axes is shown at the bottom right. A current 'I(t)' is indicated on the left side.

The basic Newman model predicts the response of a thin planar single cell, with a three-layer structure (such as illustrated in Figs 1 & 2) and, in particular, it **models four key phenomena**: (i) Li-ion transport within electrode particles; (ii) (de-)intercalation reactions taking place on the surface of the electrode particles in which Li-ions move between the electrode particles and the surrounding electrolyte; (iii) Li-ion and charge transport in the electrolyte filling the porous cell; and (iv) charge transport in the solid portion of the electrode matrix (Ohm's Law). Even though the structure of the cell is planar the model is quasi two-dimensional since it not only describes Li-ion transport in the electrolyte across the cell but also within representative microscopic electrode particles and this makes its numerical solution fairly costly.

A single planar cell (as described above) is very thin (typically around 150 μm) and so in engineering applications it is usually either layered with other planar cells, to form a pouch

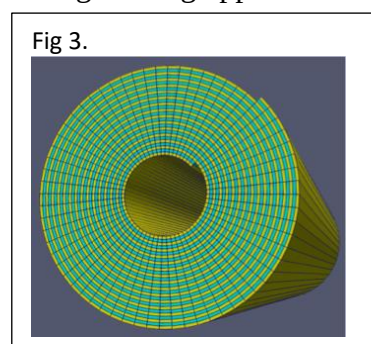


Fig 3.

cell, or wound around a central core to form a cylindrical cell (see Fig. 3). Since such *large format* cells often support significant thermal gradients, and the chemical processes occurring within a cell depend sensitively on temperature, models of these large cells are quasi 5-dimensional (in contrast to the quasi 2-dimensional models of a thin planar cell). Such high-dimensional

models are potentially extremely computationally expensive to solve accurately.

In this talk the Newman model (i.e. the standard physics-based model for Li-ion battery performance) is reviewed and its accurate and rapid numerical solution is briefly discussed². It is then shown that, a correctly parametrised model, can accurately predict real battery behaviour, even for an extremely complex discharge mimicking the current draw of a vehicle in an urban environment. In order to assess heat production in the cell a rigorous energy conservation law is derived from the Newman model³. This conservation law is used, in a quasi-5d Newman model representation of a pouch cell, to compute the heat produced as the pouch cell is discharged. Finally, we consider how Newman type models can be applied to large battery modules with integral cooling systems.

¹ M. Doyle, T. F. Fuller, & J. Newman, *J. Electrochem. Soc.*, **140**, 1526–1533, (1993).

² Korotkin, I., Sahu, S., O’Kane, S. E., Richardson, G., & Foster, J. M., *J. Electrochem. Soc.*, **168**, 060544 (2021).

³ Richardson, G. & Korotkin, I., *Electrochim. Acta*, **392**, 138909 (2021).

Mobile ions in halide perovskites: from drift-diffusion to equivalent circuit and defect chemical models

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Understanding the behavior of mobile ionic defects in halide perovskite-based devices exposed to light and/or voltage bias is an important question to advance the field of perovskite photovoltaics.^{1,2} Drift-diffusion simulations allow one to accurately define and solve the problem describing electronic charge carrier dynamics in these mixed conducting devices, including the role of mobile ions. Analysis of results, such as the time-domain and frequency-domain response of perovskite solar cells, can be complex, and the identification of the determining physical processes may require time-consuming parameter exploration. Progress in this direction relies on the development of appropriate models that can provide an accessible, yet accurate, interpretation of experimental and simulated results in terms of material properties. In practice, such models should be able to reproduce (i) the electrical response of devices based on mixed conducting materials, and (ii) trace such behavior back to the transport, storage and reaction of electronic and ionic charge carriers.

As a first step towards addressing questions (i) and (ii) above, an equivalent circuit modelling approach is presented. The model is general and can describe the small perturbation electrical response of devices based on mixed conductors under bias.³ The circuit combines the established transmission line approach, implementing the transport and storage of charge carriers,⁴ with resistive and transistor elements describing electron-hole recombination (Figure 1). The result is a network extending the concept of ionic-to-electronic current amplification in mixed conducting devices under bias.⁵

¹ D. Moia, J. Maier, Ion Transport, Defect Chemistry, and the Device Physics of Hybrid Perovskite Solar Cells, *ACS Energy Lett.* 6 (2021) 1566–1576.

² T.Y. Yang, G. Gregori, N. Pellet, M. Grätzel, J. Maier, The Significance of Ion Conduction in a Hybrid Organic-Inorganic Lead-Iodide-Based Perovskite Photosensitizer, *Angew. Chemie - Int. Ed.* 54 (2015) 7905–7910.

³ D. Moia, arXiv:2405.10477 [physics.app-ph] (2024)

⁴ J. Jamnik, J. Maier, Generalised equivalent circuits for mass and charge transport: chemical capacitance and its implications, *Phys. Chem. Chem. Phys.* 3 (2001) 1668–1678. <https://doi.org/10.1039/b100180i>.

⁵ D. Moia, I. Gelmetti, M. Stringer, O. Game, D. Lidzey, E. Palomares, P. Calado, J. Nelson, W. Fisher, P.R.F. Barnes, Ionic-to-electronic current amplification in hybrid perovskite solar cells: ionically gated transistor- interface circuit model explains hysteresis and impedance of mixed conducting devices, *Energy Environ. Sci.* 12 (2019) 1296–1308.

The presented approach ensures analytical correspondence with the linearized Nernst-Planck-Poisson model, which is tested here using drift-diffusion simulations of perovskite solar cells. The analysis of calculated impedance spectra based on the proposed model allows the clarification of several anomalous experimental observations, including inductive behavior and multiple low frequency features reported for perovskite solar cells.⁶

More complex interactions between electronic and ionic defects under non-equilibrium conditions imply that ions influence device response beyond considerations related with electrostatics. To explore this question, we focus on aspects relevant to the quasi-equilibrium of photoactive mixed conductors under light, in terms of their defect behavior. By combining defect chemical models of hybrid perovskites^{7,8} with the relevant description of their optoelectronic properties, the effect of light on the steady-state defect concentrations is investigated, including a systematic analysis of the key kinetic parameters in the model. The results highlight guidelines for the design of materials used in solar cells. More in general, they point towards the potential of controlling the defect chemistry of active materials (e.g. via control of component partial pressures) to optimize the performance of solar energy conversion devices.

Finally, an outlook on how drift-diffusion simulations, as well as equivalent circuit and defect chemical models can help the understanding of more complex perovskite solar cell structures, such as mesoscopic and tandem devices, is presented.

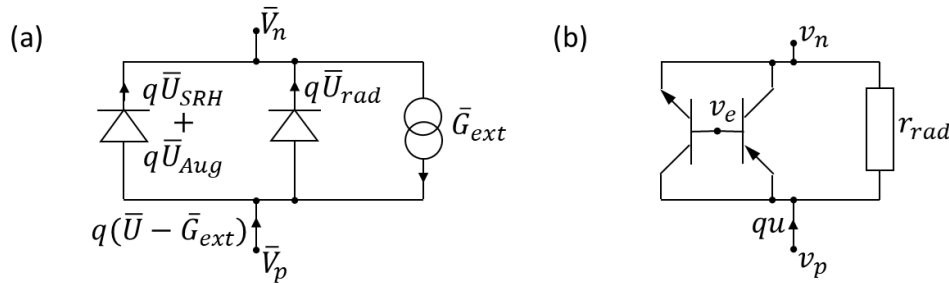


Fig. 1 (a) Equivalent circuit model of local net recombination U in a semiconductor using two diodes for the different recombination processes (rad: radiative, SRH: Shockley-Read-Hall, Aug: Auger). **(b)** Proposed model describing the small perturbation regime of the local net recombination u . Besides the small signal quasi-Fermi levels of electrons and holes (v_n and v_p) local changes in electrostatic potential (v_e) affect the small signal Shockley-Read-Hall and Auger rates. In the large perturbation model (a), such dependence is encapsulated in the ideality factor of the diode. In the figure, q is the elementary charge and G_{ext} the generation rate due to external illumination.

⁶ H. Wang, A. Guerrero, A. Bou, A.M. Al-Mayouf, J. Bisquert, Kinetic and material properties of interfaces governing slow response and long timescale phenomena in perovskite solar cells, *Energy Environ. Sci.* 12 (2019) 2054–2079. <https://doi.org/10.1039/c9ee00802k>.

⁷ D. Moia, J. Maier, Ionic and electronic energy diagrams for hybrid perovskite solar cells, *Mater. Horizons*. 10 (2023) 1641–1650.

⁸ A. Senocrate, T.Y. Yang, G. Gregori, G.Y. Kim, M. Grätzel, J. Maier, Charge carrier chemistry in methylammonium lead iodide, *Solid State Ionics*. 321 (2018) 69–74.

Revisiting the Working Mechanism of Perovskite Memristors

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Memristors are two-terminal devices, where the resistance depends on previous current flow. This feature unites storage and computing capabilities in a single device, which might help address the von Neumann bottleneck of today's computers. Furthermore, such in-memory computing and features like plasticity might enable simple realizations of neuromorphic computing.

