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SWISS PHOTONICS

Scientific Program

	Wednesday, 09.09.26	Thursday, 10.09.26	Friday, 11.09.26
	OLED/PV	*PV*	*PV/Batteries*
08.45-09.00	Registration	Welcome	Welcome
09.00-09.15		Matthias Diethelm	Juan Anta
09.15-09.30			
09.30-09.45		Mathias Nyman	Evelyne Knapp
09.45-10.00			
10.00-10.15		Manjeet Kumar	Sharun Parayil
10.15-10.30		Tabea Krucker	Mahmoud Samadpour
10.30-10.45	Welcome	break	break
10.45-11.00	Koen Vandewael		
11.00-11.15		Sonia Ruiz Raga	Christoph Kirsch
11.15-11.30	Andreas Mischok		
11.30-11.45		Tristan Sachsenweger	Mahdi Mohammadi
11.45-12.00	Giacomo Cotelli	Philippe Baranek	
12.00-12.15	Anatolii Kuimov	Urs Aeberhard	Philip Calado
12.15-12.30	break		
12.30-12.45		break	break
12.45-13.00			
13.00-13.15			
13.15-13.30	Jens Pflaum		
13.30-13.45			August Johansson
13.45-14.00	Sandra Jenatsch		
14.00-14.15		Quentin Jeangros	Nicola Courtier
14.15-14.30	Jawid Nikan		
14.30-14.45	break	Davide Moia	Jože Moškon
14.45-15.00			
15.00-15.15		Kerttu Aitola	Lina Scholz
15.15-15.30	Anton Kirch	Pilar Lopez Varo	
15.30-15.45	Joan Rafols Ribe	break	
15.45-16.00	Yuntao Qiu		
16.00-16.15	Oskar Sandberg	Paola Vivo	
16.15-16.30			
16.30-16.45	Daniel Parsons	Ji-Youn Seo	
16.45-17.00			
17.00-17.15		João Pedro Ferreira Assunção	
17.15-17.30			

Conference dinner

Wednesday, 09.09.2026

Thursday, 10.09.2026

Friday, 11.09.2026

New organic device architectures for near-infrared detection and up-conversion imaging

Koen Vandewal

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[3]EnergyVille, IUMAT, Thor Park 8320, B-3600 Genk, Belgium

Organic opto-electronics has seen tremendous progress in the past decades: Organic light emitting diodes are a commercial product which can be found in smart-phones and TV screens, while organic photodiodes reach detectivities comparable to that of silicon in the visible wavelength range. Moreover, organic photovoltaic devices allow for an easy, light-weight integration into buildings and now reach power conversion efficiencies over 20% for lab-scale devices. This presentation will give an overview of the basic photo-physical processes occurring in such organic opto-electronic devices and sensors. Based on our current understanding of charge carrier photo-generation, recombination, and charge transport, we will link molecular and microstructural properties to device performance parameters. This allows us to determine performance limitations for organic photovoltaic and photo-detecting devices. I will further discuss novel nano-optical concepts to tune light absorption and will review our recent work on new device architectures enabling organic infrared detectors and photon up-conversion.

Strong and ultra-strong light-matter coupling in organic light-emitting diodes for applications in displays, imaging and biophotonics

Andreas Mischok

PoLightFilters & Humboldt Centre for Nano- and Biophotonics, Department of Chemistry and Biochemistry, University of Cologne, Greinstr. 4-6, DE50939 Köln, Germany

Thin-film interference is a fundamental principle in photonics and optoelectronics, governing spectral properties such as emission, transmission, and absorption through constructive and destructive interference. In microcavity systems, this enables precise spectral control but also introduces a major limitation: the pronounced angular dependence of cavity modes, typically observed as a blue shift under oblique viewing angles.

Here, we demonstrate a strategy to overcome this challenge by exploiting strong and ultra-strong coupling between cavity photons and material excitons. In this regime, the dispersion evolves from photonic to exciton-like behavior, effectively flattening the parabolic angular dispersion and enabling angle-independent and narrowband spectral responses. Organic semiconductors with high oscillator strengths are particularly well suited for this approach, allowing the realization of narrowband and broadband optical functionalities with exceptional angular stability.

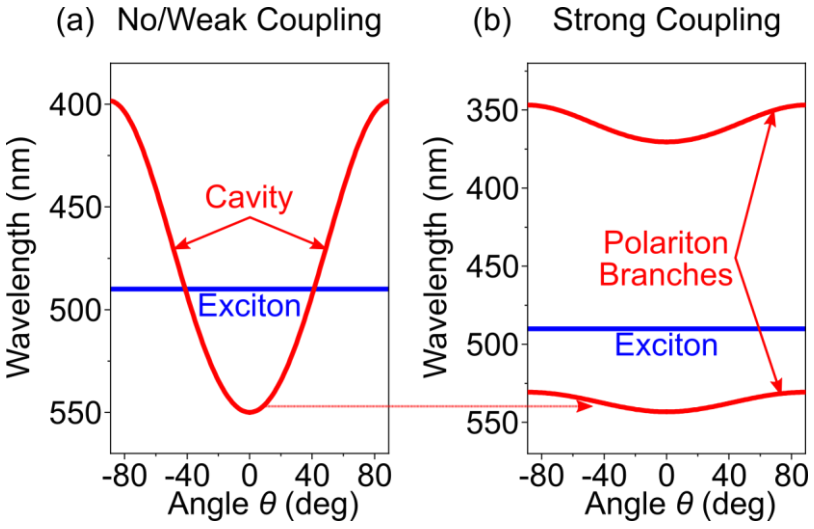

Figure 1 Angular dispersion of a weakly coupled cavity mode (a) and a polariton mode in the ultrastrong light-matter coupling regime. Through increasing the coupling strength and optimizing the cavity (de-)tuning, the angular dispersion of the polariton branches can be greatly reduced.

We experimentally demonstrate angle-independent transmission filters in both metallic and dielectric cavities, including distributed Bragg reflector architectures[1], as well as polaritonic

narrowband photodetectors with strongly suppressed spectral dispersion[2]. Furthermore, we report highly efficient polaritonic organic light-emitting diodes exhibiting narrowband, angle-stable emission across the visible and near-infrared spectral range[3,4]. We also show the compatibility of our polaritonic cavity architecture with all major device generations, including OLEDs with fluorescent[5], phosphorescent[3] and TADF-based[4] emitters.

These advances are highly relevant for applications in displays, imaging, spectroscopy, microscopy, biosensing, optical communications, and biophotonics, where angular robustness and spectral purity are critical for peak performance. Organic polaritonic devices also hold great opportunities for the realisation of stable electrically pumped lasing[6,7]. By addressing long-standing light collimation and color stability challenges, our work establishes strong light-matter coupling as a versatile and practical platform for next-generation photonic and optoelectronic devices.

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[1] Mischok et al., Nature Comm. 15, 10529 (2024)
[2] Abdelmagid et al., Adv. Opt. Mater. 13, e01727 (2025)
[3] Mischok et al. Nature Phot. 17, 393 (2023)
[4] Mischok et al., Light: Science & Application, in press (2026), arXiv: 2505.06057
[5] Witt et al., ACS Photonics 11, 1844 (2024)
[6] Le Roux et al., Nature Comm. 16, 811 (2025)
[7] Witt et al., Small Structures 7, e202600009 (2026)

The rates are not what they seem: understanding the time dependence of exciton-exciton annihilation “constants” in a TADF system

Giacomo Cotelli and Anna Köhler
Soft matter Optoelectronics, University of Bayreuth, 95440 Bayreuth, Germany

Exciton-exciton annihilation is a key non-radiative loss mechanism in organic optoelectronic devices, responsible for the efficiency roll-off in organic light-emitting diodes (OLEDs) at high luminance and implicated in the photochemical degradation of active layer materials. An accurate quantification of exciton-exciton annihilation is essential for the characterisation of organic semiconductors and for the parametrisation of device-level models. We investigate the kinetics of exciton-exciton annihilation in systems comprising a thermally activated delayed fluorescence (TADF) emitter dispersed in an inert host. Using kinetic Monte Carlo simulations, we show that the annihilation kinetic coefficients are in time-dependent and scale as t^(-0.5) for realistic parameters. A larger exciton diffusivity reduces the exponent of the time dependence, but a truly time-independent regime requires exceptional energy transfer parameters. We furthermore show that, when fitting transient PL data with time-independent rate constants, the fit quality is an unreliable indicator of the accuracy of the fitted parameters, hence cautioning against their use without appropriate scrutiny.

Exploring Pixel Isolation as a Strategy to Control OLED Operational Degradation

Anatolii Kuimov[1], Edoardo Stanzani[2], Sandra Jenatsch[2], Rishabh Saxena[3], Anna Köhler[1]

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OLED operational lifetime is governed by intrinsic material stability, charge balance, current distribution, and local ageing pathways. While some processes are defined by the molecular and electronic properties of the active materials, others are strongly affected by fabrication conditions, contact geometry, and local imperfections introduced during device preparation. Here, we investigate the role of edge-related degradation and pixel isolation by comparing conventional OLED pixels with photoresist-defined isolated cavities. Using modern characterization tools, including Paios and Vitios, together with standard optoelectronic measurements, we study sky-blue neat DBA-DI OLEDs and host-guest single-emissive-layer devices aged under constant-luminance conditions. For neat DBA-DI devices, isolated cavities show promising indications of improved stability, with lifetime enhancement of approximately 20%. In contrast, doped mCBP-CN devices exhibit more complex behaviour under the same isolated-contact geometry. These observations suggest that pixel isolation can modify OLED ageing dynamics and, in selected device stacks, may improve operational lifetime. However, it does not act as a universal lifetime-enhancement strategy. Instead, the results highlight contact geometry as an important parameter for OLED degradation studies.

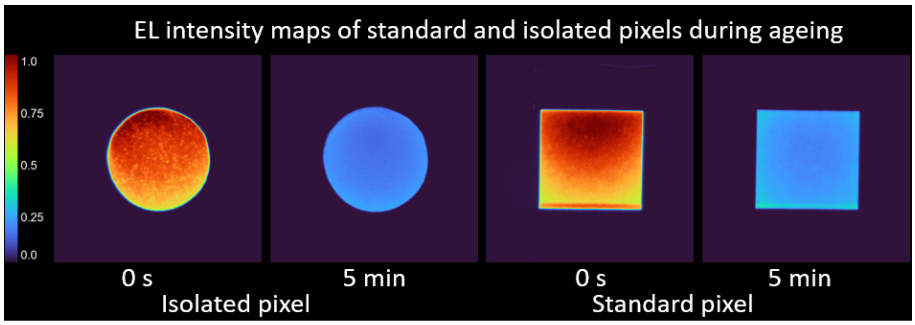

Fig. 1. EL maps of isolated and standard OLED pixels before and after 5 min under accelerated high-current stress at 7 V. The standard pixel shows a pronounced edge-localized bright region, suggesting local current concentration or enhanced emission near the pixel boundary. This feature is suppressed in the isolated geometry, indicating reduced edge-related inhomogeneity and a modified early-stage degradation pathway.

Subwavelength Organic Light-Emitting Diodes Pixels: Physical Principles, Challenges and Their Solutions

Jens Pflaum

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The advanced miniaturization of pixel architectures is a key requirement for the use of organic light-emitting diodes (OLEDs) in Ultra HD or 4K displays for applications in the field of augmented and virtual reality (AR & VR). While classical theory of electromagnetism reaches its limits for emitting dipole structures smaller than half the wavelength of the emitted light, this boundary can be overcome by utilizing metallic nanostructures. Such structures can act as plasmonic antennas that efficiently couple the light generated by the radiative decay of the excited molecular species into the far-field as well as spectrally shape the emission and direct the radiation in distinct spatial directions. Moreover, by their metallic nature, the antennas can be directly used as electrical contacts to inject the charge carriers necessary for electroluminescent recombination.

This promising approach, however, comes along with problems of an inhomogeneous distribution of charge carriers leading to parasitic currents and, thus, low external quantum efficiencies (EQE). Moreover, the formation of low-ohmic filaments caused by the migration of metal atoms in the high local electric fields (s. Figure 1) leads to unstable device operation and, ultimately, to failure of the entire OLED pixel.

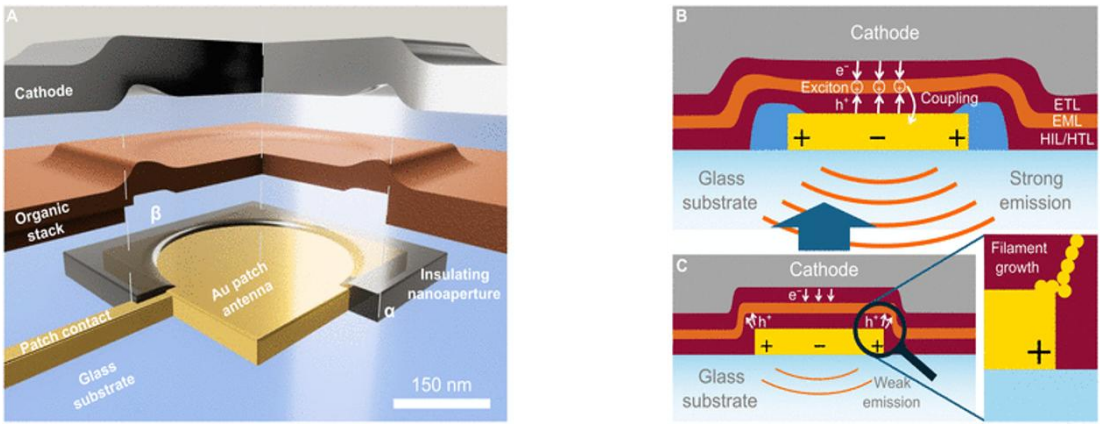

Figure 1. Conceptual nano-OLED pixel design (left), illustrating the passivation of the plasmonic antenna periphery by a dielectric cover layer and the central nanoaperture. Cross-sectional scheme with (top) and without (bottom) antenna passivation, indicating the inhomogeneous charge distribution and filament formation in case of the latter.

To cope with these challenges, we have developed a new approach, in which the periphery of the nanosized metal contact is selectively passivated by a dielectric layer while a circular aperture is prepared in the center of the patch antenna (s. Figure 1). As demonstrated by prototypical hole-only devices, this structure results in efficient charge carrier injection accompanied by stable diode operation. Extending this concept to a full OLED stack, we were able to successfully operate, for the first time, a 300 x 300 nm^2 pixel with a maximum luminance of 3000 cd/m^2 and a stable, non-optimized EQE of about 1 %.[1]

Aiming for further optimization of the metallic nanostructures, we report on a simple yet efficient approach towards plasmonic antennas that combine the advantages of silver, namely its low optical losses and ability to access a broad spectral range in the visible, with the high stability and durability of gold nanostructures. For this purpose, $Ag_{100-x}Au_x$ alloy films were grown by thermal co-evaporation under high vacuum and analyzed for their structural and optical characteristics (s. Figure 2).[2] Already at an Au content of only 5 at.%, stable plasmonic nanoantennas with resonances across the entire visible spectrum and low optical losses could be demonstrated.

Finally, in addition to these primarily technological aspects, we will present a new method for analyzing the optical properties of the thermally-activated delayed fluorescent (TADF) emitters, which were also applied in our stacks.[3] By photon-correlation measurements, we can determine the influence of the local matrix, in particular its rigidity and polarity, on the photophysical behavior of the TADF emitters at the single-molecule level.

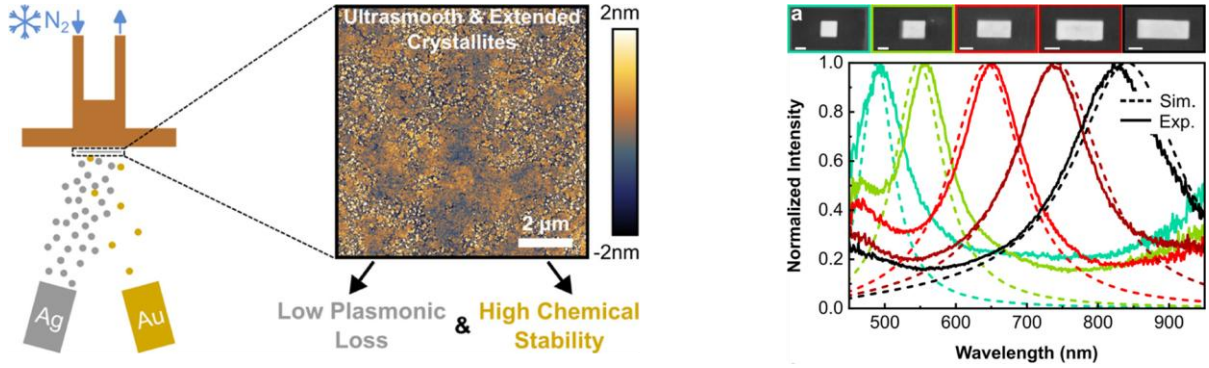

Figure 2. Co-evaporation of silver (Ag) films with small amounts of gold (Au) enable the fabrication of ultrasmooth, chemically stable thin films with excellent plasmonic properties.

[1] C. Zhang, B. Ewald, L. Siebigs, L. Steinbrecher, M. Rödel, T. Fleischmann, M. Emmerling, J. Pflaum, and B. Hecht, "Individually addressable nanoscale OLEDs", Sci. Adv.11, eadz8579 (2025)
[2] B. Ewald, L. Siebigs, C. Zhang, J. Graf, A. Tiwari, M. Rödel, S. Hammer, V. Stepanenko, F. Würthner, B. Gompf, B. Hecht, and J. Pflaum, "$Ag_{100-x}Au_x$ Alloy Films: An Approach to Fixing Silver for Durable, Low-Loss Plasmonics", ACS Photonics 12, 6161, (2025)
[3] B. Ewald, T. Kaiser, T. Fleischmann, and J. Pflaum, "Disclosing the impact of local host effects on TADF dynamics", J. Mater. Chem. C 14, 6884, (2026)

Enhancing the efficiency of ultrathin-EML OLEDs via double-emitter configuration

Edoardo Stanzani[1,2], Michele Forzatti[2], Sergio Martìnez Saiz[2], Daniel Tordera[2], Henk J. Bolink[2], Simon Zeder[1], Vasileios Georgakopoulos Paltidis[1], Balthasar Blülle[1], Beat Ruhstaller[1,3], Sandra Jenatsch[1]

[1]Fluxim AG, Katharina-Sulzer-Platz 2, 8400 Winterthur, Switzerland

[2]Instituto de Ciencia Molecular, Universidad de Valencia, Paterna 46980, Spain

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Recently, organic light emitting diodes (OLEDs) employing undoped ultrathin emitting layers (UEMLs) have attracted considerable interest because they enable highly simplified device architectures, straightforward fabrication and low material consumption. Nevertheless, concentrating charge recombination and excitons within a sub nanometer region enhances exciton–polaron and exciton–exciton annihilation, which leads to efficiency roll off and shortened operational lifetimes, especially at high luminance. To address these limitations, a range of strategies has been developed that focus on both molecular design and exciton management at the device level.

Here, an ultrathin EML OLED is investigated that employs a double emitter structure exploiting Förster energy transfer (FRET) via three routes: (i) intralayer donor to emitter FRET, (ii) interlayer exciplex to emitter FRET and (iii) interlayer ν-DABNA to ν-DABNA FRET across the mCP based interface. Fig. 1 shows that the resulting EQE for the double-UEML OLED is enhanced by approx. 25% compared to the single UEML OLED. By functionally decoupling the emission region from the main recombination region, the double emitter design reduces non radiative quenching pathways and enhances radiative exciton feeding at high current density. The novel architecture yields the highest peak external quantum efficiency (EQE) among the tested stacks: the single emitter reference reaches an EQE_{max} of 9.6%, whereas the double emitter configuration achieves 14.15% EQE_{max}, corresponding to a substantial efficiency gain from multi path exciton feeding.[1] The experimental observations are modelled with a coupled

[1] E. Stanzani, M. Forzatti, S. Martìnez Saiz, D. Tordera, H. J. Bolink, S. Zeder, V. Georgakopoulos Paltidis, B. Blülle, B. Ruhstaller, S. Jenatsch, ACS Applied Electronic Materials (accepted)

3D master equation and 1D drift-diffusion approach implemented in the software SETFOS for advanced OLED modelling to further confirm the operational mechanism.[2,3]

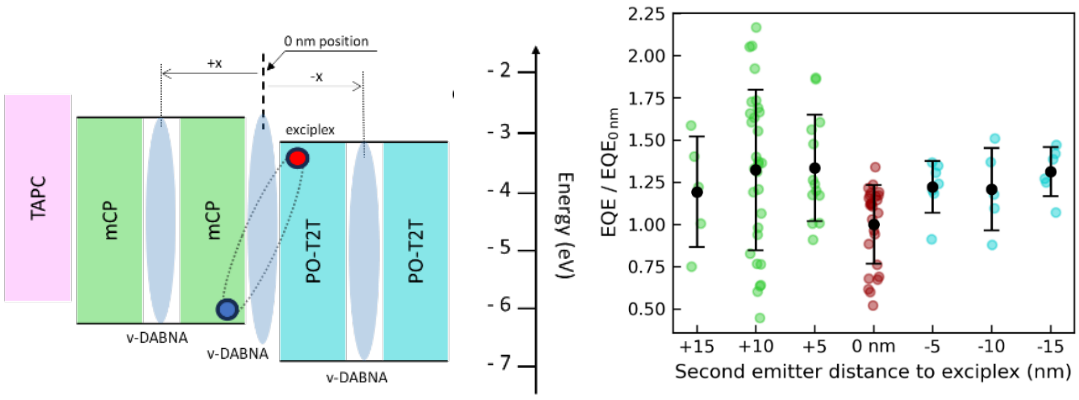

Fig. 1 a) Schematic representation of the double-emitter device structure with the UEML in the center (x=0) and a systematic variation of the second v-DABNA UEML within the mCP (positive x) or the PO-T2T layer (negative x), respectively, to investigate the energy transfer processes and b) measured EQE values of the double-emitter devices, normalized to reference OLED with x=0 nm.

Acknowledgement

This project has been partly funded by the European Union Horizon 2021 research and innovation programme under grant agreement No. 101073045 (TADFsolutions).

[2] S. Zeder, C. Kirsch, U. Aeberhard, B. Blülle, S. Jenatsch, B. Ruhstaller, Journal of the SID, Vol. 28, Issue 5, (2020)

[3] Simulation software SETFOS (version 6.0) by Fluxim AG, www.fluxim.com

Integrated Optoelectronic Model to Predict the External Quantum Efficiency of Single-layer TADF Organic Light-emitting Diodes

Jawid Nikan, Kaiwen Guo, Yungui Li, Paul W.M. Blom, Gert-Jan A.H. Wetzelaer
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The performance of single-layer thermally activated delayed fluorescence (TADF) organic light-emitting diodes (OLEDs) is governed by a complex interplay between charge transport, exciton dynamics, and optical outcoupling. In this work, we present a fully integrated optoelectronic modeling framework that enables quantitative prediction of the external quantum efficiency (EQE) of single-layer TADF OLEDs without relying on empirical fitting parameters[1]. All input parameters are based on separately determined experimental values. A single-layer OLED based on the TADF emitter 9,10-bis(4-(9H-carbazol-9-yl)−2,6-dimethylphenyl)−9,10-diboraanthracene (CzDBA), known for its nearly trap-free transport and high photoluminescence quantum yield, is used as the experimental model system.

The model self-consistently couples drift–diffusion charge transport with exciton rate equations describing singlet and triplet populations[2]. Key microscopic processes are explicitly included, such as Langevin recombination, singlet–triplet intersystem crossing (ISC), reverse intersystem crossing (RISC), as well as exciton–exciton annihilation channels including triplet–triplet and singlet–triplet annihilation. This allows a spatially resolved description of exciton generation and decay within the emissive layer.

To bridge electrical and optical properties, the exciton distribution is combined with a dipole-based optical model accounting for position-dependent outcoupling efficiency and microcavity effects[3]. This unified treatment enables direct computation of the EQE as a function of current density, device geometry, and material parameters.

The model is validated against experimental data from single-layer TADF OLEDs, showing excellent agreement in current–voltage characteristics, EQE magnitude, and efficiency roll-off behavior (**Figure 1**). In particular, the analysis reveals that efficiency loss at high current

[1] Jawid Nikan, Kaiwen Guo, Yungui Li, Paul W. M. Blom, and co-authors, “Integrated Optoelectronic Model to Predict the External Quantum Efficiency of Single-layer TADF Organic Light-emitting Diodes”, Adv. Electron. Mater. (2026), 2500729.
[2] B. van der Zee, Y. Li, G.-J. A. H. Wetzelaer, and P. W. M. Blom, “Numerical Device Model for Organic Light-Emitting Diodes Based on Thermally Activated Delayed Fluorescence”, Adv. Electron. Mater. 8, 2101261 (2022).
[3] Y. Li, N. B. Kotadiya, B. van der Zee, P. W. M. Blom, and G.-J. A. H. Wetzelaer, “Optical Outcoupling Efficiency of Organic Light-Emitting Diodes with a Broad Recombination Profile”, Adv. Opt. Mater. 9, 2001812 (2021).

densities originates from the combined effects of exciton–polaron interactions and annihilation processes, while interference effects and position-dependent outcoupling efficiency additionally influence the measured EQE.

This framework provides a predictive tool for linking material properties and device architecture to OLED performance, and offers a pathway toward systematic optimization of TADF-based emitters and device structures. Furthermore, it establishes a foundation for future extensions including degradation mechanisms and long-term operational stability.

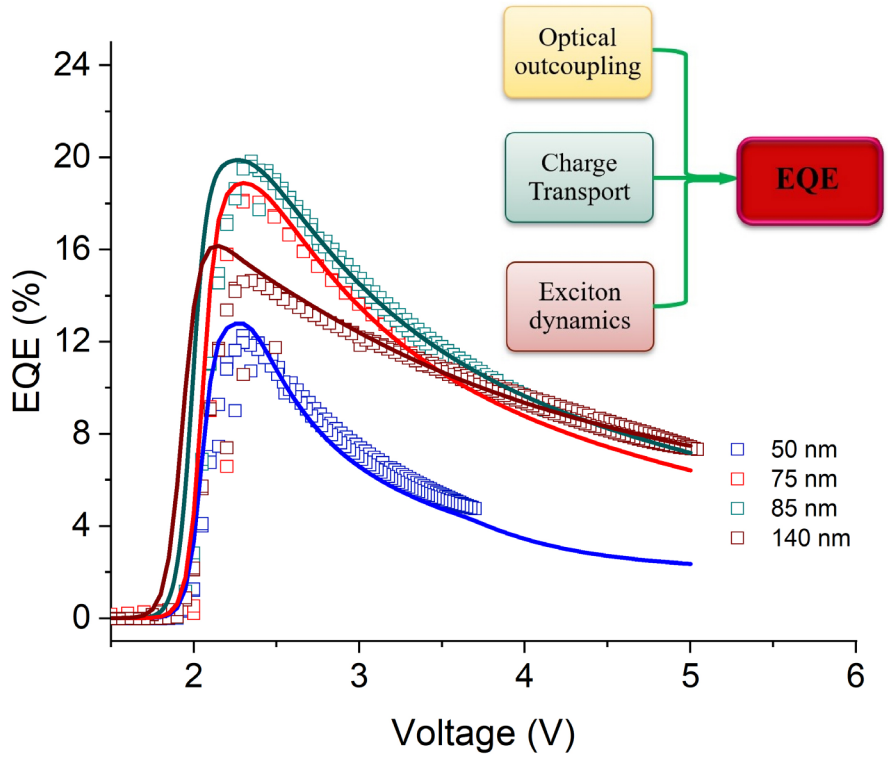

Fig. 1 Experimental and simulated EQE of a CzDBA OLED device for varying emissive layer thicknesses and applied voltage.

Ion dynamics in light-emitting electrochemical cells (LECs): What we can learn from perovskite-based devices

Anton Kirch[1,3], Joan Ràfols Ribé[1], Preetam Dacha[1], Agustin O. Alvarez[2], Ludvig Edman[1], Bruno Ehrler[2], and Sebastian Reineke[3]

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[2] LMPV - Sustainable Energy Materials Department, AMOLF, Amsterdam, The Netherlands
[3] Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute of Applied Physics, Technische Universität Dresden, Germany

The evolution of efficient light-emission concepts based on organic semiconductors has been a major research focus in recent decades. While the performance of organic LEDs (OLEDs) is outstanding, their fabrication usually requires energy-intensive vacuum processing. The light-emitting electrochemical cell (LEC) is a promising candidate for a recyclable and low-cost alternative, as it can be processed from solution using biocompatible materials.

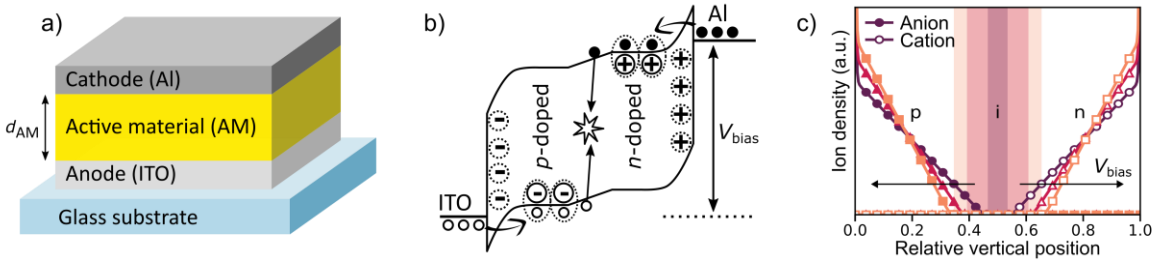

Figure 1. a) Sketch of the LEC stack used in this work. b) Electron potential energy diagram of the semiconductor's frontier energy levels over the vertical LEC dimension when the LEC is operated at a voltage V_{bias}. c) Modelled ion distribution (doping structure) in an LEC depending on V_{bias}.[1]

LECs feature a single electrochemical layer sandwiched between two electrodes and are therefore simpler to fabricate than OLEDs, cf. Fig. 1a. The active layer comprises a blend of mobile ions and a luminescent semiconductor. Under an applied voltage, V_{bias}, the mobile ions redistribute, producing a self-organized structure of injection-facilitating electric double layers (EDLs) at the electrode interfaces, electrochemically doped transport layers, and an intrinsic emission zone (dynamic *p-i-n* structure),[1] cf. Fig. 1b and 1c. While mobile ions are a decisive ingredient for the operation of LECs, they are generally regarded as detrimental in perovskite-based devices.[2] Hence, both research branches have an inherent interest in understanding ion dynamics and follow similar approaches.

In this paper, we discuss how impedance spectroscopy, complemented by drift-diffusion and equivalent-circuit modeling, can help us understand the dynamic doping structure in LECs and highlight how understanding ion dynamics can be of mutual interest to the perovskite and LEC communities.

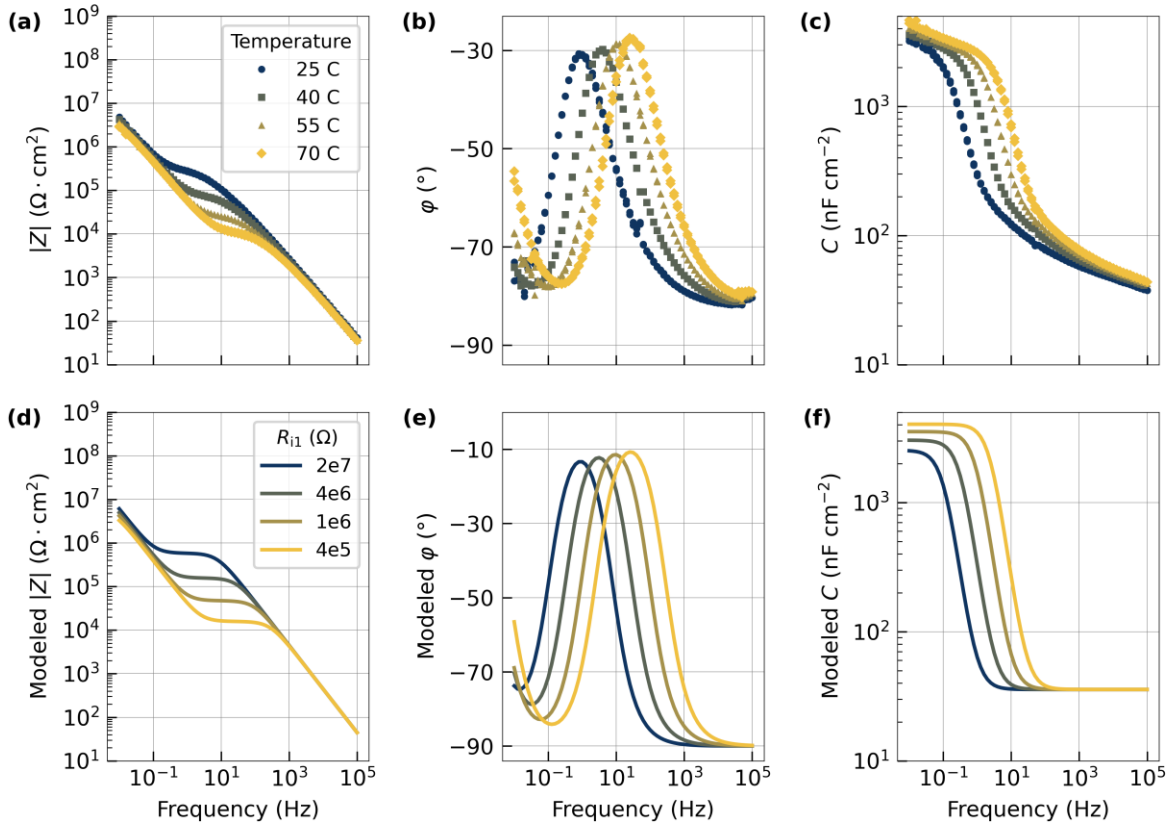

Figure 2. (a-c) Experimental absolute impedance, voltage-to-current phase angle, and capacitance density. (d-f) Corresponding data as acquired by an adapted Debye equivalent circuit, with Ri1 denoting the anionic resistance (conductivity).

Figure 2 shows an example of how impedance spectroscopy can reveal ionic properties in an LEC using a Debye-equivalent circuit, with R_{i1} denoting the temperature-activated anionic resistance (or the corresponding anionic conductivity).[3] Drift-diffusion modeling is subsequently applied to discern between the impact of ionic mobility and concentration on their conductivity.

References

1. Ràfols-Ribé J, Sato A, Kirch A, et al. Pinpointing the Dynamic p-i-n Junction. *PRX Energy*. 2025;4(3):033015. doi:10.1103/2vyr-4yp3

2. Schmidt MC, Alvarez AO, de Boer JJ, van de Ven LJM, Ehrler B. Consistent Interpretation of Time- and Frequency-Domain Traces of Ion Migration in Perovskite Semiconductors. *ACS Energy Lett*. 2024;9(12):5850-5858. doi:10.1021/acsenergylett.4c02446

3. Kirch A, Ràfols-Ribé J, Qiu Y, et al. In-operando dipole orientation for bipolar injection from air-stable electrodes into organic semiconductors. *Mater Horiz*. 2026;13(10):5050-5060. doi:10.1039/D6MH00161K

Pinpointing the dynamic *p-i-n* junction

Joan Ràfols-Ribé[1], Yuntao Qiu[1], Atsushi Sato[2], Anton Kirch[1], Xiaoying Zhang[1], Christian Larsen[1], Sandra Jenatsch[3], Kazuhiro Marumoto[2], Ludvig Edman[1]

[1]Umeå University, The Organic Photonics and Electronics Group, Department of Physics, Umeå, Sweden

[2]Division of Materials Science, University of Tsukuba, Tsukuba, Ibaraki 305-8573, Japan.

[3]Fluxim AG, Katharina-Sulzer-Platz 2, Winterthur 8400, Switzerland

The light-emitting electrochemical cell (LEC) efficiency depends heavily on the *p-i-n* structure that develops dynamically via electrochemical doping (ECD) under an applied bias.[1] While the complex electronic and ionic processes that govern the transient *p-i-n* formation have been extensively studied using experiments and drift-diffusion (DD) modeling, the steady state has been largely overlooked. In this study[2], we characterize the formed *p-i-n* structure of a polymer LEC at steady state for voltages above the energy gap through its most distinctive feature: the *IVL* characteristics, acquired via fast voltage sweeps (snapshots) that outpace ionic motion—effectively probing a static *p-i-n* junction. Unexpectedly, we find that the effective conductance of the developed junction scales with applied bias in an opposite direction to that predicted by conventional DD models (c.f. Fig.1). In this talk, I will discuss how we resolve this discrepancy using a modified phenomenological DD model, later validated using electron spin resonance spectroscopy. Yet, a key open challenge remains: the reconciliation of the measured *IVL* snapshots with the impedance spectroscopy data. These findings advance our understanding of the operational mechanism of LECs—and to the broader community of organic mixed ionic-electronic conductor (OMIEC) devices—while also emphasizing the need for a more realistic ion-transport model that addresses the limitations of the current deterministic DD LEC framework.