Perovskites became interesting for memristors due to the hysteresis, they show in their current-voltage curve. Additionally, filamentary switching has been observed. Here, conductive nanofilaments are created, which can be reversibly ruptured and closed, turning the memristor on and off. These filaments are created either by defect ions in the perovskite or metal ions.

In this work, we report highest-performance and highly stable perovskite memristive switches (millions of cycles), whose switching behavior is further analyzed (Fig. 1). This includes voltage-scan-rate and temperature dependent measurements to understand which parameters govern the values of SET and RESET voltage, as well as the switching dynamics. The effect of heat generation is measured by photoluminescence and thermography imaging and analyzed using a combined electrical and thermal model, showing strong local heating, an effect so far less investigated.

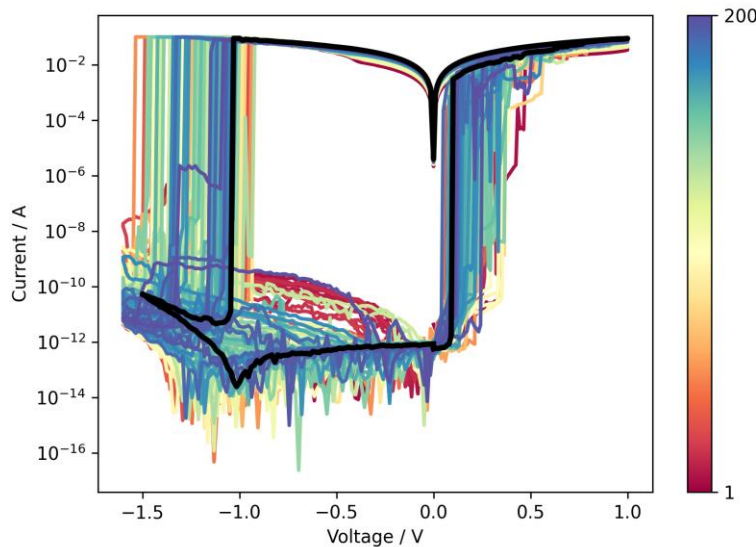


Fig. 1 200 current-voltage loops of a perovskite memristor, showing a SET voltage of 0.1 to 0.5 V and a RESET voltage of -1.0 V to -1.5 V.

Machine Learning Analysis of Perovskite Solar Cell Stability with Low-Dimensional Light-Absorbing Layers

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Abstract

The stability of perovskite solar cells is a critical factor for their practical deployment in outdoor applications¹. This study investigates the stability of perovskite solar cells by applying various machine learning (ML) methods to assess the aging effects on perovskite layers and complete cells. We compared the stability data of perovskite layers with that of whole solar cells under aging conditions. The complete cell stability dataset was curated from extensive literature reviews of research articles that included aging test reports on perovskite solar cells.

To explore the aging effects on perovskite layers, various structures of 3D/Low-dimensional (LD) perovskite layers were fabricated in a nitrogen-filled glove box. These layers were subjected to aging under controlled humidity and temperature at dark condition. The optical and structural properties of the layers were investigated by UV-visible absorption spectroscopy, photoluminescence (PL) analysis, X-ray diffraction, and scanning electron microscopy before and after aging.

To quantify the aging rate of various structures, we measured the PL maps of the layers before and after aging, comparing the shifts in PL peak positions and changes in the full width at half maximum (FWHM) of the peaks (Figure 1). Model inputs (X) were normalized using the StandardScaler algorithm from the scikit-learn library. Various ML models, including linear regression, ridge, lasso, k-nearest neighbors, support vector regression (SVR), random forest, gradient boosting, and neural networks, were applied and their performance was evaluated using cross-validated root mean squared error (RMSE).

Results indicated that the XGBoost regressor and random forest models exhibited the best performance on both training and test data. To identify the most influential features affecting model

¹ Zhu, H., Teale, S., Lintangpradipto, M.N. et al. Long-term operating stability in perovskite photovoltaics. *Nat Rev Mater* 8, 569–586 (2023).

outputs, SHAP (SHapley Additive exPlanations) analysis was performed². SHAP analysis revealed that molecular features such as branched amines, rotatable bonds, and halogen type significantly impact the cell stability.

Our findings provide insights into designing and manufacturing more stable perovskite solar cells, suggesting pathways for enhancing their longevity in outdoor applications. This research highlights the potential of machine learning to uncover critical stability factors and accelerate the development of durable perovskite solar technologies.

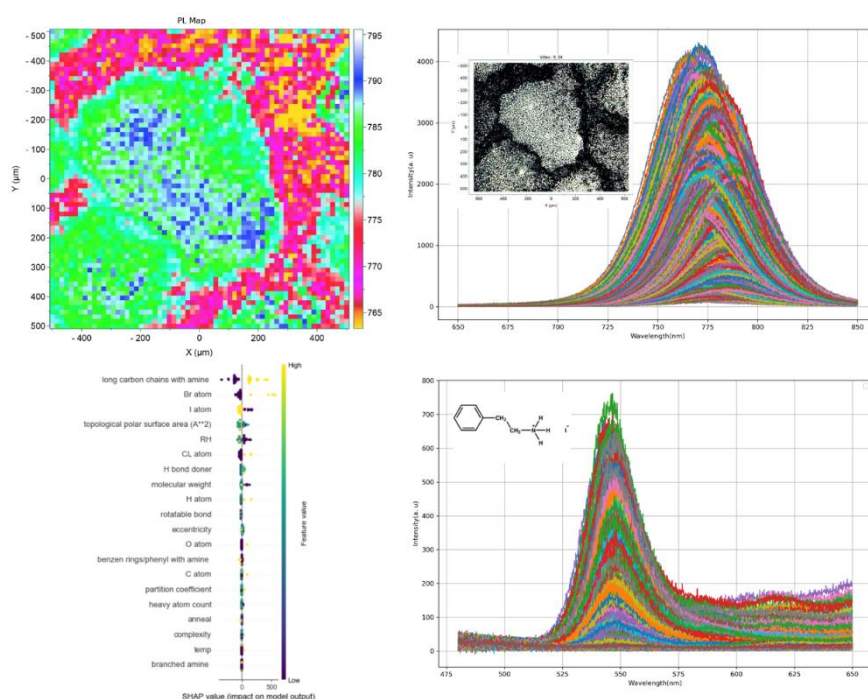


Fig. 1 Typical PL map of aged perovskite layers and corresponding PI spectrum of various points. Typical SHAP analysis results to explore the effect of molecular characteristic on the cells stability.

² Lundberg, S.M., Erion, G., Chen, H. et al. From local explanations to global understanding with explainable AI for trees. Nat Mach Intell 2, 56–67 (2020).

Ultra-Broadband THz Time-Domain Spectroscopy Based on Organic Crystals for Materials Testing

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Terahertz (THz) spectroscopy has been established as a powerful technique to study phonon modes and charge transport mechanisms of various materials, including materials for organic electronics and photovoltaics.¹ We report on our approach using organic crystals as THz generators and detectors for the emerging ultra-broadband THz range, extending beyond the few-THz limit of commercial systems.² By optimizing both the organic crystals and the experimental configurations, we achieved THz-wave generation and detection in a broad THz range up to 15 THz, well above the limits of the inorganic standard ZnTe crystals (Fig. 1). Employing a compact and a relatively low-cost telecom femtosecond pump laser at 1560 nm and a high repetition rate of 100 MHz, we can achieve a dynamic range up to 80 dB with frequency components up to 20 THz at a resolution below 3 GHz. Using this system, we report on ultra-broadband THz time-domain spectroscopy and imaging of different materials interesting for optoelectronic applications.

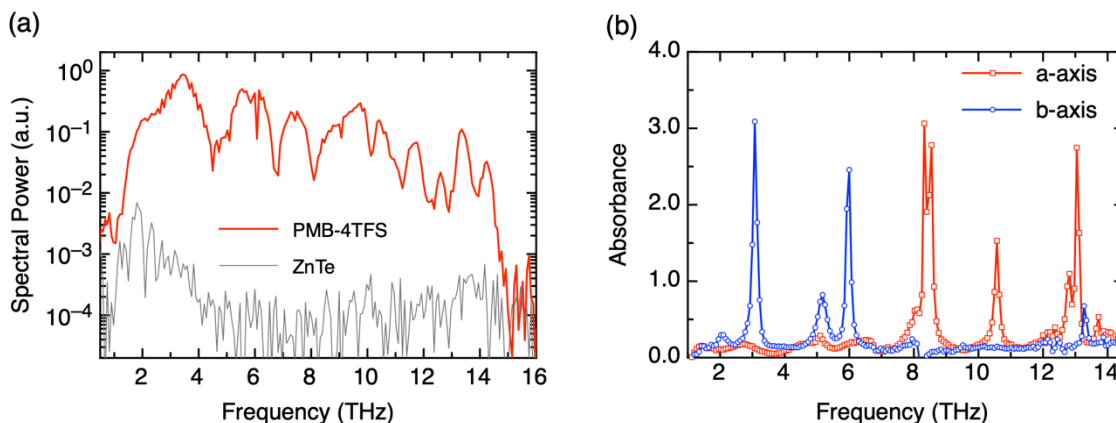


Fig. 1 (a) Ultra-broad THz spectrum generated in a 0.29 mm thick benzothiazolium ionic organic crystal PMB-4TFS³ compared to a 1.0 mm thick inorganic standard ZnTe. (b) Strongly anisotropic THz phonon modes in an organic electron transporting material, as measured using the ultra-broadband THz system at ZHAW.