[1] P. Matyba, K. Maturova, M. Kemerink, N.D. Robinson, & L. Edman, The dynamic organic p–n junction. Nature Mater 8, 2015, 672–676

[2] Ràfols-Ribé, J.; Sato, A.; Kirch, A.; Zhang, X.; Jenatsch, S.; Larsen, C.; Marumoto, K.; Edman, L., Pinpointing the Dynamic p-i-n Junction. PRX Energy 2025, 4 (3)

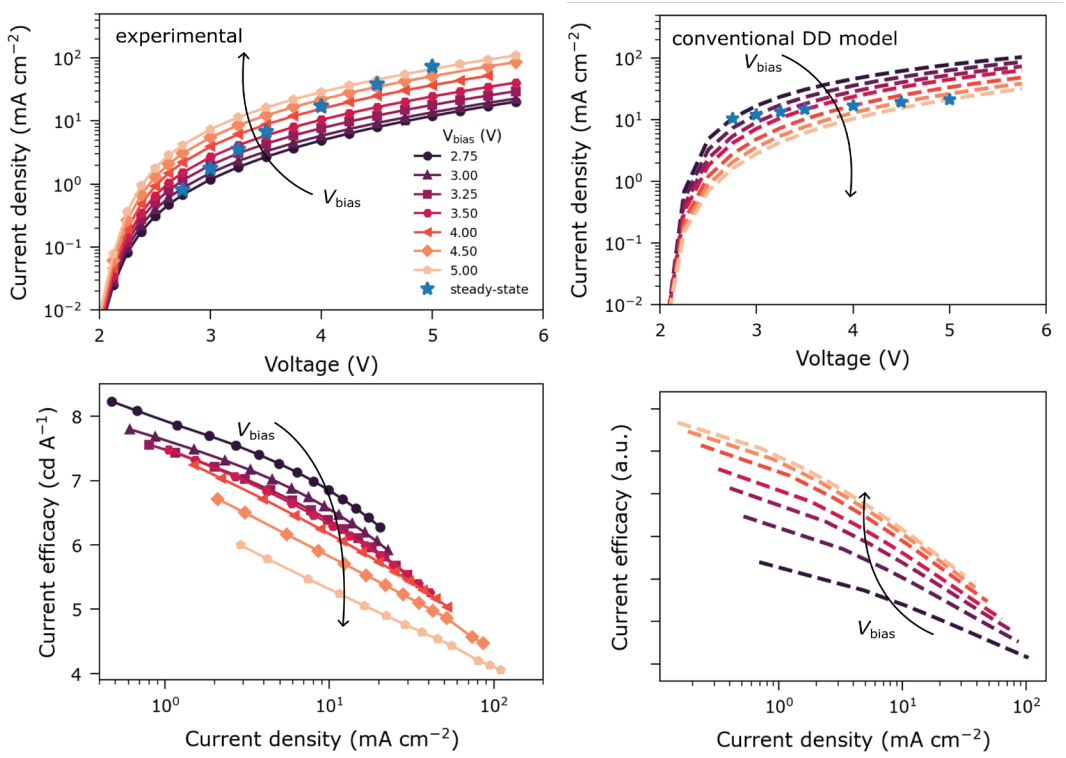

Fig. 1. Current-voltage and current efficiency (CE) snapshots of the dynamic *p-i-n* junction formed under different applied voltages, revealing opposite trends in effective conductance between the experimental data (left column) and simulations using conventional DD assumptions (right column).

Dynamic Emission Zone Width Extraction in Light Emitting Electrochemical Cells

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The emission zone (EZ) of light-emitting electrochemical cells (LECs) originates from in-situ electrochemical doping, forming a dynamic p–i–n junction. Its position and width strongly impact light outcoupling, spectral features and overall device performance.[1] Characterizing the EZ profile is thus significant to improve the efficiency and stability of devices and understand the loss mechanisms, such as exciton-polaron quenching. In OLEDs, EZ profiles are resolved by combining device operating at the optical minimum, angle-dependent electroluminescence spectroscopy and optical simulations. Applying this approach to LECs is considerably more challenging because their EZ evolves during operation,[2] continuously changing the optical interference condition. In this contribution, we demonstrate that the accuracy of EZ width extraction strongly indeed relies on the proximity of the EZ to its optical minimum condition by using a polymer-based LEC. Building on our previous work on EZ position, we tailor the active-layer thickness to place the EZ position close to the optical minimum during its operation. Subsequently, by fitting the simulation results from Setfos optical model with experimental angle-resolved electroluminescence spectra, we show clear spectral distinguishability close to the optical minimum, drastically reducing uncertainty in EZ width extraction in Fig 1. Finally, we use this approach to track the evolution of EZ width in a polymer-based LEC during device operation. The emission zone gradually narrows as electrochemical doping progresses, accompanied by a reduction in current efficiency relative to the initial state, indicating a trade-off between EZ width and exciton-quenching losses.

[1] Zhang, X. *et al.* Efficiency roll-off in light-emitting electrochemical cells. *Adv. Mater.* **36**, 2310156 (2024).

[2] Jenatsch, S. *et al.* Time-dependent p–i–n structure and emission zone in sandwich-type light-emitting electrochemical cells. *ACS Photonics* **5**, 1591–1598 (2018).

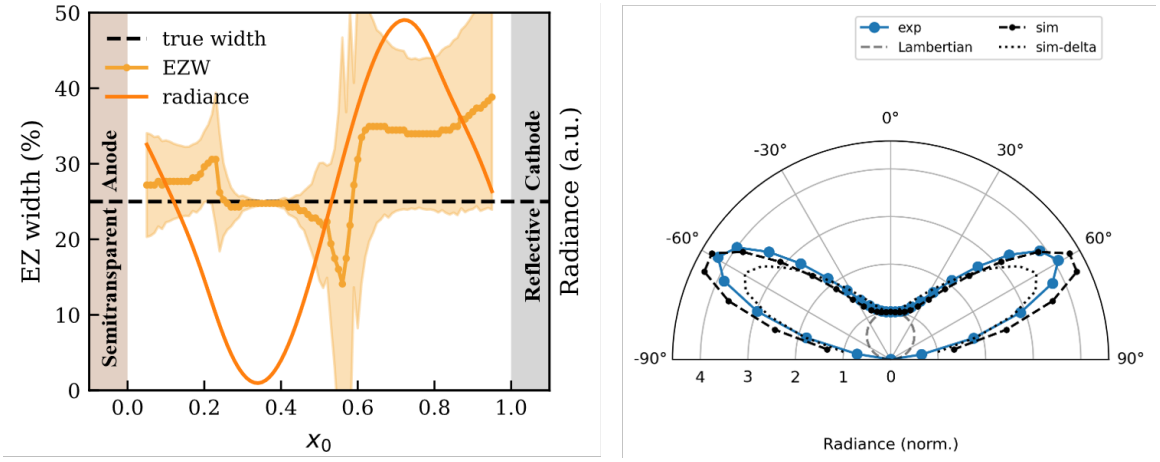

Fig 1. Left: Simulation of the EZ width extraction as a function of the EZ peak position. The shape of the EZ was assumed to be a Gaussian, and its FWHM is used as a proxy for the EZ width. The dashed horizontal line is the true width. The orange circles and the shadowed area indicate the predicted width and its uncertainty. The optical minimum is identified by the minimum in radiance. **Right:** Polar plot of experimental angular radiant intensity of an LEC. Solid lines denote experimental results; dashed lines represent simulations adopting a Gaussian emission profile, while dotted lines correspond to simulated data based on an ideal delta-function emission profile.

Contact Effects Limit the Photocurrent Collection in High-Efficiency Organic Solar Cells

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The contacts play a vital role in thin-film photovoltaics such as organic solar cells. Importantly, the contacts supply a built-in electric field within the active layer, necessary for efficient collection of photogenerated charge carriers in organic photovoltaic devices. In addition, ohmic contacts enhance the conductivity for majority carriers near the contact regions, minimizing losses in quasi-Fermi level splitting and the open-circuit voltage. As such, contact-related degradation typically manifests as a reduction of either the open-circuit voltage and/or the Fill Factor[1,2]. Here, we find that contact-related effects can also give rise to considerable losses in the photocurrent, limiting the short-circuit current densities in high-efficiency organic solar cell systems[3,4,5]. Further, we show that these photocurrent losses can be reduced by contact passivation. The underlying loss mechanisms are clarified by electrical measurements and validated by drift-diffusion simulations.

[1] O. J. Sandberg, A. Sundqvist, M. Nyman, and R. Österbacka, ”Relating charge transport, contact properties, and recombination to open-circuit voltage in sandwich-type thin-film solar cells”, Phys. Rev. Appl. 5, 044005 (2016)

[2] A. Sundqvist, O. J. Sandberg, M. Nyman, J.-H. Smått, and R. Österbacka, ”Origin of the S-Shaped JV Curve and the Light-Soaking Issue in Inverted Organic Solar Cells”, Adv. Energy. Mater. 6, 1502265 (2016)

[3] Y. R. Kim, O. J. Sandberg, S. Zeiske, G. Burwell, D. B. Riley, P. Meredith, and A. Armin, ”Mitigating detrimental effect of self-doping near the anode in highly efficient organic solar cells”, Adv. Funct. Mater. 33, 2300147 (2023)

[4] O. J. Sandberg and A. Armin, “Diode equation for sandwich-type thin-film photovoltaic devices limited by bimolecular recombination”, PRX Energy 3, 023008 (2024)

[5] B. Liu, O. J. Sandberg, et al, “Inverted organic solar cells with an in situ-derived SiO_xN_y passivation layer and power conversion efficiency exceeding 18%”, Nat. Photon. 19, 195-203 (2025)

Multi-modal imaging and electro-thermal simulations of indoor organic PV mini-modules

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In the indoor photovoltaics (IPV) community, commercialization efforts have already begun, and there are currently prototypes integrating third-generation photovoltaic technologies to provide power to low consumption electronic applications. A promising solution for upscaling the fabrication of indoor organic photovoltaic modules is through roll-to-roll thin film deposition processes and lamination; a technique that can be applied to fully organic devices and performed under ambient conditions. Maximising shunt resistance is a necessity for indoor light-harvesting but attention must also be given to series resistance, as this reduces the total harvesting efficiency to power an IoT device[1]. In this work, we combine multiple imaging techniques with electrothermal simulations to spatially characterize shunt and series resistance losses in roll-to-roll laminated organic devices. Figure 1a. shows a dark lock-in thermography (DLIT) measurement on a mini-module, displaying significant thermal losses close to the interconnects[2]. Electrothermal simulations with the LAOSS software confirm that this observation can be modelled by including regions of enhanced sheet resistances. We discuss this result in relation to the de-doping of the cathode, which is an undesired effect arising from the fabrication process[3]. Using this foundation, the same procedure is applied to cells and modules with more evident defective features (Figure 1b.), also reflected in their current voltage response, to deduce the corresponding failure modes. A combination of 1D electrothermal simulations in the SETFOS software and current mapping were also conducted to investigate how these failure modes affect out-of-plane charge transport. This work highlights the poten-

[1] Grandhi, G. K. *et al.* Underexplored Dimensions of Emerging Indoor Photovoltaics. *ACS Energy Lett* https://doi.org/10.1021/acsenergylett.5c03760 (2026) doi:10.1021/acsenergylett.5c03760.

[2] Breitenstein, O., Warta Wilhelm & Langenkamp M. *Lock-in Thermography: Basics and Use for Evaluating Electronic Devices and Materials (2nd edition)*. Springer Series in Advanced Microelectronics (2010).

[3] Cai, W. *et al.* Dedoping-induced interfacial instability of poly(ethylene imine)s-treated PEDOT:PSS as a low-work-function electrode. *J Mater Chem C Mater* **8**, 328–336 (2019).

tial and limitations of DLIT for the spatial characterization of shunts and series resistance effects in IPVs.

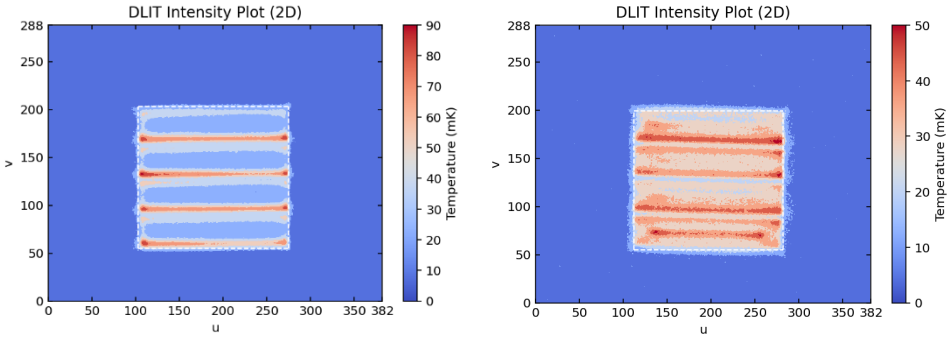

Fig. 1 Dark lock-in thermography (DLIT) amplitude measurement of (a) a good-performing and (b) defective mini-module

Towards practical quantification of ion density and mobility in perovskite solar cells

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Mobile ions strongly influence the performance and stability of perovskite solar cells, yet their density and mobility are difficult to quantify reliably because many electrical measurements probe them only indirectly. We previously analysed the bias-assisted charge extraction (BACE) method for the case of a screened bulk electric field.[1] The initial current density and current-decay dynamics depend on the ion conductivity, that is, the product of ion density and mobility, while the integrated current reflects the ionic charge required to screen the bulk electric field. In this study, we expand our analysis to include the extraction of ion density using BACE, low-frequency Mott-Schottky analysis (LFMS) and impedance spectroscopy on p-i-n perovskite solar cells [2,3], supported by drift-diffusion simulations (Figure 1a) [4]. We place particular emphasis on the role of transport layers, an aspect that has received little attention in the context of these ion-extraction methods. The results confirm that BACE is reliable only when the ion density is low enough such that the bulk electric field is not fully screened, whereas LFMS, which is more suitable in the high ion density regime, is dominated by transport layer capacitance and substantially underestimates the true bulk ion density relative to the expected ~10^{19} cm^{-3} range [4], both experimentally and computationally (Figure 1b). Although drift-diffusion simulation-based work reported a bulk ion density threshold for electric field screening of around ~10^{16} cm^{-3}, recent studies on similar device structures link degradation to increasing ion density and report extracted bulk ion densities far above that level. We discuss why these experimental findings are still qualitatively meaningful, and explore how bulk field screening and transport layer limitations can be circumvented in ion density

[1] M. Diethelm, T. Lukas, J. Smith, A. Dasgupta, P. Caprioglio, M. Futscher, et al. Probing ionic conductivity and electric field screening in perovskite solar cells: a novel exploration through ion drift currents. Energy Environ Sci. 18, 1385–97, (2025)

[2] M. Othman, Q. Jeangros, D. A. Jacobs, M. H. Futscher, S. Zeiske, A. Armin, et al. Alleviating nanostructural phase impurities enhances the optoelectronic properties, device performance and stability of cesium-formamidinium metal–halide perovskites. Energy Environ Sci. 17, 3832-3847, (2024)

[3] M. Diethelm, https://www.fluxim.com/research-blogs/reverse-bias-stressing-of-perovskite-solar-cells, (2025).

[4] D. Moia, https://www.fluxim.com/research-blogs/stutorial-setfos-pscs-ionic-properties, (2025).

and mobility extraction measurements, with transport layer thickness variation providing a route to separate bulk and contact contributions.

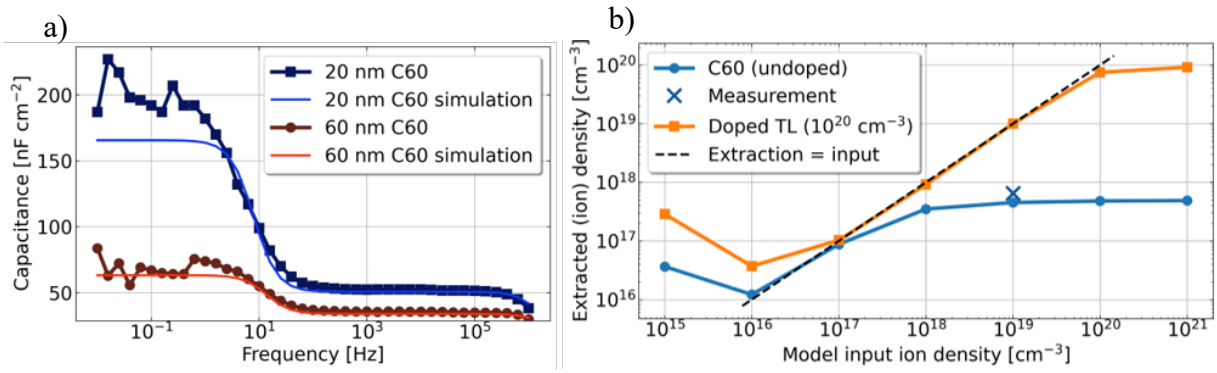

Fig. 1 a) Comparison of experimental and simulated capacitance-frequency sweeps measured in the dark at 0 V for different C60 layer thicknesses.[4] b) Simulated LFMS analysis at 1 Hz for a swept model input ion density in the perovskite layer for different transport layer doping levels.

Understanding capacitance-frequency spectra of Perovskite solar cells

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Perovskite solar cells hold great potential for future large scale energy production. However, several challenges remain to be solved before Perovskite solar cells are ready for the market. In particular, long-term device stability is still a concern. It has been shown that stability of Perovskite solar cells is mainly related to slow-moving ionic species within the Perovskite bulk, therefore, it is essential to have reliable characterization techniques to determine ionic properties such as ion density and mobility [1]. Impedance spectroscopy in the low-frequency regime is a technique frequently used to determine the ion depletion-layer capacitance, from which the ion density can be inferred. However, operating Perovskite solar cells typically have several interlayers, which complicates the analysis.

In this work, we present a framework for understanding the capacitance as function of frequency (*C-f*) of Perovskite solar cells, taking into account both ionic and electronic contributions in the Perovskite active layer as well as the interlayers. By varying the temperature, the ion mobility as well as the conductivity of the interlayers can be varied, which yields additional possibilities. Computer simulations using SETFOS are used to both rationalize the results, and to extract the ion density and mobility from the low-frequency *C-f*. We furthermore relate the ionic properties to simulated and experimentally determined hysteresis index. Our results indicate that the ion mobility is a broad distribution, rather than a uniquely defined fixed number, which is in agreement with a broader than expected hysteresis behavior [2].

[1] J. Thiesbrummel, *et al*, *Nature Energy* **2024**, *9* (6), 664–676. https://doi.org/10.1038/s41560-024-01487-w

[2] Manjeet Kumar, Changzeng Ding, Jiansheng Yang, Oskar J. Sandberg, Mathias Nyman, Chang-Qi Ma, Ronald Österbacka, *J. Phys. Chem. Lett.* **17, 5**, 1527–1533 (2026)

Simulation-Based Study of Ion Migration in Perovskite Solar Cells

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Ion migration is a key phenomenon that influences the performance and stability of metal halide perovskite solar cells (PSCs). Mobile species such as halide ions and organic cations migrate by hopping between vacant lattice sites under internal or applied electric fields, leading to redistribution of ionic charge within the material. This leads to current–voltage (J–V) hysteresis, as ions respond more slowly than electronic carriers, causing nonequilibrium behaviour during measurements. The accumulation of ions at interfaces or within the bulk affects the electrical potential landscape, which influences charge extraction, recombination[1], and overall efficiency. This typically leads to time-dependent performance and challenges in accurate characterization.

Drift–diffusion simulations are performed to understand the capacitance–frequency (C–f) response and hysteresis behaviour of perovskite solar cells. C–f analysis provides a powerful, non-destructive way to probe these ionic effects by separating slow ionic responses from fast electronic processes. At low frequencies, capacitance is dominated by ion accumulation and interfacial polarization, whereas at high frequencies it mainly reflects electronic charge dynamics. This frequency-dependent response enables the extraction of key parameters such as ion mobility and ion density, ion mobility primarily determines the scan-rate regime at which hysteresis becomes pronounced, while ion density governs the magnitude of the hysteresis[2]. Since hysteresis in PSCs originates from the coupling between ionic motion and electronic transport, it leads to transient behaviour and performance variation over time. A comprehensive understanding of ion-induced hysteresis, supported by techniques like C–f analysis, is essential for improving the accuracy of device characterization and for designing stable, high-performance perovskite solar cells suitable for practical applications.

References:

1. O. Sandberg, M. Kumar, M. Stolterfoht, D. Neher, & A. Armin "*Analytical model for interface recombination limited ideality factors in p -i -n perovskite solar cells*" APL Energy 3, 036107 (2025).

2. M. Kumar, C. Ding, J. Yang, O. Sandberg, M. Nyman, C. Ma, & R. Österbacka "*Effect of thermal stress on the ion density and mobility distribution in perovskite solar cells*" Journal of Physical Chemistry Letters, 17(5), 1527–1533 (2026).

Mixed but Not Fully Hybrid? - Toward Understanding Lateral Inhomogeneity in Me-4PACz/F-4PACz SAMs

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Self-assembling molecules (SAMs) are widely employed to tailor interfacial energetics and surface properties in perovskite solar cells, yet their multifunctional role remains difficult to disentangle. In this work, we investigate mixed SAMs composed of Me-4PACz and F-4PACz, with a particular focus on their degree of hybridization at the interface.

While pristine F-4PACz provides favorable wettability but introduces an extraction barrier that limits device performance, Me-4PACz enables efficient charge extraction but typically requires additional treatments (e.g. nanoparticles) for a higher wettability and optimal film formation. Mixed SAMs combine key advantages of both systems, enabling device efficiencies comparable to Me-4PACz while eliminating the need for nanoparticles.

Structural and optoelectronic characterization reveal that perovskite film morphology and crystallinity are largely unaffected by the change of the functional group of the underlying SAM, suggesting that device performance is primarily governed by interfacial energetics. However, some measurements indicate a tendency toward increased variability for mixed SAMs compared to their pristine counterparts.

These observations suggest that mixed SAMs may not form a fully homogeneous hybrid layer but instead exhibit lateral inhomogeneities. To test this hypothesis, ongoing work focuses on combining optical simulations (Setfos), modeling lateral combinations of Me-4PACz and F-4PACz domains, UPS measurements and KPFM measurements performed directly on the SAM layer.

This approach aims to clarify whether mixed SAMs form truly hybridized interfaces or retain lateral heterogeneity, and how this impacts interfacial energetics and device performance.

Lattice and ions: understanding the perovskite solar cell degradation with in-operando XRD and impedance spectroscopy

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Understanding performance loss during operation, beyond extracting a T80 lifetime metric, is crucial for developing strategies that address underlying degradation mechanisms. Non-destructive operando characterization enables real-time correlation of device performance with physical and material properties while capturing reversible processes driven by ionic motion in perovskites.[1] Electrochemical impedance spectroscopy (EIS) probes key processes in operating solar cells, from charge transfer and recombination to ion migration and chemical (redox) reactions. In this talk, practical examples will be presented demonstrating how EIS can be used to investigate the evolution of physical processes under operational conditions. First, we examine the origin of light-soaking-induced performance enhancement in devices employing a low-doped hole-transport material (HTM). Combined EIS and in situ photoluminescence (PL) measurements are used to evaluate the hypothesis of spiro-OMeTAD photodoping and the role of perovskite ions in governing its kinetics.[2] Second, we discuss the evolution of ionic and electronic processes during a standard maximum power point tracking (MPPT) degradation study.[3] Finally, operando X-ray diffraction (XRD) measurements are used to reveal how perovskite lattice strain and crystallinity evolve during operation and correlate with device performance, placing these observations in the context of parallel EIS findings.[4-5]

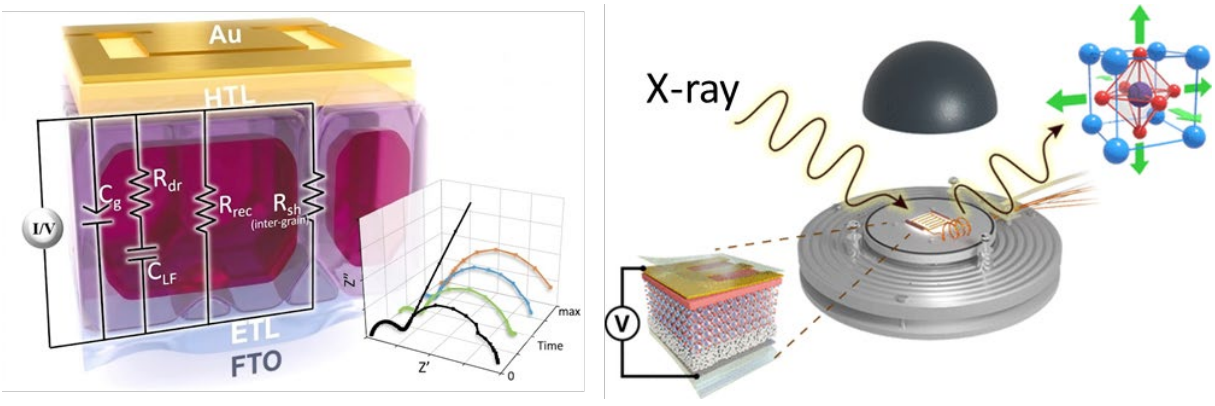

Fig. 1 Scheme representing the equivalent circuit of a perovskite solar cell (left) and in-situ XRD setup to measure complete devices under light, N2, T and bias (right)

References:

1. Baumann, F.; Raga, S. R.; Lira-Cantú, M., Monitoring the Stability and Degradation Mechanisms of Perovskite Solar Cells by in Situ and Operando Characterization. *APL Energy* **2023**, *1*.
2. Tan, B.; Raga, S. R.; Rietwyk, K. J.; Lu, J.; Fürer, S. O.; Griffith, J. C.; Cheng, Y.-B.; Bach, U., The Impact of Spiro-Ometad Photodoping on the Reversible Light-Induced Transients of Perovskite Solar Cells. *Nano Energy* **2021**, *82*, 105658.
3. Tanko, K. T.; Raga, S. R.; Vahedigharehchopogh, N.; Baumann, F.; Karimipour, M.; Miranda-Gamboa, R. A.; Lira-Cantú, M., The Roles of Ion Migration on Perovskite Solar Cell Operational Stability at Various Illumination Intensities. *Solar RRL* **2025**, *9*, 2500162.
4. Baumann, F.; Karimipour, M.; Padilla-Pantoja, J.; Chávez-Angel, E.; Caicedo Roque, J. M.; Pouteaux, R.; Alcalá Ibarra, A.; R. Raga, S.; Santiso, J.; Lira-Cantu, M., Strain in Halide Perovskites and Solar Cell Stability: Accelerated Stress Tests under Bias Voltage. *ACS Energy Letters* **2025**, *10*, 476-483.
5. Baumann, F., et al., Stabilizing Perovskite Solar Cells at 85 °C Via Additive Engineering and Mxene Interlayers. *EES Solar* **2025**.

ChargeFabrica: A Python-based Finite Difference Multidimensional Electro-Ionic Drift Diffusion Simulator applied to Mesoporous Perovskite Solar Cells

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Modelling non-planar perovskite solar cells (PSCs) in 1D is very challenging due to strong interfacial and geometric interactions. This affects especially mesoporous, structured tandem, phase segregated and bulk heterojunction solar cells. We present ChargeFabrica[1], an open source, two dimensional electro-ionic drift-diffusion simulation tool designed to address these challenges by simultaneously solving the coupled electronic and ionic transport equations across complex device geometries. Using ChargeFabrica, we successfully replicate experimentally observed thickness-dependent trends in current–voltage (JV) curves, the influence of ionic prebiasing and associated EQE, which cannot be fully captured by conventional one-dimensional models. By incorporating realistic device morphologies and experimentally demonstrated defect densities, the simulator accurately predicts performance losses, field inversion effects, and the impact of geometric and interfacial properties. ChargeFabrica thus provides a robust platform for understanding and optimizing the interplay between ion migration and charge collection in mesoporous PSCs and will aid future development of perovskite device architectures.

[1] Sachsenweger, T. et al, Materials Futures 2026, 5(2), 025602

Computational insights into the influence of the $MAPbI_3$ crystal order on the solar cell performance

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We present a multiscale approach to evaluate perovskite solar cell performance which determines material properties at the atomistic scale with first-principles calculations, and applies them in macroscale device models[1,2]. This work focuses on the $MAPbI_3$ (MA = CH_3NH_3) perovskite and how its phase transitions impact on its optical, electronic, and structural properties, which are investigated at the first-principles level. It is based on a nanoscale description of $MAPbI_3$, which allow to take the MA ordering into account, used to determine a hybrid exchange-correlation functional optimized to yield qualitatively correct and quantitatively accurate description of the structural and electronic properties of this family of perovskite in good agreement with experiment. The calculated optical indices are in better qualitative agreement[2] with experiment than the previously published ones based on a local description of the material determined with more sophisticated methods. The obtained optical indices, band gaps and affinities serve as input to a numerical drift-diffusion device model. This yields the performance of single junction devices, with a methodology aiming at evaluating the performance of these materials rather than modelling real efficiencies. The obtained results are systematically discussed in terms of atomic model and first-principles approximation, such as the spin-orbit coupling effects and other issues, which can lead to unphysical evaluation of the cell performance[2].

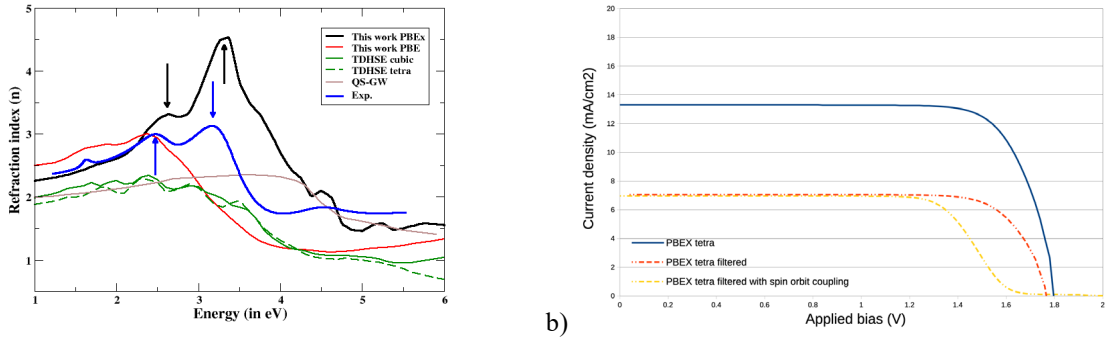

Fig. 1 : a) Refraction index and b) IV curve determined at different levels of approximation for the cubic and tetragonal phases of $MAPbI_3$, respectively.

[1] Ph. Baranek, J. P. Connolly et al., "Multiscale models for perovskite optimization", DOI: 10.4229/EUPVSEC2025/2AO.3.5 (2025).

[2] Ph. Baranek, J.P. Connolly et al., «Impact of $MAPbI_3$ phase transitions on solar cell performance», DOI: 10.48550/arXiv.2601.03737, submitted (2026).

Simulation Analysis of Recombination Junctions in Perovskite-based Tandem Solar Cells

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The recombination junction (RJ) forms an essential component of any two terminal tandem solar cell. Hence, physical models of recombination junctions are crucial ingredients in the opto-electronic simulation based on semiconductor transport equations that enables a comprehensive loss analysis and performance optimization[1,2]. While the central function of the recombination junction is always the formation of an intermediate electrical contact with minimum optical and electrical loss, a wide range of different implementations exist, from ultra-thin metal layers – popular in all-perovskite tandems[2] – to hetero-interfaces with transparent conductive oxides – widely used in perovskite-silicon tandems[1] – and to the tunnel junctions induced by heterogeneous doping as present in III-V multijunction architectures[3]. The corresponding models reflect the nature of the processes involved in the charge transfer across the junction, from non-local direct and trap-assisted tunneling to local charge hopping or pinning of the quasi-Fermi levels. While several processes might contribute in a given device, it is found that the device characteristics are rather insensitive to the choice of recombination junction model as long as the junction is not limiting the performance. On the other hand, the different physical mechanisms underlying the working principles lead to characteristic dependencies on configurational parameters of the interconnect.

Here, we discuss the characteristics of different recombination junction models used in the simulation of perovskite-based tandem solar cells within a drift-diffusion formalism. For a RJ formed by SnO_x-Au-PEDOT:PSS[4], we investigate the junction voltage required to drive a current of 13 mA/cm^2 (~ J_{MPP}) as a function of doping density and mobility in the charge transport layers as well as model-specific parameters, such as interface trap density (for the local interface recombination model), the hopping rate (for the local charge hopping model) or the work function of the ultra-thin metal (for the intermediate electrode model). To be able to screen such a large parameter space, we first validate a reduced RJ model that reproduces the junction voltage of the full tandem device for identical junction parameters. Using the reduced model, configurations are identified with junction voltage < 10 mV - or a junction specific resistance <1 mΩ cm^2 - as required for less than 1% relative PCE loss. The critical level of charge density and

mobility in the charge transport layers varies significantly between the models, with the intermediate electrode model posing less strict requirements on charge transport layer properties to reach a sufficient transfer rate than, e.g., the hopping model. Hence, in the case of thin metal films, the intermediate electrode model is found to provide both, a realistic description of the physical situation and a low-loss interconnection mechanism. On the other hand, if interface defects dominate the charge transfer, tunneling is shown to have a large impact for sizable fields in the junction region and should therefore be included in the simulation-based RJ assessment.

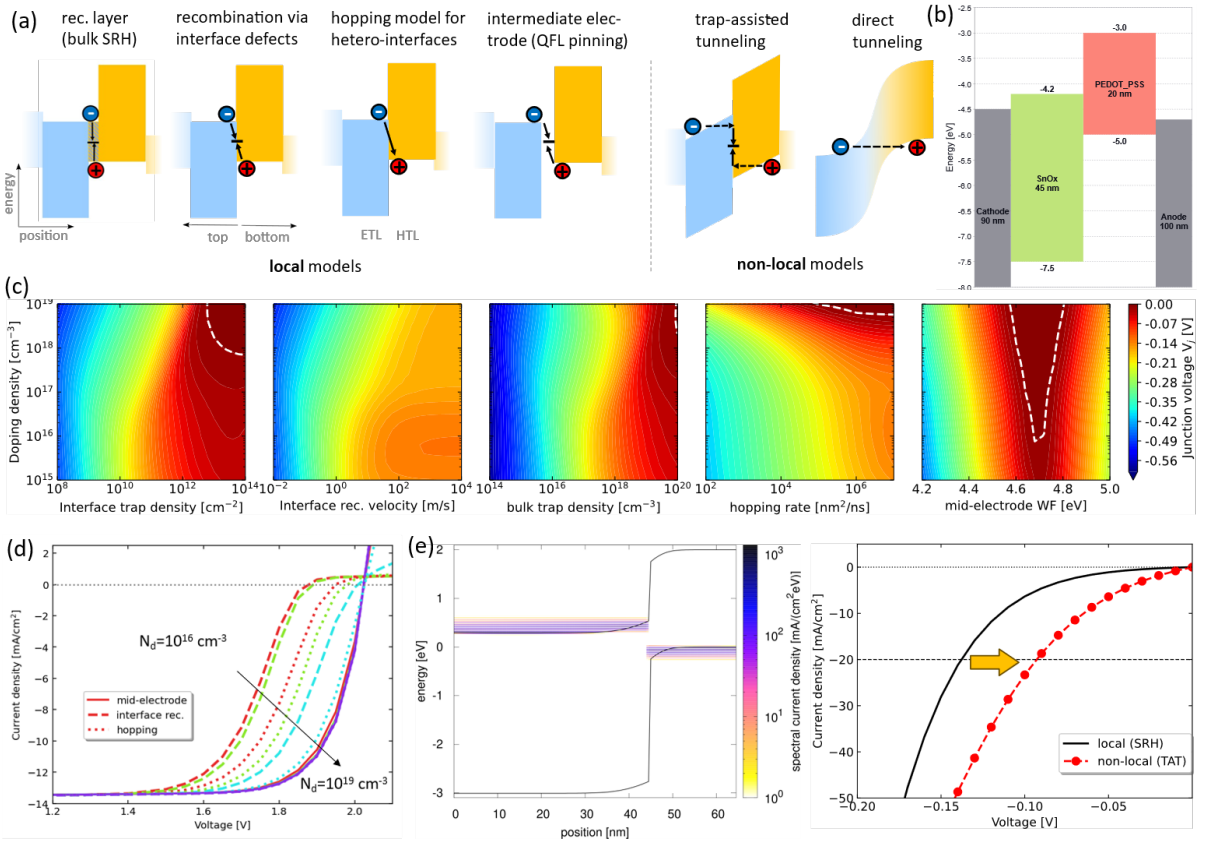

Fig. 1 (a) Local and non-local models for recombination junctions in monolithic perovskite-based tandem solar cells. (b) Implementation of a the reduced junction domain for simulation with drift-diffusion (setfos). (c) Junction voltage required to drive a current density of 13 mA/cm² (~J_{MPP}) across the RJ as a function of doping density and model-specific junction configuration (local models; dashed lines: V_j <10 mV). (d) Doping dependence of the tandem JV characteristics for different models highlights superior electrical performance of metal-based RJ. (e) The non-local trap-assisted tunneling (TAT) model provides a strongly enhanced charge transfer rate at elevated fields as compared to local interface recombination.

[1] O. Er-raji *et al.*, 'Loss Analysis of Fully-Textured Perovskite Silicon Tandem Solar Cells: Characterization Methods and Simulation toward the Practical Efficiency Potential', *Sol. RRL*, vol. 7, no. 24, p. 2300659, Dec. 2023, doi: 10.1002/solr.202300659.

[2] U. Aeberhard, S. J. Zeder, and B. Ruhstaller, 'Effects of Photon Recycling and Luminescent Coupling in All-Perovskite Tandem Solar Cells Assessed by Full Opto-electronic Simulation', *Sol RRL*, vol. 8, no. 14, p. 2400264, Jul. 2024, doi: 10.1002/solr.202400264.