¹ A. Leitenstorfer et al, “The 2023 terahertz science and technology roadmap”, J. Phys. D: Appl. Phys. 56 223001 (2023).

² U. Puc, T. Bach, P. Günter, M. Zgonik, M. Jazbinsek, “Ultra-Broadband and High-Dynamic-Range THz Time-Domain Spectroscopy System Based on Organic Crystal Emitter and Detector in Transmission and Reflection Geometry”, Adv. Photon. Res. 2, 2000098 (2021).

³ U. Puc, J.A. Yang, D. Kim, O.P. Kwon, M. Jazbinsek, “Broadband THz wave generation in organic benzothiazolium crystals at MHz repetition rates”, Opt. Mater. Express 13, 53 (2023).

Light-emitting electrochemical cells: Basic understanding for functional and sustainable devices

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The light-emitting electrochemical cell (LEC) is formally defined by the existence of mobile ions in the active material. It is the action of these ions that enables attractive properties, notably that complete LEC devices can be fabricated by energy- and material-efficient ambient-air printing and coating.¹ Specifically, the redistribution of the mobile ions in the active material causes electrochemical doping of the emissive semiconductor (p-type at anode and n-type at cathode), which results in the formation of a p-n junction doping structure. This in-situ formed doping structure enables the printing fabrication, but also poses challenges from conceptual and performance perspectives. For instance, the preferred position of the emissive p-n junction for constructive interference and minimized electrode quenching can not be controlled by conventional spatial design during device fabrication, and the doping regions comprise high concentrations of polarons that can cause severe exciton-polaron quenching. Herein, we present conceptual insights and rational design methods for the alleviation of exciton-polaron quenching² and for the identification and control of the position of the in-situ formed p-n junction for efficient light emission³. We also present new LEC concepts and novel device architectures as well as recent developments towards LEC devices, which are sustainable during both fabrication, operation and recycling.

¹ Sandström, A.; Dam, H. F.; Krebs, F. C.; Edman, L., Ambient fabrication of flexible and large-area organic light-emitting devices using slot-die coating. *Nat. Commun.* 2012, 3, 1002.

² Tang, S.; Sandström, A.; Lundberg, P.; Lanz, T.; Larsen, C.; van Reenen, S.; Kemerink, M.; Edman, L., Design rules for light-emitting electrochemical cells delivering bright luminance at 27.5 percent external quantum efficiency. *Nat. Commun.* 2017, 8 (1), 1190.

³ Ràfols-Ribé, J.; Zhang, X.; Larsen, C.; Lundberg, P.; Lindh, E. M.; Mai, C. T.; Mindemark, J.; Gracia-Espino, E.; Edman, L., Controlling the Emission Zone by Additives for Improved Light-Emitting Electrochemical Cells. *Advanced Materials* 2022, 34 (8), 2107849.

⁴ Larsen, C.; Lundberg, P.; Tang, S.; Ràfols-Ribé, J.; Sandström, A.; Mattias Lindh, E.; Wang, J.; Edman, L., A tool for identifying green solvents for printed electronics. *Nat. Commun.* 2021, 12 (1), 4510.

Simulating charge transport in the limit of high carrier densities or low disorders

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In organic semiconductors charge transport is usually controlled by static and dynamic disorder of the hopping sites. However, at high carrier densities, realized e.g. in organic field-effect transistors, electron-electron scattering becomes important and can lead to a decrease of the carrier mobility. We address this issue using kinetic Monte-Carlo simulations. The filling up of traps and tail states in the density of states smoothes the energy landscape. It turns out that for disorder parameters $\sigma < 2kT$, the commonly used Miller-Abrahams expression is no longer valid and needs replacing with a full statistical treatment. With this approach, the reduction of mobility as a function of carrier density, dimensionality and temperature is discussed.

Comprehensive Exploration of Exciton Quenching Mechanisms in OLEDs through Combined Characterization and Numerical Simulation

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Organic light-emitting diodes (OLEDs) are a leading display technology that continues to be the focus of extensive research aimed at improving efficiency and stability. Achieving these improvements requires a deep understanding of the mechanisms driving device performance under various currents and temperatures. A significant challenge faced by OLEDs is efficiency roll-off, where the light emission efficiency decreases as current density or luminance increases. This issue, especially problematic at high brightness, impacts power consumption and device lifespan. The efficiency roll-off is caused by exciton quenching, charge carrier imbalances, and Auger recombination¹, each requiring distinct investigative techniques due to their complex nature.

Examining the electroluminescence (EL) dependence on applied voltage sheds light on efficiency roll-off but falls short of distinguishing between excitonic processes such as exciton-polaron quenching and exciton-exciton annihilation (TTA, TPQh, TPQe). Recent findings suggest that Modulated Photoluminescence Spectroscopy (MPLS), a complex characterization technique that is combining Electroluminescence and Photoluminescence (PL), provides a deeper understanding of exciton quenching mechanisms in OLEDs².

In this study, we present an enhanced approach to studying exciton quenching in OLEDs through integrated experimental characterizations and device simulations. Using the all-in-one characterization system Paios³, we measured the bias-dependent PL of an Ir(ppy)₃ emitter-based OLED, along with its EL, current-voltage (IV), and capacitance-voltage (CV) characteristics. Furthermore, we utilized Setfos⁴ to simulate the EL/PL roll-off of the OLED and align the results with experimental data. This multitarget optimization enabled us to examine TPQ and TTA, even at voltages below the turn-on threshold, enhancing the precision of the extracted parameters.

As shown in Figure 1, we began with the examination of the electrical characteristics of the OLED, focusing on CV and IV data to derive reliable electrical model parameters (Figure 1a and Figure 1b). Following this, we explored the device's excitonic parameters by analysing its EL and PL characteristics (Figure 1c and Figure 1d). It is clearly visible that two different parameter sets can lead to the same current efficiency characteristic while affecting the PL characteristic differently. Therefore, a global fit of EL and PL is crucial for obtaining reliable exciton quenching parameters. Investigating the EL roll-off alone is insufficient to unambiguously determine the device's excitonic characteristics.

To further evaluate the impact of the excitonic model parameters extracted from the global fit on OLED device performance, we focus on the exciton loss diagram. Figure 2 illustrates the relative contribution of various exciton loss mechanisms at different operating voltages. In the low-voltage region, non-radiative decay is the sole loss mechanism. As the voltage increases beyond turn-on, exciton-polaron quenching and exciton-exciton annihilation mechanisms begin to contribute. Notably, around 2 V, both exciton-polaron quenching mechanisms start to become significant, though to varying extents. At approximately 2.5 V, TTA becomes prominent and, due to its quadratic scaling with exciton density, dominates at higher voltages. In contrast, TPQ mechanisms scale linearly with exciton density.

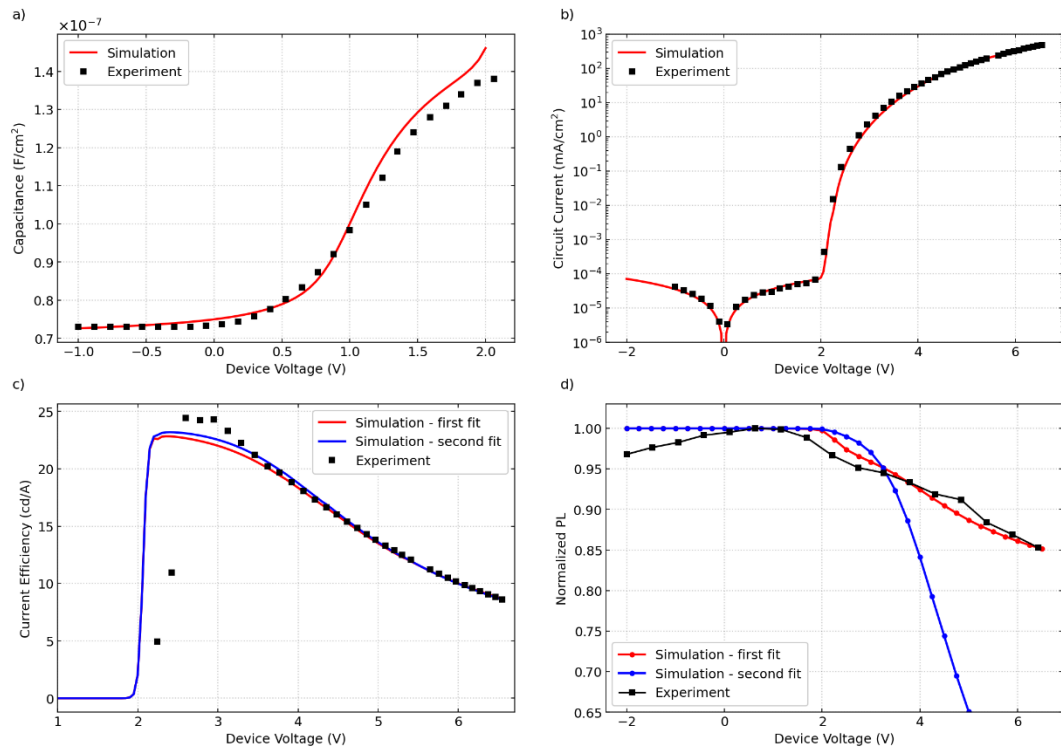


Figure 1: Opto-electrical measurements and simulations of the OLED under investigation. (a) CV and (b) IV measurements (solid lines) and simulations (symbols). (c) Current Efficiency (d) Normalized PL as a function of the applied bias.