[3] M. Hermle, G. Létay, S. P. Philipps, and A. W. Bett, 'Numerical simulation of tunnel diodes for multi-junction solar cells', *Prog Photovolt Res Appl*, vol. 16, no. 5, pp. 409–418, 2008, doi: 10.1002/pip.824.

[4] H. Lai et al., "Tailored PEDOT:PSS phase segregation for high-efficiency flexible all-perovskite tandem solar cells and mini-modules," *Nature Communications*, vol. 16, no. 1, p. 11468, 2025, doi: 10.1038/s41467-025-66479-0.

Monolithic versus mechanically stacked perovskite/Si tandem solar cells: a first benchmark

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This work compares two perovskite/silicon (Si) tandem solar cell configurations: two- and four-terminal designs. Two-terminal devices offer high efficiency under standard test conditions, driven by reduced parasitic absorption, compatibility with industrial Si module integration, resilience to partial shading, and lower balance-of-system costs. However, they may suffer from current mismatch losses during operation. Four-terminal tandems provide greater flexibility in top-cell design and can achieve higher energy yield due to the absence of current-matching constraints. Their performance under standard test conditions is typically lower because of increased parasitic absorption in thicker electrodes, and they may incur higher system costs depending on the interconnection scheme. As a result, it remains unclear which of these two architectures will ultimately prove more advantageous.

This contribution reviews CSEM's R&D activities on both device architectures, covering device development, module integration, outdoor monitoring, and failure mode analysis. In particular, recent demonstrations of two-terminal tandems with screen-printed electrodes achieving a power conversion efficiency of 34% will be presented. In addition, an experimental comparison of the energy yield of both architectures, based on the same perovskite absorber and operated side by side under outdoor conditions, will be discussed.

Evaluating ionic and opto-electronic properties of the perovskite sub-cell in silicon-perovskite tandem devices

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Experimental techniques and analysis methods addressing the mixed-conducting properties of halide perovskite-based single junction solar cells are gradually reaching maturity. However, the application of similar or novel approaches to tandem systems is still at its infancy.[1],[2] A key challenge is the fact that in typical 2-terminal tandem devices one lacks knowledge of the sub-cell voltages, requiring more sophisticated analysis and assumptions in the evaluation of experimental data.

Here, we present a dual wavelength optoelectronic characterization approach applied to lab-scale perovskite-silicon tandem devices.[3] By integrating a blue (405 nm) and a NIR (950 nm) LED in our optoelectrical measurement setup, we are able to apply independent optical bias to the two sub-cells. By further controlling the transient signal of either LED, we demonstrate a wide-range of optoelectronic transient and frequency domain techniques for the characterization of perovskite-silicon tandem cells.

First, we evaluate transient photocurrent measurements, which we use to map photo-current limitations and current-matching in the device. Next, we analyze the transient current-voltage response of the cell as a function of scan rate and pre-bias voltage, exploring the effect of having the silicon or the perovskite as the limiting sub-cell. The results highlight how the nature of an even minor current mismatch has major implications on the overall device response. We then use impedance spectroscopy under selected optical bias conditions to highlight the electron-

[1] M. Jošt, L. Kegelmann, L. Korte, and S. Albrecht, Monolithic Perovskite Tandem Solar Cells: A Review of the Present Status and Advanced Characterization Methods Toward 30% Efficiency, Advanced Energy Materials **10**, (2020).
[2] C. Messmer, D. Chojniak, A. J. Bett, S. K. Reichmuth, J. Hohl-Ebinger, M. Bivour, M. Hermle, J. Schön, M. C. Schubert, and S. W. Glunz, Toward more reliable measurement procedures of perovskite silicon tandem solar cells: The role of transient device effects and measurement conditions, Prog Photovolt Res Appl. 1 (2024).
[3] D. Turkay et al., Synergetic substrate and additive engineering for over 30%-efficient perovskite-Si tandem solar cells, Joule **8**, 1735 (2024).

hole recombination impedance in the silicon and in the perovskite sub-cells. Based on previous work on the interpretation of such data,[4] we identify the dominant loss in the perovskite sub-cell. To validate our hypothesis further, we use Setfos to perform combined optical and ionic-electronic drift-diffusion simulations of all measurements performed on the complete tandem device. The resulting model reproduces the overall experimental trend in the time and frequency-domain, also providing further insights into the role of mobile ions on the electronic charge carrier dynamics of the perovskite sub-cell. We conclude by commenting on additional chemical and electrochemical effects that could improve the description of the observed slow dynamics in frequency domain data.[5]

In summary, our study demonstrates a combined experimental-simulation approach to the investigation of sub-cell losses in silicon-perovskite tandem solar cells. The presented methodology based on optoelectronic characterization under dual wavelength optical bias shows great potential for providing key input to optimization cycles of the technology.

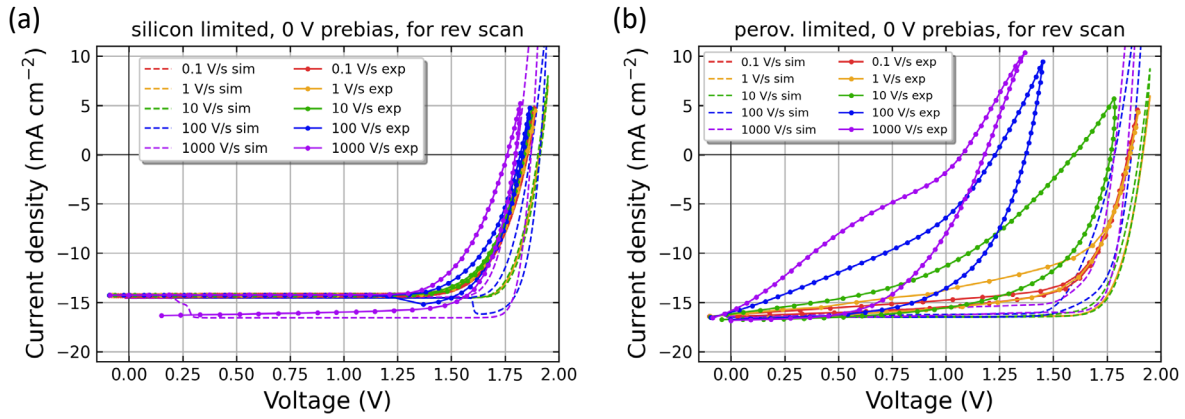

Fig. 1 Current-voltage transients performed on a perovskite-silicon tandem solar cell at different scan rates after a prebias step at 0 V for 10 s. By varying the light bias condition, either (a) a silicon sub-cell limited or (b) a perovskite sub-cell limited response is obtained. Dashed lines represent drift-diffusion simulations.

[4] D. Moia, Equivalent-circuit modeling of electron-hole recombination in semiconductors and mixed ionic-electronic conductors, Phys. Rev. Applied **23**, 014055 (2025).
[5] D. Moia and J. Maier, Defect chemistry of mixed ionic–electronic conductors under light: halide perovskites as a master example, Mater. Horiz. **13**, 763 (2026).

Industrial testing of perovskite solar cells and modules – can simulations help devise novel characterization protocols?

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Perovskite solar cells and modules require novel current–voltage (IV) characterization methods for industrial photovoltaic (PV) testing, as typical PV production line cycle times are on the order of seconds. Currently, silicon solar cell and module IV characterization is typically performed using pulsed solar simulator flashes with IV acquisition times below 100 ms. Metastable perovskite solar cells on the other hand require slow IV scans on the order of several minutes to obtain stabilized IV characteristics from which relevant PV parameters for industrial quality control and classification can be extracted.
In this work, we develop fast industrial IV characterization methods based on advanced electro-optical characterization of perovskite solar cells combined with numerical simulations. The method was tested in our laboratory and the preliminary results were encouraging, although further work is required to refine and validate the approach.

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Characterizing Ion Migration in Perovskite Solar Cells by Coupling Impedance Spectroscopy and Drift-Diffusion Simulations

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The presence of mobile ions is inherent in perovskite solar cells (PSCs), strongly influencing charge transport, recombination dynamics, and charge extraction. Despite extensive research, the interpretation of electrical characterization techniques remains challenging due to the strong coupling between ionic and electronic processes. As a result, identifying the operating conditions under which ionic and electronic contributions can be disentangled remains an open question. In this work, we present an integrated experimental-theoretical framework that combines impedance spectroscopy (IS) under different biasing conditions with drift-diffusion (DD) simulations to investigate ion migration and its impact on device operation in inverted (p–i–n) PSCs.[1,2]

By systematically analyzing the frequency-dependent response under short-circuit and open-circuit conditions, we identify characteristic signatures associated with ionic redistribution, charge-carrier transport, and recombination. The DD simulations provide a physics-based interpretation of the measured impedance spectra, enabling the disentanglement of interfacial energetic effects from ionic phenomena and allowing the extraction of key parameters such as carrier mobilities, mobile-ion density, and recombination-related characteristics. Particular attention is given to the influence of ion accumulation at selective contacts and its interaction with interfacial band offsets, which critically affect the device impedance response and ideality-factor analysis.

The results demonstrate that coupling IS with DD modeling offers a powerful route to quantitatively characterize ionic transport while avoiding common ambiguities associated with equivalent-circuit-only interpretations. This methodology provides deeper insight into the interplay between ionic and electronic processes in PSCs and establishes a robust framework

[1] O. Almora, P. López-Varo et al. "Instability analysis of perovskite solar cells via short-circuit impedance spectroscopy: A case study on NiOx passivation" J. Appl. Phys. 136, 094502 (2024)

[2] Juan Pablo Medina-Flechas, Raj Dashrath Patel et al. "Characterization of ionic–electronic transport and recombination in perovskite solar cells under multi-biasing conditions" EES Solar. (2026)

for diagnosing performance limitations and guiding the design of more efficient and stable perovskite photovoltaic devices.

Perovskite-Inspired Indoor Photovoltaics: Towards Energy-Autonomous Systems

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Indoor photovoltaics (IPVs) are emerging as a key enabling technology for powering low-energy electronics, wireless sensor nodes, and distributed Internet of Things (IoT) systems[1]. In this context, perovskite-inspired materials (PIMs) have attracted growing attention as a promising class of absorbers, combining optoelectronic properties well-suited for low-light operation with improved chemical stability and reduced toxicity compared to lead-based perovskites[2].

This talk will provide an overview of our recent work on PIM-based indoor photovoltaics, with a focus on materials design, device physics, and system-level relevance. Particular attention will be given to antimony- and bismuth-based compounds[3-5] and vacancy-ordered structures, where compositional engineering, such as A-site alloying[3,5] and bandgap tuning, has led to improved charge carrier dynamics and higher photovoltage under low-intensity illumination. These advances have recently enabled efficiencies beyond 10% under typical indoor lighting conditions, highlighting the rapid progress of the field[4].

Beyond efficiency, the talk will address underexplored aspects that are increasingly recognized as performance-limiting factors under realistic operating conditions. These include spectral mismatch effects under different artificial light sources, the role of interfacial energetics and defect tolerance at low carrier densities, and the often overlooked stability challenges specific to indoor environments, such as prolonged operation under weak but continuous illumination[6,7]. The importance of realistic testing conditions and device architectures optimized for long-term operation, rather than peak efficiency, will be emphasized[7].

Finally, I will connect these advances to the broader vision of energy-autonomous systems. By integrating efficient and stable PIM-based IPVs with ultra-low-power electronics, it becomes possible to move towards maintenance-free, battery-less IoT platforms[8]. Key research directions to bridge the gap between laboratory-scale demonstrations and scalable, deployable technologies will be outlined.

References

1. Grandhi, G.K. et al., *Nat. Rev. Clean Technol.* **2025**, *1*, 132.
2. Huang, Y.-T. et al., *Nanotechnology* **2021**, *32*, 132004.
3. Lamminen, N. et al., *Adv. Energy Mater.* **2023**, *13*, 2203175.
4. Lamminen, N. et al., *ACS En. Lett.* **2025**, *10*, 3415.

5. Krishnaiah, M. et al., *Adv. Energy Mater.* **2025**, *15*, 2404547.
6. Hoye, R. et al., *Joule* **2025**, *9*, 102127.
7. Asuo, I.M. et al., *Adv. Energy Mater.* **2026**, *16*, e06091.
8. Grandhi, G.K. et al., *ACS En. Lett.* **2026**, *11*, 3, 2474

Spatially Resolved and Subcell-Selective Characterization of Perovskite Solar Modules

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Perovskite solar modules have attracted considerable attention as a promising next-generation photovoltaic technology owing to their high power conversion efficiency, low-temperature processability, and compatibility with scalable thin-film fabrication. However, the transition from laboratory-scale single cells to module-level devices is still accompanied by substantial efficiency losses and operational instability. Since perovskite modules consist of multiple series-interconnected subcells, conventional module-level characterization tends to yield averaged device responses, masking local performance variations arising from defects, material nonuniformity, interfacial degradation, and subcell-dependent instability. Therefore, spatially resolved and subcell-selective diagnostic tools are essential for identifying the origins of performance loss during scale-up.

In this work, we present an integrated characterization platform that combines two complementary diagnostic approaches: (i) a high-speed laser beam induced current (LBIC) imaging system for spatially resolved photocurrent mapping, and (ii) a subcell-selective electrical characterization platform based on a dual-end subcell diagnostic contact architecture for current–voltage (*J–V*), electrochemical impedance spectroscopy (EIS), and maximum power point tracking (MPPT) measurements at the individual subcell level.

The high-speed LBIC system employs a 532 nm pulsed laser as the excitation source and a galvanometer-based mirror scanning mechanism to rapidly image selected regions of the solar cell module. Laser trigger, photodiode, and photocurrent signals are synchronously acquired via a high-speed digitizer controlled through a LabVIEW program, and two-dimensional LBIC maps are subsequently reconstructed in MATLAB. The system achieves a lateral resolution of approximately 60 μm, enabling the visualization of local photocurrent distributions and the identification of defect-related regions across large-area modules in a non-destructive manner.

Complementing the spatial imaging capability, the dual-end subcell diagnostic contact architecture provides selective electrical access to both terminals of individual subcells without disrupting the primary series-interconnection pathway of the module. This design enables independent J–V, EIS, and MPPT measurements at the subcell level, allowing the separation of resistive and capacitive contributions associated with charge transport, recombination, and interfacial processes, as well as the assessment of time-dependent operational stability under realistic working conditions. Systematic comparison of different dual-end contact designs further clarifies the influence of contact architecture on measurement reliability and subcell-resolved diagnostic accuracy.

Together, the high-speed LBIC imaging and subcell-selective electrical characterization provide a comprehensive, multi-scale diagnostic framework for perovskite solar modules. This integrated platform enables the correlation of spatially resolved photoelectrical responses with subcell-level impedance and stability data, offering a more precise route for identifying the origins of efficiency loss and degradation. The proposed approach is expected to support defect detection, local performance assessment, failure analysis, and rational optimization of perovskite solar modules toward reliable commercialization.

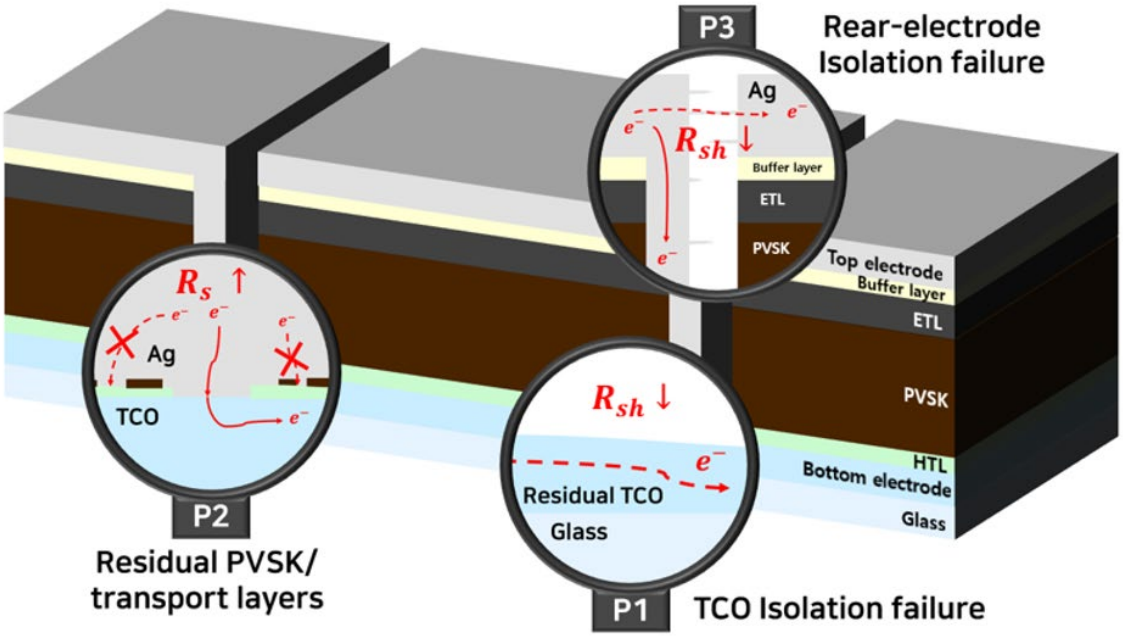

Fig. 1 Schematic of defects origin in perovskite solar module.

The use of Ti_3C_2Tx – Mxene to overcome insulating behavior in polymeric buffer layers for Perovskite Solar Cells

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Achieving inverted perovskite solar cells (PSCs) that simultaneously exhibit high power conversion efficiency (PCE) and long-term operational stability remains challenging due to intrinsic defects and the susceptibility of perovskite materials to environmental degradation. Incorporating ultrathin polymeric interlayers has emerged as an effective strategy to passivate interfacial defects, improve energy-level alignment, and provide a barrier against extrinsic degradation factors. Poly(methyl methacrylate) (PMMA) is particularly attractive because its carbonyl (C=O) groups can coordinate undercoordinated Pb^{2+} ions through Lewis acid-base interactions, suppressing trap states and mitigating ion migration. Polyethylenimine (PEI), on the other hand, is widely employed as a cathode interlayer owing to the presence of amine groups that induce molecular dipoles and lower the electrode work function, thereby facilitating electron extraction. However, the insulating nature of both polymers may increase the series resistance and limit device performance.

In this work, $Ti_3C_2T_x$ MXene nanosheets were incorporated into PMMA[1] and PEI[2] matrices to form conductive solution-processable composite interlayers (PMMA/MX and PEI/MX) for p–i–n perovskite solar cells. Structural and electrical characterization reveal that the presence of MXene improves interfacial properties, suppresses non-radiative recombination, extends carrier lifetime, and promotes more efficient extraction of photogenerated charges. Consequently, both composite layers lead to enhanced photovoltaic performance, mainly through increases in open-circuit voltage (Voc) and fill factor (FF).

The most significant improvement was obtained with PEI/MX. While devices employing pristine PEI exhibited a PCE of 18.9 ± 0.6%, MXene incorporation increased the average efficiency to 22.0 ± 0.8%, with a champion device reaching 23.1%. Figure 1 summarizes the proposed mechanism and supporting Kelvin probe measurements. Beyond the conductivity en-

hancement expected from the flakes, electrical analyses reveal that MXene acts as charge accumulation centers within the PEI matrix, generating an additional electrostatic potential at the PCBM/PEI/MX/Ag interface that reinforces the built-in electric field. Kelvin probe measurements show pronounced and reversible light-induced work-function modulation in Ag/PEI/MX/PCBM structures, substantially larger than in pristine PEI, providing direct evidence of photoinduced charge accumulation. Consistently, CELIV and capacitance-voltage (C–V) measurements reveal increased built-in potential and Voc, demonstrating that charge accumulation on MXene flakes enhances carrier extraction and overall photovoltaic performance.

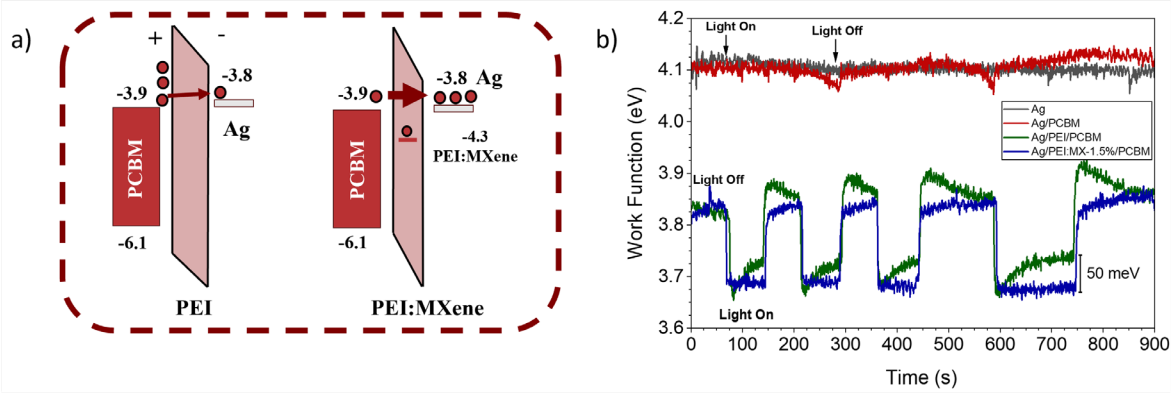

Fig. 1 (a) Schematic illustration of charge accumulation on $Ti_3C_2T_x$ MXene flakes dispersed in PEI, generating an additional electrostatic potential at the PCBM/PEI:MX/Ag interface and reinforcing the built-in electric field. (b) Kelvin probe measurements under dark and illumination conditions for Ag/PCBM, Ag/PEI/PCBM and Ag/PEI:MX/PCBM structures. The larger reversible work-function modulation observed in PEI:MX provides direct evidence of photoinduced charge accumulation associated with MXene flakes.

These findings demonstrate that MXene-containing polymer interlayers provide functionalities beyond conductivity enhancement and defect passivation. In particular, PEI/MX enables interfacial electrostatic engineering through charge accumulation, offering a powerful route to simultaneously enhance built-in voltage and carrier extraction. Conductive polymer/MXene composites thus emerge as promising multifunctional interlayers for next-generation high-efficiency and stable inverted perovskite solar cells.

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[1] J. P. F. Assunção, H. G. Lemos, et al., "Interface passivation with $Ti_3C_2T_x$-MXene doped PMMA film for highly efficient and stable inverted perovskite solar cells", J. Mater. Chem. C,12, 562-574, (2024)

[2] J. P. F. Assunção, H. G. Lemos, et al., "Charge-Transfer Enhancement by PEI/MXene Buffer Layer for Boosting Performance of Inverted Perovskite Solar Cells", ACS Appl. Mater. Interfaces, 18, 20, 28638–28650, (2026)

Inversion of the Impedance Response towards Physical Parameter Extraction using Interpretable Machine Learning

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Interpreting the impedance response of perovskite solar cells (PSCs) is challenging due to the complex coupling of ionic and electronic motion. While drift-diffusion (DD) modelling is a reliable method, its mathematical complexity makes directly extracting physical parameters from experimental data infeasible. This work uses DD modelling to generate a large synthetic dataset of impedance spectra for a standard TiO_2/MAPI/spiro configuration. This dataset trains machine learning (ML) models to predict recombination and ionic parameters from impedance measurements. A Gradient Boosting Regressor, using features from a generalized equivalent circuit, showed the best performance. Interpretative analysis indicates that open-circuit impedance experiments best probe recombination losses, while short-circuit conditions are more adequate for extracting ionic features like concentrations and mobilities. The trained ML models were tested on experimental spectra, confirming that the inferred physical parameters could reproduce the data. For the studied configuration, predicted ion concentrations were (1.3-3.3) × 10^{17} cm^{-3}, ion mobilities were (5-7) × 10^{-11} $cm^2V^{-1}s^{-1}$, and surface recombination velocities were 7-9 and 23-40 m/s. This approach provides insights into the physical information extractable from impedance measurements and paves the way for ML models to unambiguously derive efficiency-determining parameters for solar cells[1]. Other examples for functionalized perovskite interfaces will also be presented in the talk.

[1] Mahmoud Nabil, Isel Grau, Ricardo Grau-Crespo, Said Hamad and Juan A. Anta. "Inversion of the impedance response towards physical parameter extraction using Interpretable Machine Learning" Advanced Energy Materials no. 20 (2026): e06352. https://doi.org/10.1002/aenm.202506352

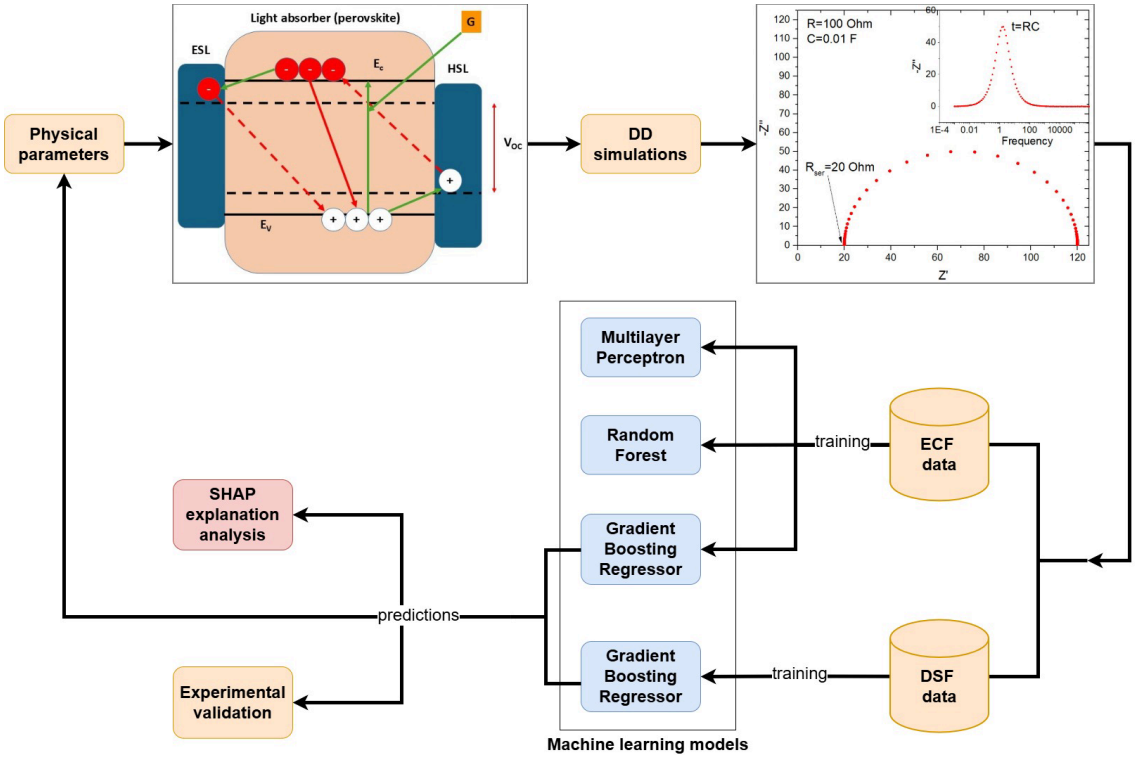

Fig. 1 Overview of the workflow used for data generation, model training, and validation. Physical parameters are first sampled and passed to DD simulations to produce two distinct feature sets: Equivalent Circuit Fitting (ECF) and Direct Signal Featurization (DSF). These simulated datasets are then used to train multiple machine learning models to learn the inverse mapping from features to physical parameters. The trained models generate predictions, which are subsequently analyzed through SHAP-based explainability and validated against experimental measurements.

Prediction of Steady-State JV Characteristics from Transient Measurements Using Physics-Based Modeling and Bayesian Optimization

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Fast and reliable prediction of steady-state device performance is essential for the characterization and optimization of perovskite solar cells. In this work, we present a methodology to derive steady-state current–voltage (JV) characteristics from transient JV measurements by combining a physics-based device model with Bayesian optimization. Material parameters are extracted from time-dependent current signals obtained at different scan rates, enabling calibration of the model and subsequent prediction of steady-state behavior.

The approach reformulates JV scans as time-dependent signals, allowing direct comparison between experimental data and simulations across multiple scan speeds. We show that parameter extraction based on a single scan speed results in poor predictive capability, whereas a multi-objective optimization framework significantly improves robustness and accuracy. Bayesian optimization accelerates parameter extraction by replacing expensive objective function evaluations with an efficient, data-driven sequential search.

Validation on synthetic datasets demonstrates excellent agreement between simulated and reference JV curves, even when extracted parameters deviate from the ground truth, indicating that the most relevant physical mechanisms are correctly captured. Application to experimental data, however, reveals limitations of the current model, particularly at high scan rates, suggesting the presence of missing physical effects or insufficient parameterization.

The results highlight the strong dependence of predictive performance on the accuracy of the underlying physical model. Future work will focus on model refinement and the integration of data-driven approaches to further improve predictive capabilities and enable rapid assessment of device performance under realistic operating conditions.

Physics-Informed Deep Learning for Non-Destructive Extraction of Depth-Resolved Charge Collection Profiles in Perovskite Solar Cells

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Spatially resolved charge-collection efficiency is a critical, yet experimentally inaccessible, descriptor of perovskite solar-cell performance. The external quantum efficiency (EQE) spectrum encodes this information implicitly through a physics-defined integral transform but inverting it reliably has remained intractable because the problem is ill-posed, and the solution space spans qualitatively distinct recombination regimes[1]. Here we present a deep-learning framework that learns this inverse mapping directly from large-scale device simulations. We introduce a five-class taxonomy of charge collection efficiency (SCE) depth profiles—ranging from severe-collapse to gentle monotonic decay and exploit it at every stage of training: stratified data splitting, class-aware sample re-weighting, and a multi-component loss that penalises gradient mismatch, back-contact accuracy, and drop-event localisation. Three progressively physics-enriched architectures are compared a hybrid CNN baseline, a physics-informed model that enforces EQE self-consistency through a differentiable forward operator, and a physics-guided cross-attention network whose attention map is biased by the depth-resolved photogeneration profile and lastly, a cross-attention model that maps the relationship between perovskite layer absorptance and EQE to predict SCE. Conformal-calibrated Monte Carlo Dropout provides per-depth uncertainty intervals with guaranteed coverage. On a held-out test set of ~450 simulated devices the best model achieves an overall RMSE of 0.0365 and reduces the RMSE around 47% on sharp-drop profiles by relative to the physics-naive baseline. Gradient-saliency analysis confirms that the networks leverage spectrally localised EQE features consistent with known absorption physics. This work establishes a practical, non-destructive route to depth-resolved charge transport diagnostics from a single spectral measurement.

[1] Segev, Gideon, et al. "The spatial collection efficiency of charge carriers in photovoltaic and photoelectrochemical cells." *Joule* 2.2 (2018): 210-224.

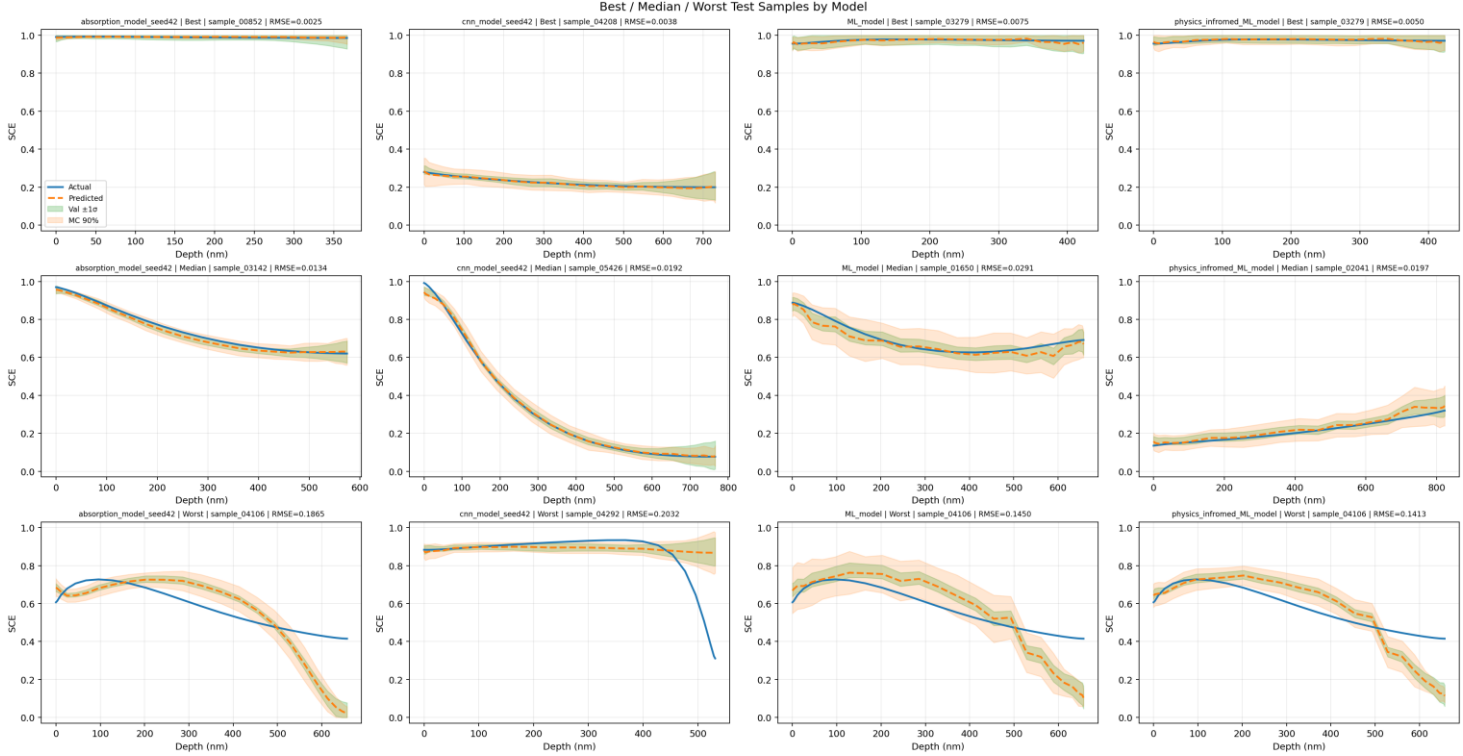

Figure 1: : Comparison of test set depth profiles across different model architectures. Columns represent the four evaluated models, while rows display representative test samples corresponding to the best (lowest RMSE, top row), median (middle row), and worst (highest RMSE, bottom row) performances. Solid blue lines indicate the actual profiles, and dashed orange lines represent model predictions. Shaded regions illustrate uncertainty estimates, distinguishing between the validation set error estimation (Val ± 1σ green) and the 90% Monte Carlo (MC) dropout confidence intervals (orange).

From Microscopic Heterogeneity to Operational Durability: Interpretable Learning for Perovskite Systems

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Perovskite photovoltaics have achieved substantial progress in power conversion performance; however, the realization of long-term operational stability remains limited by the challenge of identifying descriptors that reliably capture degradation mechanisms across different length scales[1]. Conventional characterization approaches often rely on spatially averaged measurements, which can obscure localized variations in optical or structural properties and reduce the effectiveness of predictive models.

In this study, a hierarchical data-driven framework is utilized to investigate stability-related characteristics in 3D/2D perovskite systems at both thin-film and device levels. Two independent datasets were analyzed separately using interpretable machine-learning approaches. The first dataset consisted experimentally fabricated 3D/2D perovskite films with different organic capping configurations, where spatially resolved photoluminescence distributions were used to generate descriptors sensitive to local heterogeneity and degradation evolution. The second dataset comprised a database of 3D/2D perovskite solar cells collected from the literature and used to examine factors governing long-term device behavior.

Independent machine-learning analyses were performed to determine the dominant descriptors associated with each system (Figure 1). Comparison of the extracted feature importance revealed that the parameters governing thin-film stability differ from those controlling device-level durability. At the film scale, material-related characteristics such as molecular structure and compositional properties exhibited stronger influence, whereas device-scale behavior was more strongly associated with interfacial effects and initial photovoltaic performance metrics. These observations indicate that stability-controlling mechanisms are not directly transferable across scales.

[1] Y. Rong, Y. Hu, A. Mei, H. Tan, M. I. Saidaminov, S. I. Seok,... & H. Han" Challenges for commercializing perovskite solar cells ", Science, 361(6408), eaat8235, (2018).

The proposed methodology establishes a route for linking localized material characteristics with macroscopic device behavior and highlights the importance of scale-specific descriptor selection for accelerated development of durable perovskite optoelectronic systems.