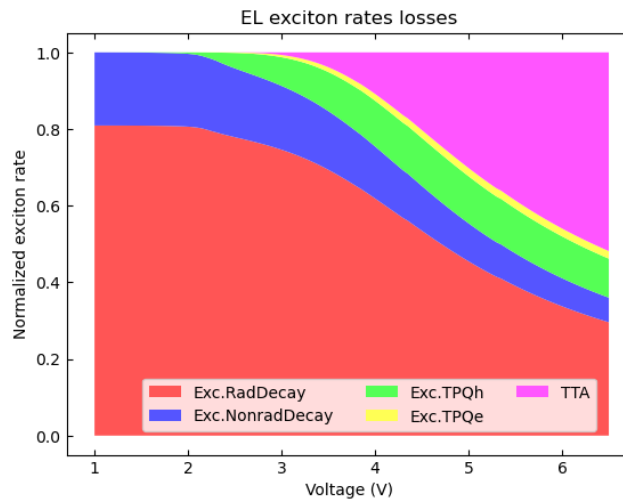


Figure 2: Exciton rate losses diagram for electroluminescence analysis.

- ¹ C. Murawski, K. LEO and M. C. Gather, Adv. Mater., 2013, 25, 6801.
- ² J. S. Bangsund, J. R. Van Sambeek, N. M. Concannon, R.J. Holmes, Sci. Adv. 2020, 6, 1.
- ³ Paios, all-in-one measurement platform by Fluxim AG, Switzerland, <https://www.fluxim.com/paios>.
- ⁴ Setfos, simulation software for LEDs and solar cells by Fluxim AG, <https://www.fluxim.com/setfos-intro>

Calibrating Operation Temperature and Voltage Relation for OLED Devices with Optimal Current Efficiency

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Displays play a critical role in military avionics, providing vital visual information to enhance situational awareness of user. Among the displays, OLEDs offer several advantages such as high contrast, wide viewing angle and low power consumption, allowing the displays to operate well-suit in harsh military conditions.¹ In this context, compatibility with NVIS (Night Vision Imaging System) determined by MIL-STD-3009 “Lighting, Aircraft, NVIS Compatible Standard” and compatibility with environmental conditions determined by MIL-STD-810 “Environmental Engineering Considerations and Laboratory Tests Standard” have critical importance. This compatibility ensures that OLED displays not only meet the standart performance criteria but also contribute to enhance operational effectiveness in military applications². On the other hand, considering the environmental conditions, temperature behavior of OLED is more critical and OLED should operate with high stability at wide range temperatures without being affected by changing temperature.

In this study, the optical and electrical simulations of monochrome yellow OLED structure for military grade displays have been achieved by using Emission and Drift-Diffusion tools in SETFOS 5.1.6 software. After obtaining ideal yellow emitting device architecture with optimal current efficiency, operation temperature and voltage of the OLED device have been calibrated such that this ideal performance of stable current efficiency is maintained all over low (-40 °C) and high (+75 °C) temperature ranges.

¹ R. Kaçar, R.B. Serin, E. Uçar, A. Ülkü, “A review of high-end display technologies focusing on inkjet printed manufacturing”, *Materials Today Communications*, 35, 105534, (2023)

² R. Kaçar, R.B. Serin, E. Uçar, A. Ülkü, “Removing crosstalk effect for high efficient polymer light emitting diode display” *Solid-State Electronics*, 192, 108253, (2022)

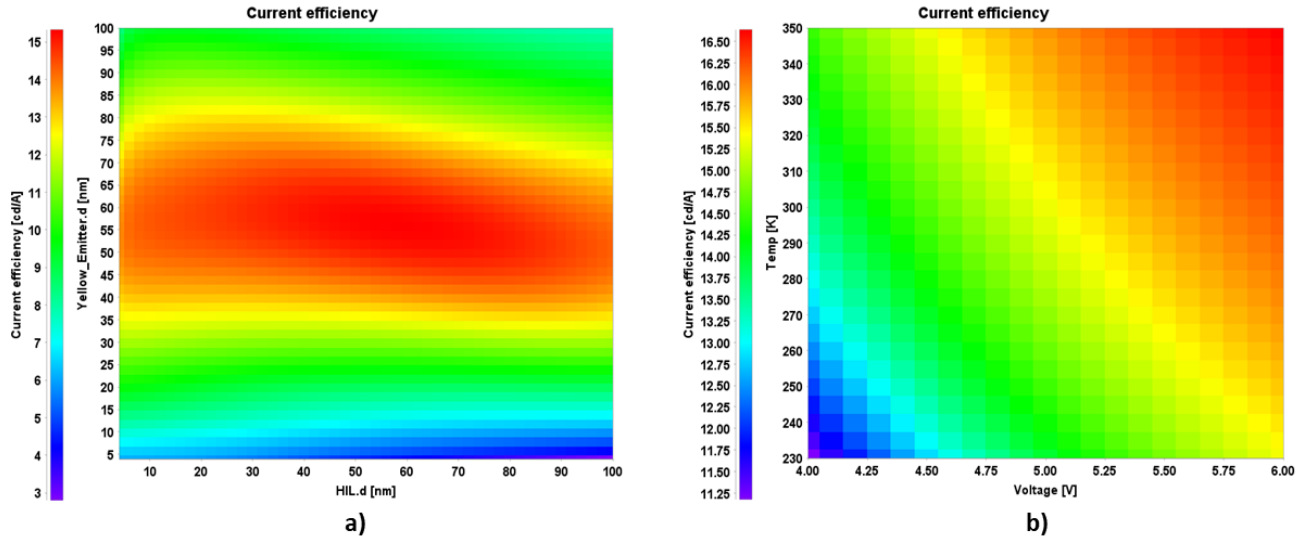


Fig. 1 2D simulations of current efficiency variation due to a) HIL-emitter thickness, b) operation temperature and voltage

It has been observed that operation temperature and voltage of OLED device has an inversely proportional linear relation. Monochrome yellow OLED device has been fabricated optimized layer structure and it has been tested. Excellent fitting between simulation and experimental results has been successfully demonstrated.

Optics and Photonics in Nano-structured OLEDs

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attention due to their low fabrication cost and high efficiency compared with inorganic light emitting diodes (LEDs) and liquid crystal displays. Typical OLEDs form a microcavity between a metal electrode and an ITO anode. In most OLEDs, the cavity length of the device is designed to achieve optimum to achieve a maximum light outcoupling efficiency, resulting in a Lambertian-like air mode emission profile due to the weak cavity effects.

To manipulate the light output, various approaches have been demonstrated in OLEDs and they can significantly enhance the cavity resonance to achieve directional emission, but the emission direction is sensitive to the cavity length and its emission spectrum is highly angle dependent. Diffractive optical elements (DOEs) have also been used to extract thin-film optical modes for directional emission, and subsequently emitted photons are coupled into a thin-film waveguide stripe and extracted by the DOE pixel, yielding directional emission.⁽⁸⁾ However, the device efficiency is very low.

Here, we demonstrate highly polarized light emission from OLEDs on grating substrates to selectively extract the TE waveguide mode by suppressing the SPP, TM waveguide, and air modes. By increasing the OLED stack thickness, the corrugation is mostly planarized at the cathode and the diffraction of TM waveguide mode and SPP mode is highly suppressed. To further suppress the emission from the air mode, the thickness of the electron transport layer (ETL) is tuned to its node position the air mode is also suppressed. Since the TE waveguide mode is highly polarized, the resulting OLED shows polarized emitted light with a high TE to TM mode extinction ratio. Using this approach, we have also demonstrated a high efficiency polarized emission from a perovskite LED.

In this paper, using OLEDs for demonstrations and different photonic structures, we demonstrated highly polarized light emission from an OLED. The highly selective diffraction of only the TE waveguide mode is possible by selectively diffracting the TE waveguide mode while suppressing other optical modes. Similar devices are made with perovskites to achieve a current efficiency of 56 cd/A.

Making Brighter OLEDs (and Lasers)

Ifor D.W. Samuel

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Many applications of OLEDs need high brightness or high light output. Obvious examples are lighting, outdoor displays and augmented reality. In addition medical applications need high intensities, and even conventional displays need higher brightness at the pixel than the range often reported in research devices.

This talk will address two aspects of high brightness operation of OLEDs. The first is efficiency roll-off in thermally activated delayed fluorescent (TADF) OLEDs. At high brightness the efficiency of LEDs and OLEDs decreases, and this can be very pronounced in TADF OLEDs because of their long emission lifetimes. Much of the literature suggests this should be addressed by increasing the rate of intersystem crossing. In this talk I will explain why this is not enough and propose a figure of merit to guide the design of materials with better performance at high brightness.

The other half of the talk will explore obtaining the highest possible light output from an OLED in order to excite a polymer laser. This requires a fluorescent OLED running at current densities of thousands of A/cm^2 i.e. approximately 10,000,000 times higher than OLEDs in displays. The construction and operation of such OLEDs will be described, together with their integration into a laser structure.

Numerical Methods for Coupled Drift-Diffusion and Helmholtz Models for Laser Applications

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D-10117 Berlin, Germany

Semiconductor lasers are pivotal components in modern technologies, spanning medical procedures, manufacturing, and autonomous systems like LiDARs. Understanding their operation and developing simulation tools are paramount for advancing such technologies. In this talk, we present a mathematical PDE model for an edge-emitting laser (see Fig. 1), combining charge transport and light propagation. The charge transport will be described by a drift-diffusion model and the light propagation by the Helmholtz equation. We discretize the drift-diffusion model using the finite volume method and solve it with a Newton solver¹. Moreover, we discretize the Helmholtz model using the finite element method and solve the resulting matrix eigenvalue problem with ARPACK². We discuss a coupling strategy for both models and showcase numerical simulations for a benchmark example. Our implementation is done in Julia, a language that combines the ease of use of e.g. MATLAB with the performance and efficiency of C++. Finally, we validate our results against a well-established software³.

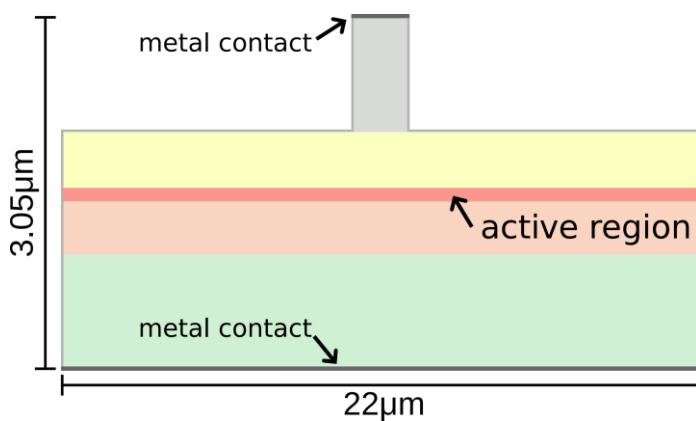


Fig. 1 Edge-emitting laser.

¹P. Farrell et al., “Drift-Diffusion Models” in “Handbook of Optoelectronic Device Modeling and Simulation”, CRC Press, pp. 733-772, (2017)

²Z. Amer, “Algorithms for computing eigenmodes in semiconductor lasers”, Master’s Thesis, Technische Universität Berlin, (2022)

³H. Gajewski et al., “WIAS-TeSCA-Two-dimensional semi-conductor analysis package”, (2016).

Simulated optimization of inverted glass substrate patterns for outcoupling efficiency enhancement and reduction of the colour shifting problem in organic light emitting diodes.

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The development of thermally activated delayed fluorescent (TADF) emissive species has led to the realization of up to 100% in internal quantum efficiencies (η_{int}) in organic light emitting diodes (OLEDs). Realizing 100% in external quantum efficiencies (η_{ext}), however, remains problematic due to the limited 20% in outcoupling efficiency (η_{out}).¹ Retrofitting OLED architecture with outcoupling structures has been successful in improving the η_{out} by redirecting substrate- and wave-guided modes into the forward viewing direction or eliminating coupling to evanescent modes altogether. Unfortunately, these structures may result in the undesirable colour-shifting phenomenon and require complex and multi-step processes for their fabrication.² The recent development of LG's 3rd generation display utilizing "META Technology 2.0" incorporates a microlens arrays (MLA), thus lifting the previously held limitations of scattering structures being used to enhance η_{out} due to image blurring or distortion concerns. The research demand has now shifted to fabricating structures from simple and quick processes which can simultaneously satisfy high η_{out} and preserve wide viewing angle colour purity. The practical incorporation of outcoupling structures into existing technologies can only be realized through high batch-processing-friendly processes. Therefore, this research prioritizes the quickness and simplicity of the outcoupling structure fabrication process as a progressive step toward achieving this goal.

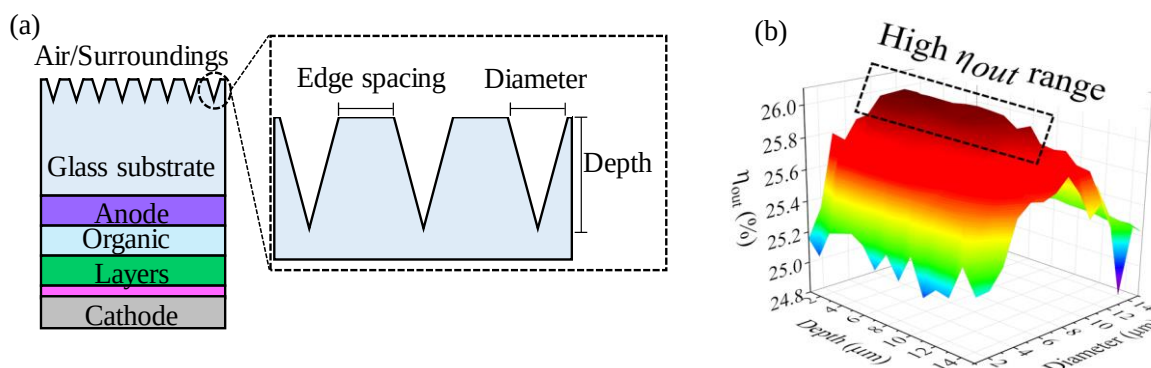


Fig. 1 (a) The simulated OLED device structure with conically shaped holes made at the air/glass substrate interface. The inset image illustrates the definition of hole pattern edge spacing, diameter and depth. (b) The simulated results of η_{out} (z-axis) achieved by varying the dimensions of diameter (y-axis) and depth (x-axis) of holes with edge-spacing of 1 μm .

The “Emission” and “Scattering” modules were coupled in FLUXiM’s SETFOS simulation programme and used to optimize the outcoupling structure (hole patterns at the air/glass substrate interface) dimensions for maximum η_{out} . **Figure 1 (a)** shows the dimensions of the hole patterns (edge distance, diameter and depth) and **Figure 1 (b)** shows an example of the systematic optimization of η_{out} by varying hole dimensions. The fabrication of the optimized micro-meter sized hole pattern structure over the OLED device was achieved using a simple and “one-step-process” femtosecond laser (IMRA America Inc.).

Compared to reference devices utilizing planar substrates, the simulation accurately predicted the best η_{out} enhancement ($\Delta\eta_{out}$) of about 30% could be achieved for conically shaped hole patterns with edge distance of 1 μm having depths and diameters ranging from 4 – 7 μm and 3 – 11 μm , respectively. The holes of patterned OLEDs were fabricated with dimensions lying within the high η_{out} range and yielded identical η_{out} results, thus validating good agreement between simulation and experiment. Practical manufacturing of flexible OLEDs, however, often requires the inclusion of thick hole transporting layers, and this significantly reduces the η_{out} due to reduced transmittance. Compared to their reference devices, a 60% in $\Delta\eta_{out}$ was achieved in their patterned OLED equivalent. In both sets of patterned devices, light rays meet the patterned air/glass interface at small contact angles, thus increasing their likelihood of being coupled into the forward viewing direction. Thus, $\Delta\eta_{out}$ is attributed to the redirection of substrate guided modes into free space. When the viewing angle of the detector relative to the device increases from 0° to 70°, the EL spectra peak of planar reference devices shifts by ~11 nm, while patterned devices demonstrate only a 3 – 5 nm shift. This favourable reduction in the viewing angle dependence is attributed to the strong light scattering ability of the hole patterns, which disarrays interference effects in weak microcavity devices that leads to EL shifting.^{3,4}

This work shows that the results of simulated outcoupling structures for OLEDs can be accurately replicated and fabricated using highly simplistic processes while simultaneously enhancing η_{out} and reducing spectral shifting. Although scattering structures may induce undesirable pixel blurring and image distortion, the recent development of complementary next generation image sharpening algorithms (ex. “META Detail Enhancer” by LG Display) have made their practical adaptation into displays a reality.