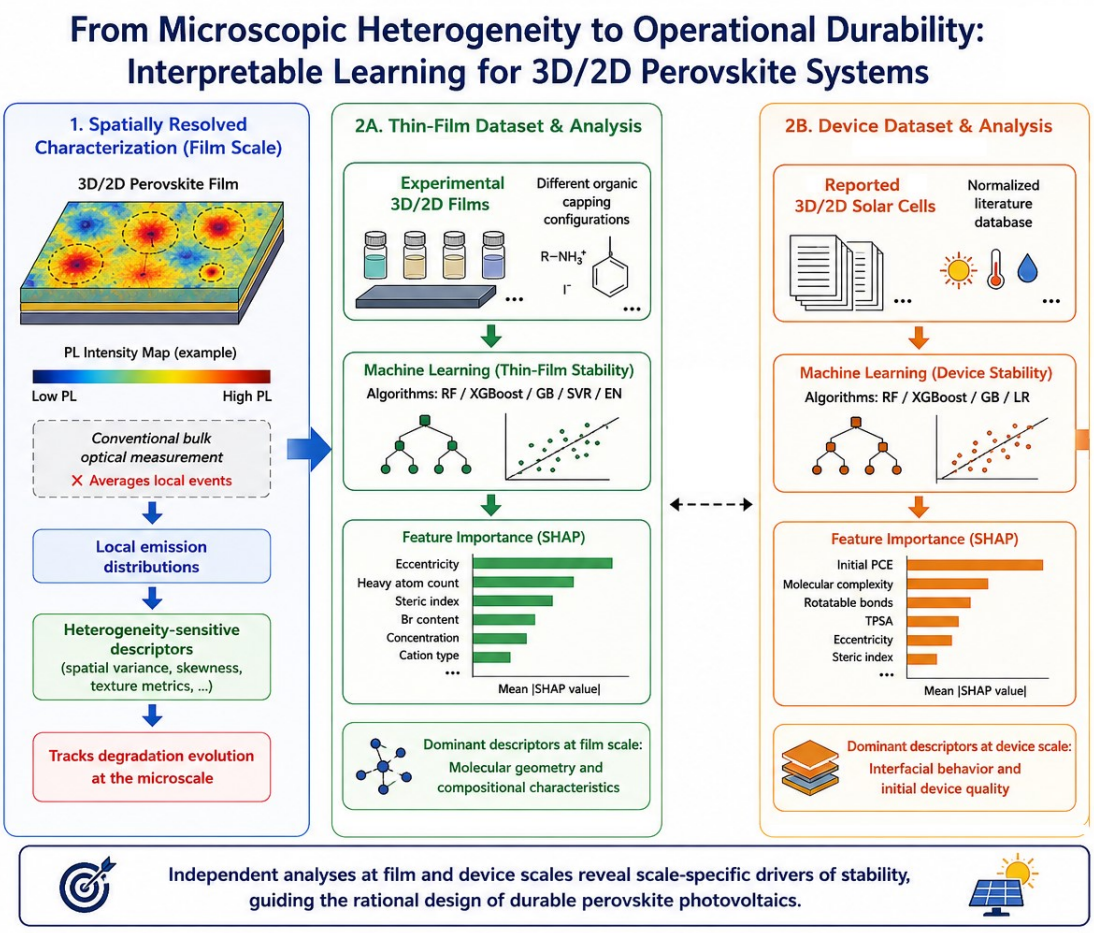

Fig. 1 Workflow of the proposed multi-scale and interpretable learning framework for 3D/2D perovskite stability analysis. Independent machine-learning models were applied to experimentally fabricated 3D/2D films and a database of reported 3D/2D solar cells, enabling identification and comparison of scale-specific descriptors governing thin-film robustness and long-term device durability.

Quantifying power loss from localized shunts in large-area perovskite-silicon tandem solar cells

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Two-terminal perovskite-silicon tandem solar cells have reached certified power conversion efficiencies above 35% and are the most promising near-term route beyond the efficiency limit of silicon photovoltaics [1]. As cells are scaled from laboratory devices to industrially relevant sizes, their performance becomes increasingly governed by two-dimensional effects: lateral current redistribution through the sheet resistance R_m of the recombination junction between the sub-cells, and the impact of localized defects ("shunts") in the perovskite top cell. A high R_m is usually regarded as detrimental, yet it can also isolate a defect from the rest of the cell — the basis of the "shunt-quenching" design concept, introduced for perovskite-silicon tandems by Blaga *et al.* [2] and recently re-examined by Fell *et al.* [3].

Within the DICE project, we extend Fluxim's large-area solver Laoss [4] to the two-terminal tandem architecture. A finite-element discretization on the cell plane resolves the lateral potentials of the two electrodes and of the recombination junction, while the local current-voltage response of each sub-cell is precomputed as a Setfos drift-diffusion lookup table. A localized defect is represented by an ohmic resistance R_{sh} on a small patch of the top cell. For each choice of R_m, shunt strength R_{sh}, and shunt position, the maximum tandem-cell power P_d^* follows from an inner maximum-power-point optimization. A discrete adjoint [5] provides the gradients with respect to all design parameters from two linear-system solves, independent of their number. For the position statistics shown in Fig. 1 below, all 4397 shunt locations of the coarse mesh are evaluated exhaustively, which remains tractable on a workstation.

Fig. 1 shows the resulting power ratio P_d^*/P_d^{ref} as a function of R_m for a fixed strong shunt, the shaded band giving the spread over all defect positions. The median follows a sigmoid across four decades of R_m: at small R_m the sub-cells are strongly coupled in the lateral direction, and the shunt loss is spread over the whole cell, whereas at large R_m the defect is laterally decoupled and the median power saturates near 0.91. This residual loss of about 9% far exceeds the area fraction of the defect, so it is electrical rather than geometric in origin. Most notably, the position-induced spread is largest — and markedly right-skewed — in the transition regime ($R_m \approx 10^2$–10^3 Ω/sq): the cell is most sensitive to *where* the defect sits not in the worst or the best case, but in between. A high recombination-junction sheet resistance thus simultaneously raises the worst-case power and collapses its dependence on defect position.

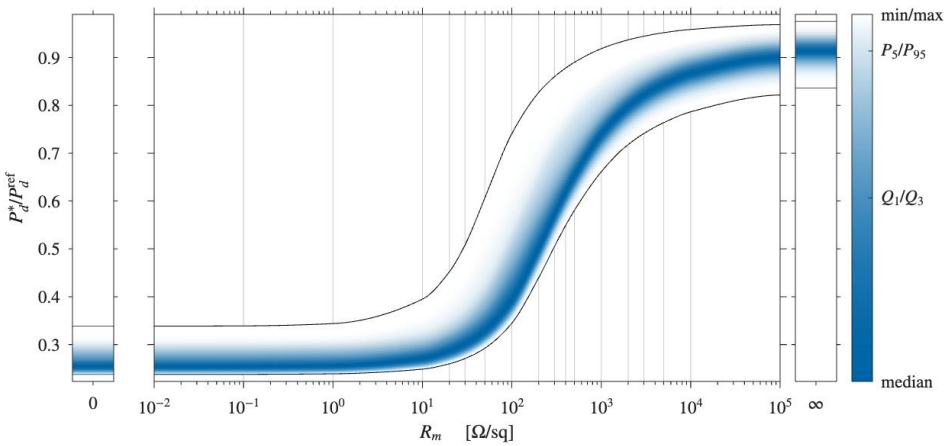

Fig. 1 Normalized maximum tandem-cell power P_d^*/P_d^{ref} over all 4397 shunt positions versus the recombination-junction sheet resistance R_m, for a fully shorting top-cell shunt ($R_{sh} = 0$). Color encodes the spread of the power over all shunt positions (darkest at the median, white at the extremes; see color bar), black curves the min/max envelope, thin gray lines the computed R_m values. The narrow side columns are the limits $R_m = 0$ and $R_m = \infty$; in the latter the median power saturates near 0.91. Power is normalized to the shunt-free 1×1 cm^2 cell with maximum power $P_d^{ref} \approx 29.2$ mW.

From the same framework we obtain design curves $R_{sh}^*(R_m)$ that give, for a prescribed power tolerance, the shunt strength still admissible at each R_m (shown in the talk). This complements earlier equivalent-circuit [2] and device-simulation [3] studies of shunt quenching: rather than assessing whether resistive isolation suppresses a shunt for a given configuration, we treat the defect position as a random variable and map the full R_m dependence into quantitative tolerance bounds. The adjoint machinery will further serve to extract local material parameters from the multispectral electro- and photoluminescence images acquired in the project, linking shunt-tolerant design rules to quantitative defect characterization in industrially relevant tandem cells.

[1] J. Werner *et al.*, Perovskite/silicon tandem solar cells: marriage of convenience or true love story?, Adv. Mater. Interfaces 5, 1700731 (2018).
[2] C. Blaga *et al.*, Palliating the efficiency loss due to shunting in perovskite/silicon tandem solar cells through modifying the resistive properties of the recombination junction, Sustain. Energy Fuels 5, 2036–2045 (2021).
[3] A. Fell *et al.*, Is shunt quenching relevant to minimize shunt losses in perovskite-silicon tandem solar cells?, Sol. RRL 8, 2400571 (2024).
[4] M. Diethelm *et al.*, Finite element modeling for analysis of electroluminescence and infrared images of thin-film solar cells, Sol. Energy 209, 186–193 (2020).
[5] G. Chavent, Identification of functional parameters in partial differential equations, in: R. E. Goodson, M. Polis (Eds.), Identification of Parameters in Distributed Systems, ASME, New York, 1974, pp. 31–48.

Integrated memristor for mitigating reverse-bias in perovskite solar cells

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Main text: Perovskite solar cells (PSCs) with power-conversion efficiencies comparable to established technologies, hold huge promise for becoming the future photovoltaic technology, also given their versatile low-cost and energy-efficient fabrication processes. However, PSCs are not stable under moderate reverse bias, an unavoidable situation under real-world operation, for instance caused by partial shading of a module or installation with PSCs connected in series. Approaches to address this issue have focused on engineering the device architecture to enhance the break-down voltage and mitigate the detrimental effects of reverse bias. Here we present a completely different approach that fully solves the reverse-bias issue. With our Memsol, we developed a novel concept of a solar cell with integrated memristor, which protects the solar cell and simultaneously works as a bypass element (Fig.1). The memristor is realized by area-selective deposition of an additional metal-insulator stack and shares the perovskite and electrodes with the solar-cell part. Reverse-bias and shading tests show that the Memsol remains stable and automatically toggles between low-resistance bypass state and full-efficiency solar-cell operation dependent on the illumination and bias conditions. We anticipate that our Memsol concept, which we demonstrated on a nine-cell string in the lab, will find implementation into large-scale modules accelerating their commercialization and potentially making external bypass diodes unnecessary. [1]

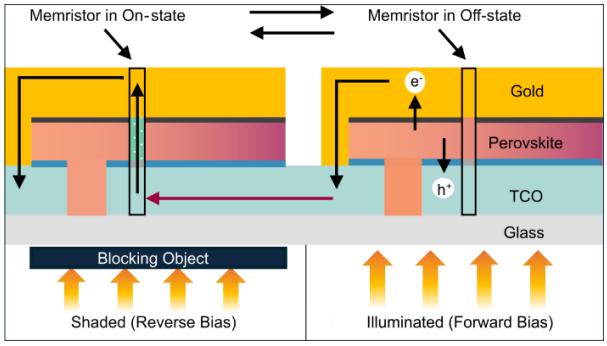

***Figure 1**: A schematic of two Memsols (solar cell with integrated memristor) connected in series, with one experiencing reverse bias due to shading.*

1. Mohammadi, M. *et al.* Integrated memristor for mitigating reverse-bias in perovskite solar cells. *Nature* **651**, 933–939 (2026).

Modelling Mixed Ionic-Electronic Memristive Systems for Hardware Neural Networks

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Artificial Intelligence (AI) is driving a rapid rise in global energy demand, largely due to inefficiencies in conventional computing architectures. Neuromorphic chips, which emulate the structure of biological neural networks, offer a promising route toward more energy-efficient AI computation[1]. Memristors (memory-resistors) are the leading candidates for realising the electronic synapses in these hardware neural networks. Memristors are passive circuit elements characterised by their ability to change resistance in response to electrical stimuli such that the device current at any point in time is a function of both the applied voltage and a history-dependent state variable[2]. Electronic currents within mixed ionic-electronic conductors (MIEC), such as hybrid organic-inorganic perovskites, can be modulated through the redistribution of slow-moving ionic carriers, making them prime candidates for use as memory materials in memristive devices[3,4]. Many challenges remain for the research field, however, including understanding the underlying resistance modulation mechanisms, device stability, and state retention.

In this presentation, I will show that increases and decreases in currents (potentiation and depression) across inert perovskite memristors (IPMs), i.e. those employing unreactive electrode materials, can be successfully reproduced using both a numerical drift-diffusion device simulator[5] and an analytical model (Figs 1 and 2).

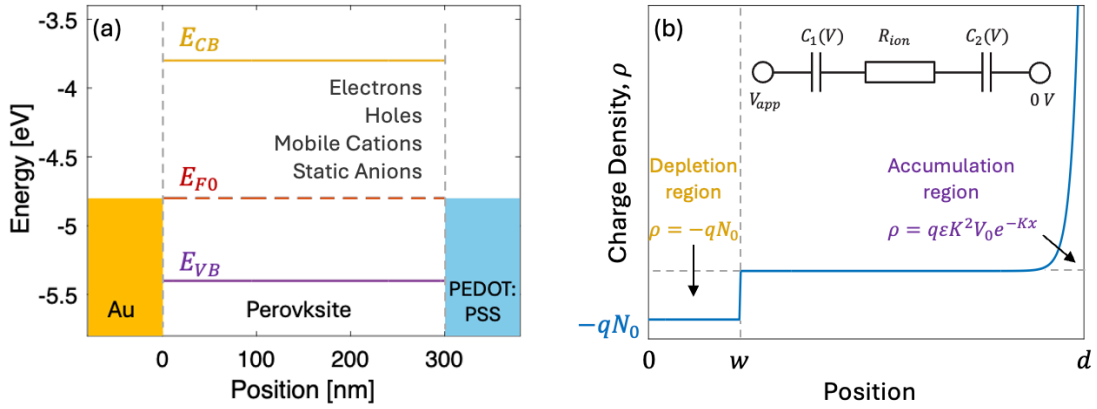

Figure 1. Schematics of the models. a) Energy level diagram of the simulated MIEC device at equilibrium. E_{CB}, E_{VB}, and E_{F0} are the conduction band, valence band, and equilibrium Fermi energies respectively. **b)** Schematic of ionic space charge as a function of position x for the analytical model. In the accumulation region the small voltage approximation to the charge density ρ is used. For the depleted region, a uniform charge density across the depletion width w is assumed. N_0 denotes is the intrinsic Schottky defect density. Inset: The equivalent circuit model used for time evolution.

The memristor device models developed for the study include both electronic carriers and relatively high concentrations of intrinsic mobile ionic carriers ($N_{SD} > 10^{17}$ cm^{-3}), compensated by static counter ions, modelling Schottky defects. The results indicate that the potentiation and depression of currents observed within IPMs can be attributed to Schottky defect migration in response to the time-averaged internal electric field generated during a series of voltage pulses applied to the device. The models show that potentiation in IPMs can be explained by confinement of the electric field to the interface regions as opposed to energetic (Schottky) barrier

modulation as previously proposed[6]. Depression of currents is achieved via the inverse process during which the potential drop becomes spatially distributed across the device. Notably, the state variable controlling the resistance in IPMs is explicitly identified as the ionic depletion width (Figs 2a and 2b). These findings provide new insight into the resistive switching mechanism underlying inert MIEC memristors more generally and suggest new design strategies for the optimisation of real-world devices.

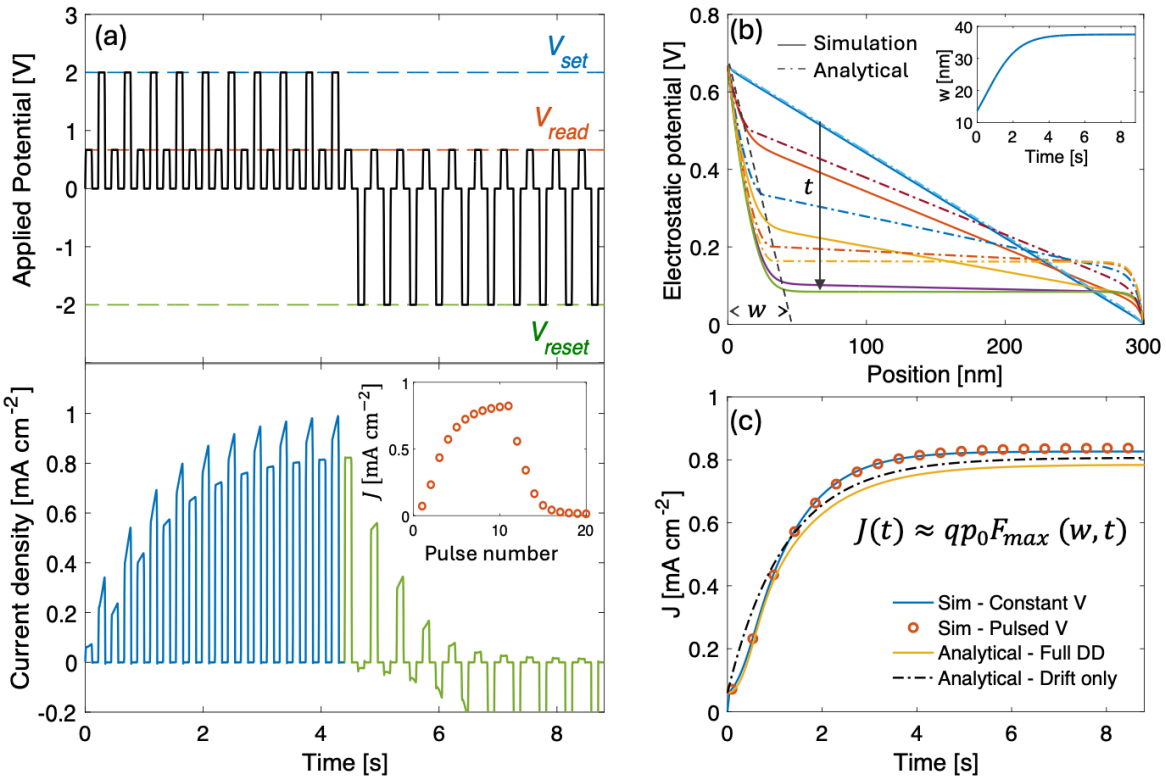

Figure 2. Potentiation and depression in the simulated and analytical models. a) Pulsed potential scheme and output current density for the simulated inert perovskite memristor. The potential scheme consists of 10 potentiation and read cycles followed by 10 depression and read cycles. The resulting current density $\boldsymbol{J(t)}$ exhibits potentiation and depression. Inset: $\boldsymbol{J}$ extracted from the penultimate data point of each read pulse. **b)** Numerical simulation and analytical solutions to the electric potential profiles as a function of time following a jump in voltage from short circuit to $\boldsymbol{v = -0.67\,V}$. Inset: The ionic depletion width transient. **c)** Current density transients for the different models. At high injection the $\boldsymbol{J}$ is proportional to the electric field at the electrode interfaces $\boldsymbol{F_{max}}$, defined by the depletion width $\boldsymbol{w}$.

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[1] Kumar, S., Wang, X., Strachan, J. P., Yang, Y. & Lu, W. D. Dynamical memristors for higher-complexity neuromorphic computing. *Nat. Rev. Mater.* **7**, 575–591 (2022).

[2] Chua, L. O. Memristor-The Missing Circuit Element. *IEEE Transactions on Circuit Theory* **18**, 507–519 (1971).

[3] Xiao, Z. & Huang, J. Energy-Efficient Hybrid Perovskite Memristors and Synaptic Devices. *Adv. Electron. Mater.* **2**, 1–8 (2016).