¹ H. Sasabe, and J. Kido, “Development of high performance OLEDs for general lighting,” J Mater Chem C Mater **1**(9), 1699–1707 (2013).

² G. Gomard, J.B. Preinfalk, A. Egel, and U. Lemmer, “Photon management in solution-processed organic light-emitting diodes: a review of light outcoupling micro- and nanostructures,” J Photonics Energy **6**(3), 030901 (2016).

³ S. Lloyd, T. Tanigawa, H. Sakai, and H. Murata, “Patterning of OLED glass substrate for improving light outcoupling efficiency,” IEICE Transactions on Electronics **E102C**(2), 180–183 (2019).

⁴ S. Lloyd, K. Higashimine, T. Tanigawa, and H. Murata, “Optimized femtosecond laser patterning of organic light-emitting diode substrates for the extraction of substrate guided modes,” Jpn J Appl Phys **60**, SBBG01-1 (2021).

TurboLED: Efficient Display Design

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Beat Ruhstaller**, Andrew Monkman***, Donal Bradley***

*Excyton Limited, Orbit Research Institute, NETPark, Durham, UK

**Fluxim AG, Winterthur, Switzerland

***University of Durham, Durham, UK

Displays consume approximately 50% of the battery in smartphones, tablets, laptops and other portable electronic devices. This is inconvenient for consumers, who must frequently recharge their devices, and damaging for the environment, with display consuming approximately 5% of all household electricity. In this work, we demonstrate that display power can be reduced by 45.0% using a novel pixel design which we have named TurboLED[®].

Fig. 1(a) shows the RGB pixel design typically used in OLED smartphones. Fig. 1(b) shows an equivalent stacked TurboLED pixel design that comprises independently addressable stacked light and deep RGB sub-pixels¹. The light sub-pixels are much more efficient and stable than the deep sub-pixels because of greater overlap with the photopic curve. These can be used to render the majority of display pixels. The less efficient deep sub-pixels are only used where needed to render display pixels with saturated colors.

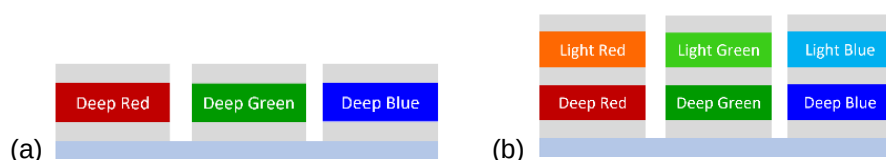


Fig. 1 Pixel Designs for (a) RGB and (b) TurboLED.

Fig. 2 shows two side-by-side 10 mm x 10 mm TurboLEDs emitting (a) light blue and (b) deep blue light with CIE 1931 (x, y) coordinates of (0.113, 0.118) and (0.151, 0.043), respectively. This demonstrates the viability of the TurboLED design.

Simulations of TurboLED display power compared to a standard RGB display were performed with Fluxim AG. The deep RGB chromaticities were set at approximately the DCI-P3 primaries (0.680, 0.320), (0.229, 0.741) and (0.130, 0.057), while the light RGB chromaticities (0.536, 0.463), (0.374, 0.614) and (0.118, 0.129) were optimized to reduce display power. These chromaticities and efficacy data for deep red, green and blue (79 cd/A, 215 cd/A and 14 cd/A) were

¹ Peter Levermore et al., Proc. SID Int. Symp. Dig. Tech. Papers. 54 (9.2) 93 (2023).

estimated from commercial OLEDs provided by Summer Sprout Technology. Efficacy data for light red and green (157 cd/A and 244 cd/A) were calculated by translating the spectra for deep red and green assuming constant EQE. Light blue efficacy (60 cd/A) assumes a phosphorescent emitter with 3x higher EQE than the fluorescent deep blue emitter, as reported by Universal Display Corporation².

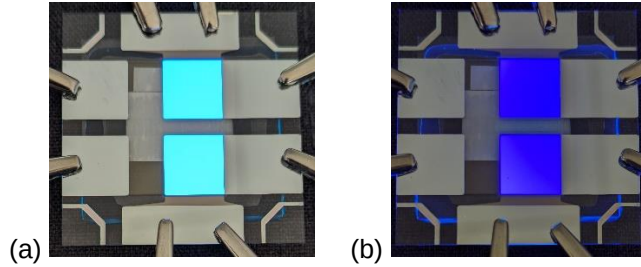


Fig. 2 TurboLEDs emitting (a) light and (b) deep blue light.

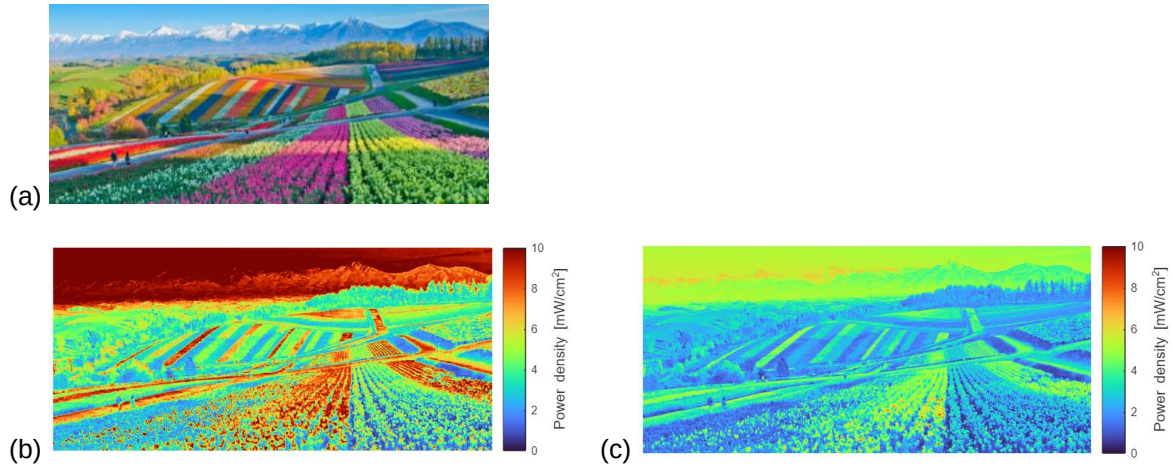


Fig. 3 (a) Image and power maps for (b) RGB and (c) TurboLED displays.

Fig 3 shows (a) an input image and simulated power maps for (b) RGB and (c) TurboLED displays. We assume a 2796 x 1290 (460ppi) display at 1,000 cd/m² with DCI-P3 color gamut and a diamond pixel array as in the iPhone 14 Pro Max. The TurboLED display consumes 45.0% less power than the standard RGB display (3.25 mW/cm² compared to 5.92 mW/cm²) because the deep RGB colors are used so infrequently. This corresponds to an estimated 3-4 hours extra daily batter life for most portable electronic device. TurboLED has the potential to dramatically reduce display power, and the light colors are also expected to extend display lifetime. Color gamut can also be extended beyond Rec. 2020 because the infrequently used deep RGB colors can be of higher saturation without significantly increasing display power consumption.

² Zhaoqun Zhou, International Conference of Display Technology, Hefei, China (2024).

Probing Blue MR-TADF OLED Stability with Electrooptical Simulations

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The advent of OLEDs has brought about a new era in displays, owing to their light-weight, flexibility, great image quality, and easy colour tunability by changing the constituent photoactive materials. Achieving the required colour gamut while maintaining high efficiencies can be achieved by using multi-resonant thermally activated delayed fluorescence emitters (MR-TADF), as these materials are both narrowband emitters and efficient exciton harvesters. However, despite being an active area of research, the stability of blue OLEDs remains insufficient due to the high photon energy accelerating degradation¹. Herein we report a methodical investigation into the stability of blue MR-TADF OLEDs aided by a set of experimental and simulation data, including steady-state, time-resolved and impedance measurements. Detailed electrooptical characterisation of MR-TADF OLEDs and single-carrier devices was used to fit experimental results simulated with Setfos², achieving a global fit over a large range of variation of device configurations. Simulations were subsequently extended to stress-tested devices, allowing a determination of the rate of degradation for each material. This provides direct insight into the stability of individual device layers and allows the pinpointing of the main degradation pathway. Additionally, the intrinsic stability of constituent materials is shown to be as important to device lifetime as the positioning of the emission zone. Employing this approach, further device iterations can be implemented deliberately, and hopefully lead to rapid improvements in OLED lifetime without significant sacrifices in efficiency.

¹ E. Tankelevičiūtė, I. D. W. Samuel and E. Zysman-Colman, “The Blue Problem: OLED Stability and Degradation Mechanisms”, *J. Phys. Chem. Lett.* 15, 1034-1047, (2024)

² Fluxim, Setfos User Manual, Version 5.3, (2023)

Formation of Electron Traps in Semiconducting Polymers via a Slow Triple-Encounter between Trap Precursor Particles

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Already in 2012, Blom et al. reported (Nature Materials 2012, 11, 882) in semiconducting polymers on a general electron-trap density of $\approx 3 \times 10^{17} \text{ cm}^{-3}$, centered at an energy of ≈ 3.6 eV below vacuum. It was suggested that traps have an extrinsic origin, with the water-oxygen complex $[2(\text{H}_2\text{O})\text{-O}_2]$ as a possible candidate, based on its electron affinity. However, further evidence is lacking and the origin of universal electron traps remained elusive. Here, in polymer diodes the temperature-dependence of fully reversible electron traps is investigated that develop under bias stress slowly over minutes to a density of $2 \times 10^{17} \text{ cm}^{-3}$, centered at an energy of 3.6 eV below vacuum. The trap build-up dynamics follows a 3rd-order kinetics, in line with that traps form via an encounter between three diffusing precursor particles. The accordance between universal and slowly evolving traps suggests that general electron traps in semiconducting polymers form via a triple-encounter process between oxygen and water molecules that form the suggested $[2(\text{H}_2\text{O})\text{-O}_2]$ complex as the trap origin.

In this talk, we will explain experimental implications of this result for future work, e.g., concerning the voltage scan rate used in current-density vs. voltage and hysteresis measurements. We will also discuss the conducted simulation procedure in some detail. The electron trap density over time is simulated from the decaying current via numerical drift-diffusion simulation. The simulation procedure is straightforward for electron-only devices. However, consistent simulation over the full temperature range for light-emitting diodes is more difficult because the current decay due to the presence of electron traps is much smaller than for an electron-only device. In addition, the simulated current sensitively depends on both capture coefficients for electrons and holes, and the exact values for these two simulation input parameters are up for discussion.

¹ M. Diethelm, M. Bauer, W.-H. Hu, C. Vael, S. Jenatsch, P. W. M. Blom, F. Nüesch, R. Hany, "Electron Trap Dynamics in Polymer Light-Emitting Diodes", Adv. Funct. Mater. 32, 2106185 (2022).

² M. Sedghi, C. Vael, W.-H. Hu, M. Bauer, D. Padula, A. Landi, M. Lukovic, M. Diethelm, G.-H. Wetzelaer, P. W. M. Blom, F. Nüesch, R. Hany, "Formation of Electron Traps in Semiconducting Polymers via a Slow Triple-Encounter between Trap Precursor Particles", Sci. Technol. Adv. Mater. 25, 2312148 (2024).

Numerical study of trap induced capacitance in polymer light emitting diodes

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Impedance spectroscopy (IS) methods are readily employed in the investigation of trap dynamics [1] due to their ease of implementation compared to more elaborate methods like thermally stimulated current (TSC) [2]. The device capacitance is often indicative of the charge accumulation inside the device. In the past, organic semiconductor devices have displayed negative capacitance (NC) at low frequencies [3]. Several microscopic explanations have been proposed including injection through interfacial states [3], charge trapping [4]. In this contribution, we focus on charge-trapping at bulk defects and highlight how the dynamic carrier capture and release process can express itself as a strong positive or negative capacitance, depending on the detailed trap interaction. Drift-diffusion simulations of IS are performed on a reference polymer LED structure, a single layer device replicating the state-of-the-art PPV-based copolymer super yellow (SY). SY has been shown to possess negative-positive capacitance at low frequencies and exhibits considerable charge trapping [5]. Qualitative agreement is found with Capacitance-Voltage (C-V) characteristics from literature. Emphasis is given to explaining the physics of such mechanisms beyond simple mechanistic descriptions like equivalent circuits. Different capacitive contributions are broken up according to particle species figure 1, charge balance has a strong effect on the cumulative total capaci-

tance sign by modulating individual positive-negative contributions.

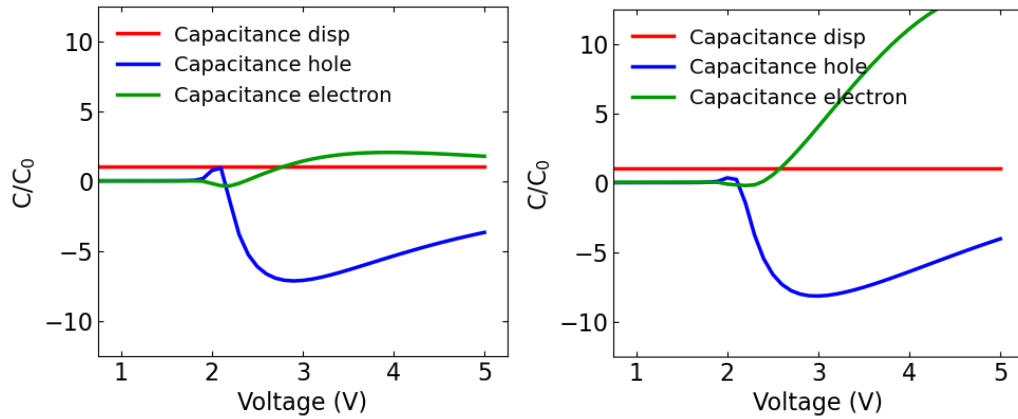


Figure 1 Capacitive contributions for a N-Majority (left), $n_{\text{anode}} \gg p_{\text{-cathode}}$ carrier and Balanced (right), $n_{\text{anode}} \sim p_{\text{-cathode}}$ device charge carrier densities showcasing charge imbalance effects on the C-V spectra. Contributions are broken up according to the AC current components displacement, electron and hole. Overall capacitance sign therefore depends on the bias voltage and charge Injection parameters.

Trap density displaces the C-V curve progressively to more negative values, a feature that can be employed during degradation as a gauge for trap generation figure 2. These findings allow us to obtain information about trap state evolution during full device operation.

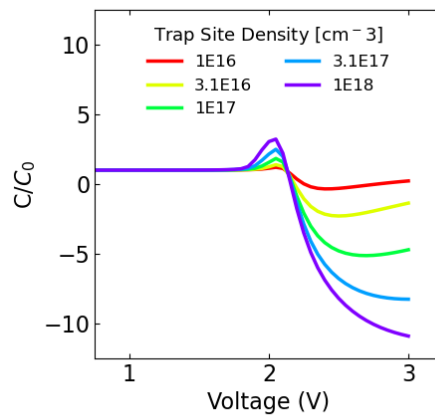


Figure 2 Capacitance-voltage curve with regards to trap site density. Negative capacitance increases in magnitude with the increase of trap site density. Minima of capacitance is also displaced to higher voltages.

- [1] Q. Niu, G.-J. A. H. Wetzelaer, P. W. M. Blom, and N. Irina Crăciun, “Quantification of hole-trap concentration in degraded polymer light-emitting diodes using impedance spectroscopy,” *Appl. Phys. Lett.*, vol. 114, no. 16, p. 163301, Apr. 2019, doi: 10.1063/1.5083036.
- [2] C. Vael, S. Jenatsch, and S. Züfle, “Scrutinizing thermally stimulated current transients originating from trapped charges in organic semiconductors: A drift-diffusion study,” *Appl. Phys.*, 2022.
- [3] J. Bisquert, G. Garcia-Belmonte, Á. Pitarch, and H. J. Bolink, “Negative capacitance caused by electron injection through interfacial states in organic light-emitting diodes,” *Chem. Phys. Lett.*, vol. 422, no. 1–3, pp. 184–191, Apr. 2006, doi: 10.1016/j.cplett.2006.02.060.
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- [5] M. Diethelm *et al.*, “Electron Trap Dynamics in Polymer Light-Emitting Diodes,” *Adv. Funct. Mater.*, vol. 32, no. 27, p. 2106185, Jul. 2022, doi: 10.1002/adfm.202106185.

Simulation of Quantum-Dot down-conversion Films and the Impact of the Backlight Illumination Geometry on the Light Conversion Efficiency

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With the application of quantum dot (QD) down-conversion films in LCD displays the color quality could be strongly improved, leading to a revival of this display technology. A key figure of such QD down-conversion film is the light conversion efficiency (LCE), which gives the ratio of down-converted QD emission to absorbed backlight illumination. To achieve a high LCE, the quantum dot concentration in the QD film and its layer thickness are usually optimized.

We present here measurement and simulation results of the angle-dependent characterization of a QD down-conversion film on a blue backlight unit. In detail we will show the impact of different illumination geometries on the LCE determination of such QD film. For the experimental data dedicated QD samples were fabricated at InnoQD¹, consisting of following layer structure: PET film / Resin + red-emitting QDs in capsules/ PET film. For the angle-dependent characterization we used Phelos², a gonio-spectrometer from Fluxim AG.

In Fig. 1a, the two different illumination geometries are depicted. In case 1, the backlight illumination unit is covered with a mask having a centered hole, resulting in an illuminated area on the QD film, which is smaller than the measurement spot of the spectrometer.