[4] Kim, S. J. *et al.* Linearly programmable two-dimensional halide perovskite memristor arrays for neuromorphic computing. *Nat. Nanotechnol.* https://doi.org/10.1038/s41565-024-01790-3 (2024) doi:10.1038/s41565-024-01790-3.

[5] Calado, P. *et al.* Driftfusion: an open source code for simulating ordered semiconductor devices with mixed ionic-electronic conducting materials in one dimension. *J. Comput. Electron.* **21**, 960–991 (2022).

[6] Guan, X. *et al.* Light-Responsive Ion-Redistribution-Induced Resistive Switching in Hybrid Perovskite Schottky Junctions. *Adv. Funct. Mater.* **28**, (2018).

A Two-Stage Calibration Strategy for DFN Battery Models

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Physics-based battery cell models, such as the Doyle-Fuller-Newman (DFN) model, can be used for predicting battery performance, identifying bottlenecks, and optimizing cell design. However, the accuracy of these models depends on the accurate parameterization. This contribution describes a two-stage approach for calibrating DFN models against experimental data where we separate parameters into equilibrium and rate-dependent subsets. The algorithms are implemented in the open-source software BattMo (see https://github.com/battmoteam).

First, a low-rate calibration is performed to determine thermodynamic parameters. If the data is at sufficiently low rate, we can avoid simulation of the DFN model but only calibrate and shift the underlying half-cell potentials without interference of the dynamic parameters. This procedure is often called cell balancing.

Second, the remaining parameters are associated with rate-dependent processes such as charge and mass transport in the solid electrodes, transport in the electrolyte and interfacial electrochemical reactions. For each process we choose one representative parameter to calibrate. The calibration that follows can be computationally expensive as the DFN model must be solved at each optimization step. To reduce the number of DFN solves, BattMo employs gradient-based optimization techniques, where we solve an auxiliary adjoint problem to efficiently obtain the gradients. The adjoint problem is automatically derived using automatic differentiation.

Calibrating all rate-dependent parameters simultaneously may lead to convergence to local minima. To improve robustness, we introduce a strategy where we divide the parameters into groups based on their sensitivity: first we group the parameters and calibrate the parameters with the highest sensitivity, then select the group of parameters of lower sensitivity and so forth. Finally, we perform a global calibration with all the parameters. This grouping and re-calibration procedure can be repeated until desired accuracy.

The method is demonstrated on two commercial cells: a 3.5 Ah cylindrical cell and a 64 Ah pouch cell. The results show that the proposed two-stage calibration approach provide a structured and computationally efficient methodology for calibration of DFN model parameters from experimental data.

Identifying Model Limitations via Systematic Parametrisation of Charge Transport in Lithium-ion Batteries

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Alongside cell models for diagnostics and design, robust parametrisation methods are needed to accurately predict and compare the performance of novel and commercial cell chemistries. Without standardisation, turning experimental data into useful models remains a bottleneck.

Electrochemical models are more challenging to parametrise than equivalent circuits, having more states and coupled, nonlinear dynamics, but extrapolate well to unseen conditions. The Doyle-Fuller-Newman (DFN) model, plus its reduced-order variations, is the field-standard for lithium-ion batteries[1]. For parametrisation, the effects of different processes on cell-level behaviour must be isolated e.g. by timescale separation. We employ a series of grouped-parameter models[2] to iteratively parametrise the open-circuit, thermal, diffusion, and resistance behaviour of two types of cylindrical cell (Gr-SiO_x/NCA, Gr/$LiFePO_4$) using the open-source tool, PyBOP[3]. This extends our previous half-cell parametrisation[4]. Discrepancies between experiment and simulation reveal common model limitations such as the inability of the "effective" diffusivity to describe lithium transport in a heterogeneous electrode active material.

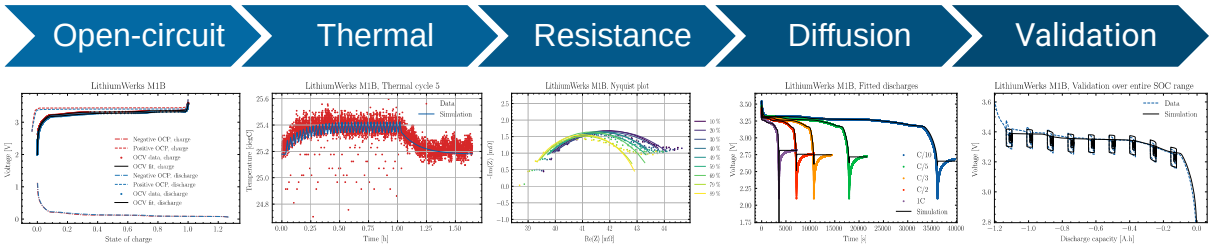

Fig. 1 Step-by-step parametrisation of a 1-D Doyle-Fuller-Newman model applied to electrochemical testing of a commercial Gr/$LiFePO_4$ battery cell.

[1] F. Brosa Planella, W. Ai, A. M. Boyce, A. Ghosh, I. Korotkin, et al. A continuum of physics-based lithium-ion battery models reviewed. Prog. Energy 4:042003 (2022)
[2] N. Hallemans, N. E. Courtier, C. P. Please, B. Planden, R. Dhoot, et al. Physics-based battery model parametrisation from impedance data. J. Electrochem. Soc. 172:060507 (2025)
[3] B. Planden, N. E. Courtier, M. Robinson, A. Khetarpal, F. Brosa Planella, and D. A. Howey. PyBOP: A Python package for battery model optimisation and parameterisation. J. Open Source Soft. 10(116):7874 (2025)
[4] R. Jackowska, N. E. Courtier, Y. Chen, B. Planden, D. Howey, et al. Transport limitations in single-crystal NCM cathode electrodes. J. Power Sources 663:238881 (2026)

Physics-Based Transmission Line Modeling of Porous Insertion Battery Electrodes: Development, Verification, and Application

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Over the past years, we have developed a comprehensive physics-based Transmission Line Model (TLM) framework for the analysis of impedance spectra of porous insertion battery electrodes. Starting from the generalized Poisson-Nernst-Planck (PNP) equations, we constructed a versatile TLM that explicitly accounts for the transport of electrons, active lithium ions, and non-active counter-ions (anions) on three separated, coupled rails [1]. This approach inherently captures all essential transport and reaction steps, including ionic migration in electrolyte-filled pores, electronic conduction in the solid phases, charge transfer at the electrolyte/particle interface, salt diffusion in electrolyte phase, and solid-state diffusion within active material particles. A key advantage of our framework is its direct physical foundation, which allows for the quantitative extraction of meaningful parameters such as chemical capacitance(s), exchange currents, and for example electrode tortuosity [2] from impedance data. To reduce computational cost without sacrificing accuracy, we derived a planar (2D) simplification of the full 3D TLM, demonstrating its equivalence to the more complex scheme for practically relevant parameter ranges [1]. In a subsequent review, we systematically compared our upgraded TLM (uTLM) with the conventional de Levie model, highlighting that only uTLM can reproduce the full low-frequency response, which includes diffusional contributions from both the electrolyte in the electrode pores and the separator – features that are often overlooked but are critical for a complete physical interpretation [3].

The practical utility of our TLM framework was verified through a systematic study on Ni-rich NMC cathodes with varying mass loadings [4]. We validated the theoretically predicted scaling laws for all model parameters, demonstrating how electrode geometry governs the detectability and magnitude of individual impedance contributions [5]. Critically, this analysis revealed that for a given mass loading, only a subset of impedance processes emerges above the measurement sensitivity threshold. Consequently, accurate parameter extraction requires impedance spectra collected from electrodes spanning a wide and well-controlled range of mass loadings. Furthermore, the analysis uncovered an unexpected additional diffusion feature – predominantly visible in thin electrodes – which we attributed to ion diffusion within micropores inside the NMC aggregates. As part of this verification, we also introduced a scaling-based normalization approach that enables a fast preliminary estimation of the total chemical insertion capacitance, C_{total}, from mass-normalized Nyquist plots. We experimentally confirmed for Ni-rich NMC that C_{total} obtained from sufficiently low-frequency impedance measurements is quantitatively equivalent to the differential capacitance $C_{\text{d}}(x)$ extracted from the equilibrium open-circuit voltage (OCV) curve [4], demonstrating that low-frequency EIS can directly probe the thermodynamic properties of single-phase insertion materials in realistic porous electrodes.

A crucial consideration arises when aiming to quantitatively interpret impedance parameters in terms of fundamental physical properties. TLMs, grounded in the PNP framework, are

strictly valid under conditions of thermodynamic ideality and infinite dilution – assumptions that are violated in real battery electrolytes. To address this, we discuss the conceptual and practical implementation of a correction step to translate PNP-derived electrolyte parameters into their Concentrated Solution Theory (CST)-consistent counterparts, as pioneered by Newman. Using representative Li-ion electrolytes, we demonstrate that this alignment is essential for obtaining physically sound and quantitatively meaningful interpretations of impedance-derived parameters, such as the cation transference number, which differs between the two frameworks due to the cation-anion interactions. This integrated methodology provides experimenters with directly applicable tools, scaling relations, and modeling strategies for developing intuitive and physically grounded interpretations of impedance responses in porous Li-ion insertion cathodes.

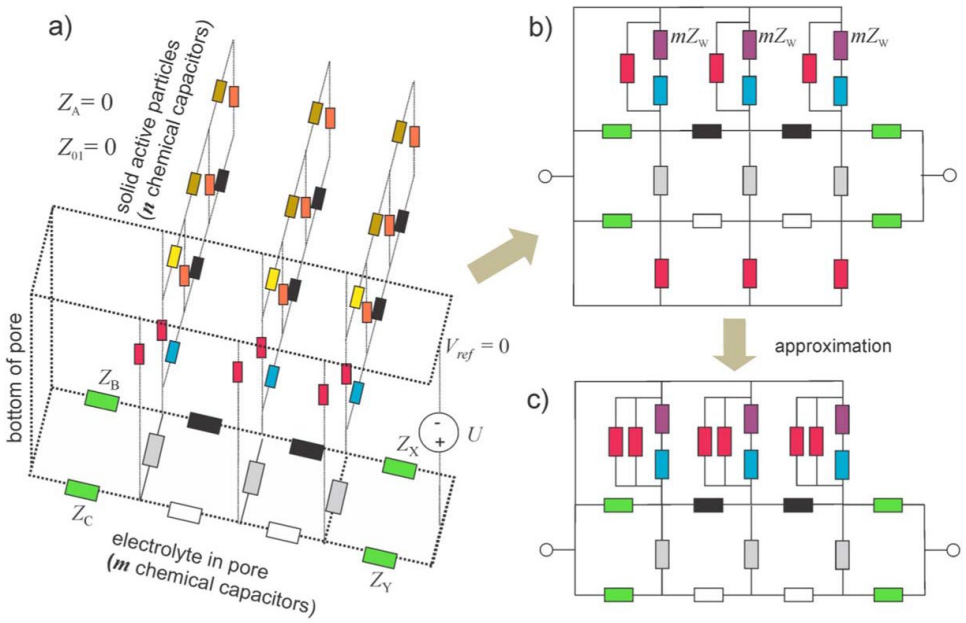

Fig. 1 Transformation of the full 3D TLM (a) into its planar simplification (b). This simplification is possible if the solid-state resistance of one charge is much lower compared to the other (i.e., resistances in one rail are set to zero). Then the whole branch representing solid active particles can be replaced by the conventional Warburg impedance (purple element). (c) Further simplification of planar model (b) by joining the individual double layer contributions of each mobile species into single capacitor for double layer.

References:

[1] Moškon, J.; Žuntar, J.; Talian, S. D.; Dominko, R.; Gaberšček, M. A powerful transmission line model for analysis of impedance of insertion battery cells: a case study on the NMC-Li system. *J. Electrochem. Soc.* 2020, 167, 140539.

[2] Submitted to *J. Electrochem. Soc.*

[3] Moškon, J.; Gaberšček, M. Transmission line models for evaluation of impedance response of insertion battery electrodes and cells. *Journal of power sources advances* 2021, 7, 1.

[4] Firm, M.; Moškon, J.; Kapun, G.; Talian, S. D.; Kamšek, A. R.; Štefančič, M.; Hočevar, S.; Dominko, R.; Gaberšček, M. Novel Methodology of General Scaling-Approach Normalization of Impedance Parameters of Insertion Battery Electrodes – Case Study on Ni-Rich NMC Cathode: Part I. Experimental and Preliminary Analysis. *J. Electrochem. Soc.* 2024, 171, 120540.

[5] Firm, M.; Moškon, J.; Dominko, R.; Gaberšček, M. Novel Methodology of General Scaling-Approach Normalization of Impedance Parameters of Insertion Battery Electrodes – Case Study on Ni-Rich NMC Cathode: Part II. Detailed Analysis Using a Transmission Line Model. *J. Electrochem. Soc.* 2024, 171, 120543.

Experimental determination of equilibrium and kinetic parameters for lithium-ion batteries modeling

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Accurate parameterization is essential for predictive physics-based lithium-ion battery models; however, experimentally determining a complete and consistent parameter set for the most common electrode materials remains challenging and time-consuming.[1] In this work, a systematic and experimental methodology, following established approaches in the literature [2] [3], is applied to extract key thermodynamic, kinetic, and structural parameters required for the Doyle–Fuller–Newman (DFN) model. The approach focuses on four widely used electrode materials – graphite, lithium titanate (Li4Ti5O12), lithium nickel manganese cobalt oxide (LiNi0.83Mn0.10Co0.07O2), and lithium iron phosphate (LiFePO4) – which are investigated in three-electrode half-cell configurations against lithium metal. Equilibrium potential curves are determined using low-current galvanostatic measurements at multiple C-rates to minimize kinetic contributions while maintaining high data resolution. Measurements are performed in EL-Cell half-cells with lithium reference electrodes and validated against measurements from coin cells. Kinetic parameters, including lithium diffusion coefficients and charge transfer resistances, are extracted using galvanostatic intermittent titration technique and electrochemical impedance spectroscopy, respectively. Electrode structural parameters such as particle size are obtained from scanning electron microscopy, porosity is determined from electrode composition and density data, and tortuosity is derived from impedance measurements. The extracted parameter sets are implemented in the PyBaMM framework and validated using experimental and simulated rate capability measurements of half-cell configurations. The simulations reproduce the overall electrochemical behavior across a wide range of operating conditions, demonstrating the internal consistency of the parameterization workflow. At the same time, deviations between simulation and experiment highlight the influence of model assumptions, measurement limitations, and material-specific transport mechanisms, particularly in electrodes exhibiting

[1] Wang, A. A.; O'Kane, S. E. J.; Brosa Planella, F.; Houx, J. L.; O'Regan, K.; Zyskin, M.; Edge, J.; Monroe, C. W.; Cooper, S. J.; Howey, D. A.; Kendrick, E.; Foster, J. M. *Progress in Energy* **2022**, 4, 032004
[2] Chen, C.-H.; Brosa Planella, F.; O'Regan, K.; Gastol, D.; Widanage, W. D.; Kendrick, E. *Journal of The Electrochemical Society* **2020**, 167, 080534
[3] O'Regan, K.; Brosa Planella, F.; Widanage, W. D.; Kendrick, E. *Electrochimica Acta* **2022**, 425, 140700

two-phase transformations. Overall, this work provides a reproducible framework for systematic battery parameter extraction and validation across different electrode chemistries. The results demonstrate that the proposed methodology can be generalized to materials with diverse electrochemical behavior, while also emphasizing that the predictive accuracy of physics-based battery models depends critically on parameter quality, measurement design, and the validity of underlying model assumptions.

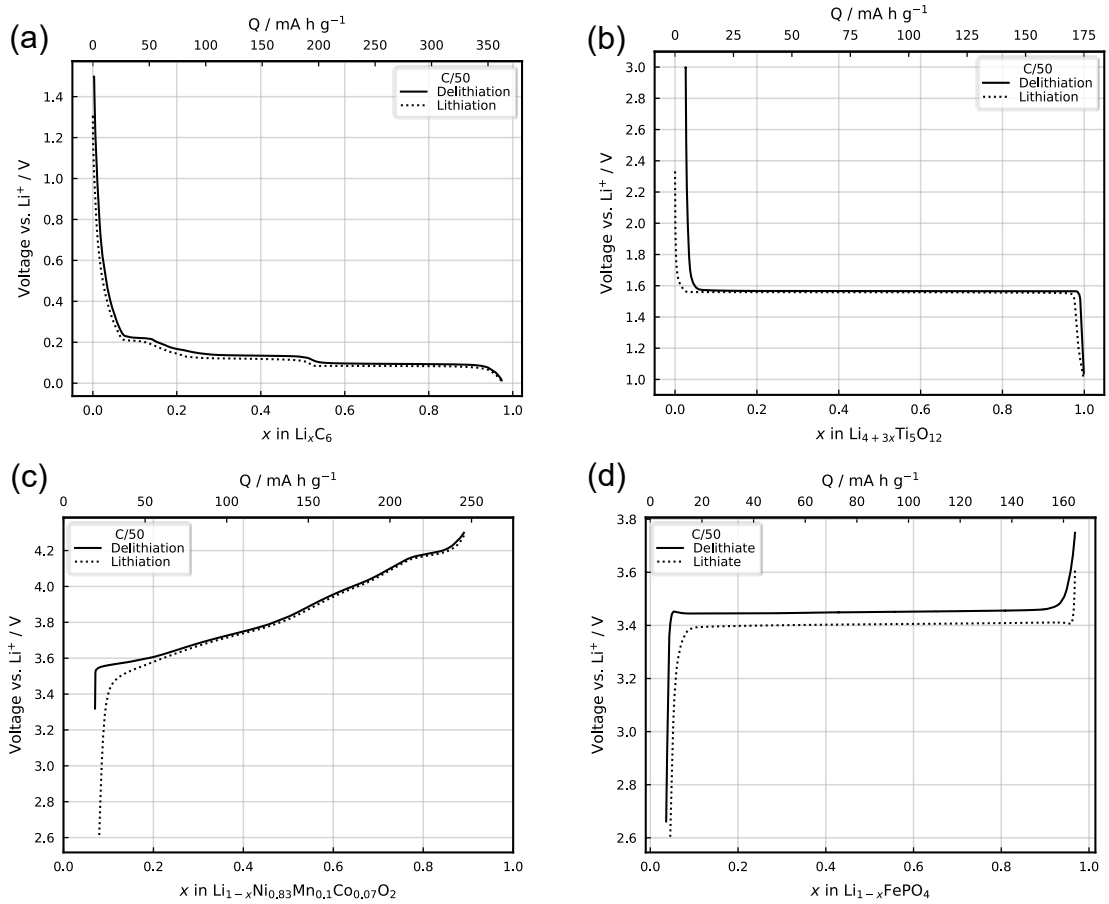

Fig. 1 Pseudo-equilibrium potential measurement in EL-Cell half-cell with Li-ref electrode: (a) graphite, (b) LTO, (c) NMC83, (d) LFP