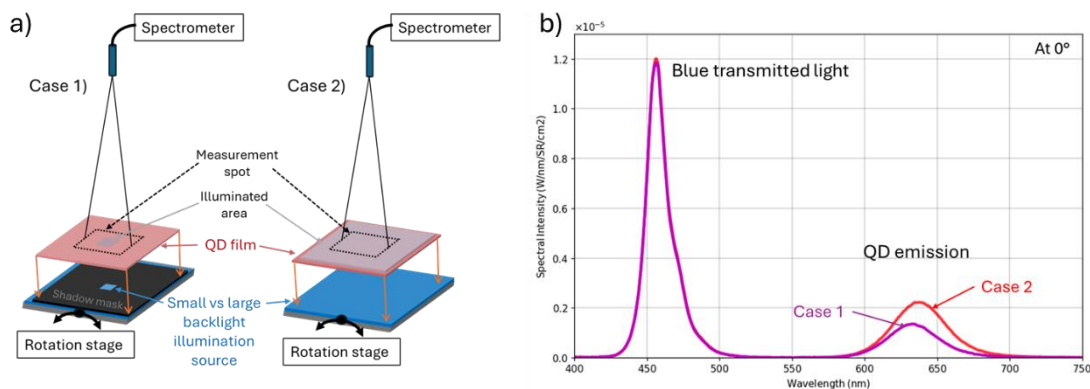


Fig. 1, a) Measurement setups with different illumination geometries for the QD film. **b)** Measured spectral intensities at 0° viewing angle for both cases.

¹ QD samples fabricated at Inno QD & Construction Co. LTD., <http://innoqd.com/eng/>

² Gonio-spectrometer Phelos from Fluxim AG, <https://www.fluxim.com/phelos>

In contrast, in case 2, the QD film is placed directly on the blue illumination source, leading to an illuminated area on the QD film, which is larger than the measurement spot.

In Fig. 1b, the measured spectral intensities for 0° viewing angle for both cases are plotted. Surprisingly, for case 2, a higher QD emission is observed. Also, the LCE for both cases, using hemispherical integration of the integrated photon density fluxes, shows a significantly higher LCE for case 2 compared to case 1 (0.39 vs 0.19), indicating a strong impact of the illumination geometry on the LCE determination.

In Fig. 2a, preliminary results with the large-area simulation software LAOSS³ show an increased QD emission (compare ratio of labelled blue/red peaks) when having a large, illuminated area, such as in case 2. This outcome strengthens our hypothesis that for case 2, additional QD excitation from outside the measurement spot is taking place, leading to the increased QD emission intensity and higher LCE, as sketched in Fig. 2b.

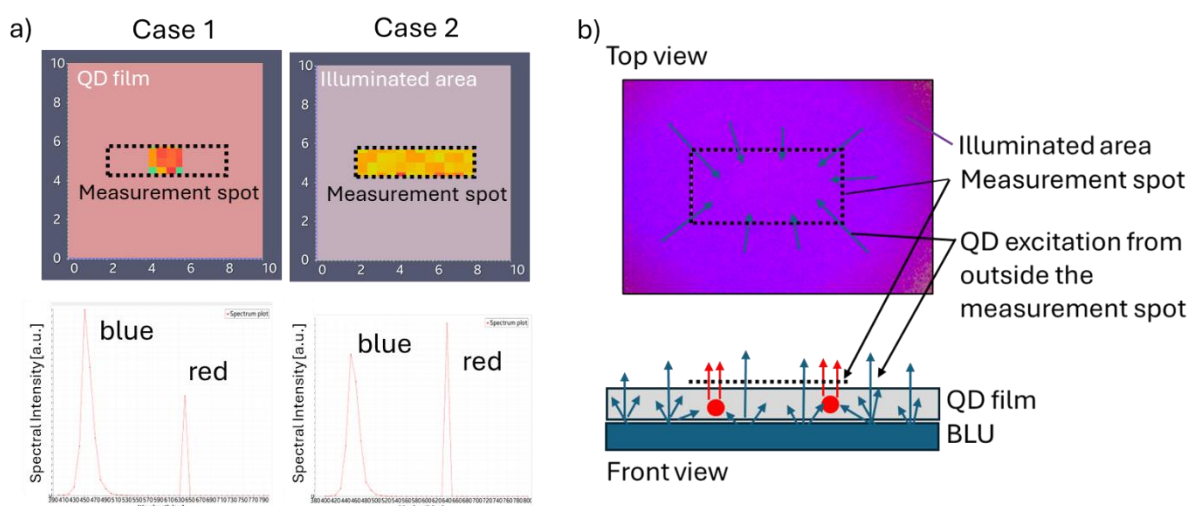


Fig. 2a) Preliminary results for case 1 and case 2 obtained with the large-area simulation software LAOSS, showing an increased QD emission (red labelled peak) for case 2. **b)** Sketched hypothesis of increased QD emission due to QD excitation from outside the measurement spot, leading to the increased LCE.

More detailed simulations will be presented at the conference, as well as a description of the LCE determination and the optical model used in the LAOSS software.

Highlighting the impact of the illumination geometry on the determination of the LCE can help to improve the design/implementation of QD films in displays.

³ Large-area organic semiconductor simulation (LAOSS) software from Fluxim AG, <https://www.fluxim.com/laoss>

Measuring HOMO and LUMO Levels in Small-Molecular Thin-Film Semiconductors Using a Novel Integrated Reference-Counter Electrode

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Characterizing the intrinsic electronic properties of organic semiconductors used in organic light emitting diodes (OLEDs) remains a formidable challenge. Among these properties, the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) levels are crucial, as they strongly influence device performance. Traditional techniques to measure these energy levels, such as photoemission yield spectroscopy or inverse photoemission spectroscopy are often complex, expensive, and not feasible for routine measurements.

In this work, we introduce a novel integrated reference-counter electrode (IRCE) specifically designed for electrochemical measurements of HOMO and LUMO levels in small-molecular thin-film semiconductors. The IRCE illustrated in the inset to Fig. 1 employs a gel polymer electrolyte with an embedded silver quasi-reference electrode, providing a stable potential during cyclic voltammetry measurements. We calibrated the IRCE against ferrocene, enabling the establishment of an absolute energy scale for these measurements.

Our experimental results demonstrate that the IRCE performs reliably, with stability comparable to the standard Ag/AgNO₃ reference electrode. We applied the IRCE to several prototypical OLED materials, including NPB, TCTA, and PO-T2T, as well as an NPB:PO-T2T exciplex. Fig. 1 shows the cyclic voltammogram of an ITO/PEDOT:PSS/NPB film measured with the IRCE, partially covered with ferrocene to obtain an absolute energy reference. The measured HOMO and LUMO levels were found to be in good agreement with values obtained from more complex methods, such as UV photoemission spectroscopy. Notably, the IRCE also allowed us to observe in-situ electropolymerization processes in TCTA, highlighting its potential for real-time monitoring of degradation phenomena.

The ability to accurately measure the frontier energy levels of organic semiconductors in thin films using the IRCE represents a significant advancement. We suggest that the IRCE could become a practical tool for OLED research, enabling routine and reliable electrochemical measurements of frontier energy levels of organic semiconducting films. The use of this method across various small-molecular thin-film semiconductors enables better characteriza-

tion of materials and promises to deepen our understanding of these materials, leading to improved modeling and understanding of electronic processes.

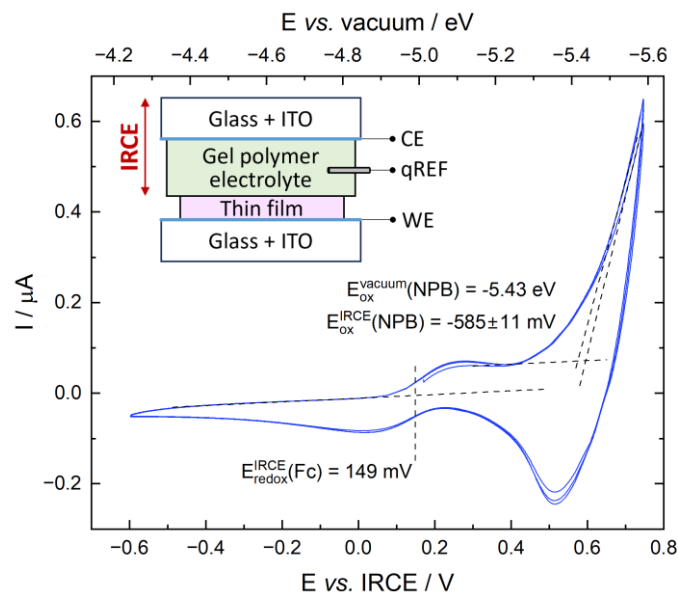


Fig. 1 Cyclic voltammogram of an ITO/PEDOT:PSS/NPB film measured with the integrated reference-counter electrode (IRCE), partially covered with ferrocene to obtain an absolute energy reference. The HOMO level is determined from the onset of NPB oxidation, as indicated by the dashed lines, and converted to the vacuum scale (top axis). The insert shows the schematic of the IRCE comprising the gel polymer electrolyte with the quasi-reference electrode.