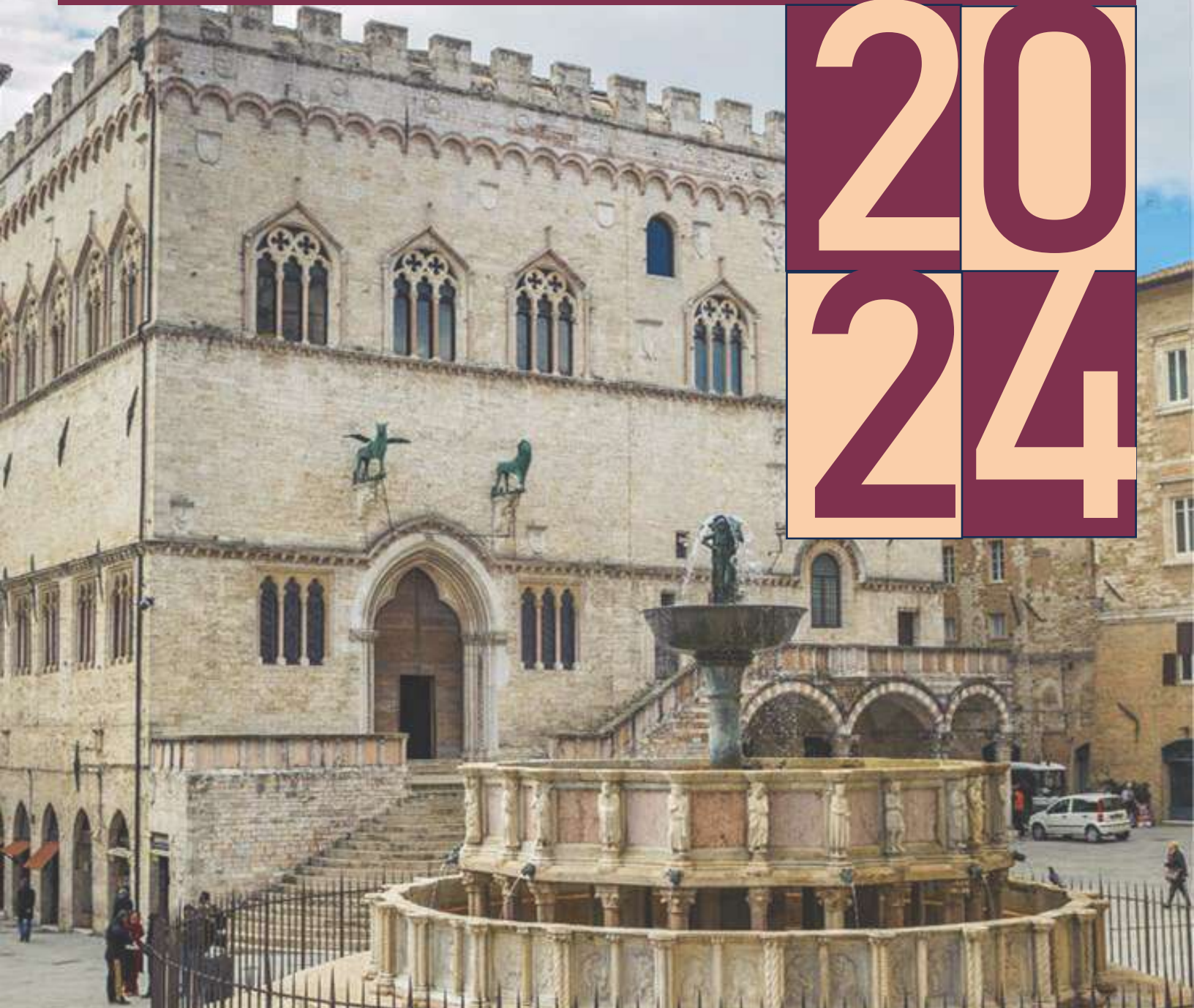


**7TH INTERNATIONAL CONFERENCE ON
PEROVSKITE SOLAR CELLS AND
OPTOELECTRONICS - PSCO**

**20
24**



BOOK OF ABSTRACT

**From 16th to 18th September 2024
Hotel Giò - Centro Congressi
Perugia, Italy**

SCIENTIFIC COMMITTEE

PSCO 2024

Henry Snaith

University of Oxford, UK

Filippo De Angelis

University of Perugia, Italy

Annamaria Petrozza

IIT, Italy

Md. K. Nazeeruddin

EPFL, Switzerland



INVITED LECTURES

PSCO 2024

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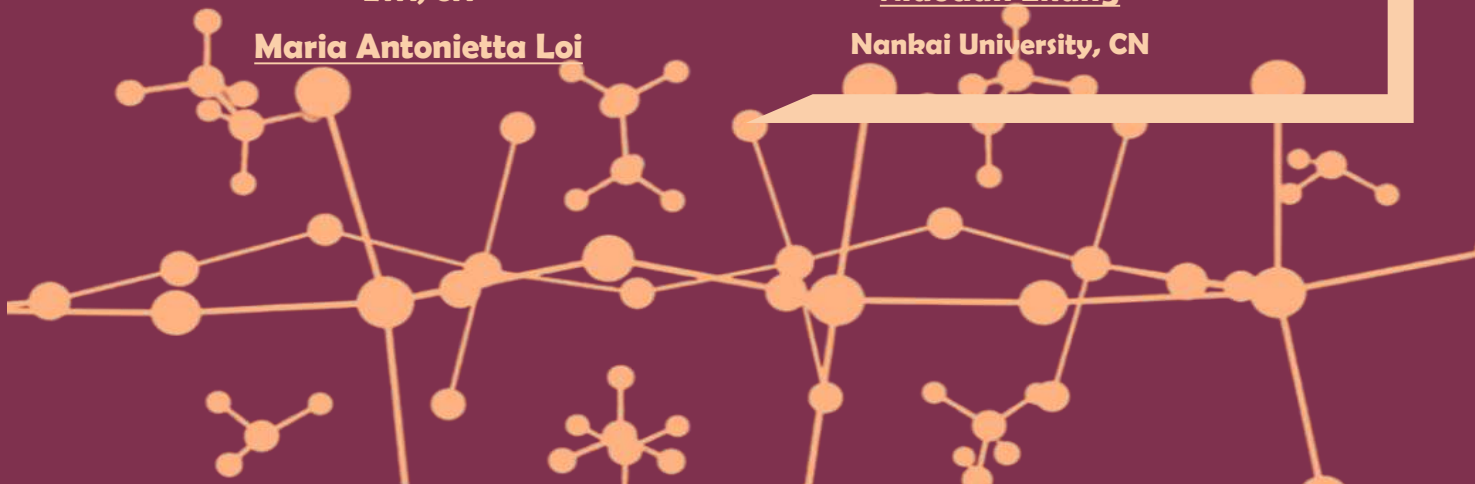
University of Freiburg, DE

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Nankai University, CN



Day 1 - Monday, September 16th, 2024

Session Chair: *Annamaria Petrozza, Istituto Italiano di Tecnologia, Italy*

WELCOME & REGISTRATION

08:00 08:30

08:30 08:45 *Welcome marks by Dr. Annamaria Petrozza*

08:45 09:00 1° PERSEPHONE Speaker **Yarong He**,
Photophysical properties of 2D tin perovskites

09:00 09:15 2° PERSEPHONE Speaker **Chunsheng Wu**, Istituto Italiano di Tecnologia, Italy
Simulated emission in perovskite: defects Management and Thin-Film Stoichiometry

09:15 09:30 3° PERSEPHONE Speaker **Oscar Adrian Jimenez Gordillo**, Nokia Solutions and Networks Italia s.p.a, Italy
From ESR to industry: a tale of two worlds

09:30 09:45 4° PERSEPHONE Speaker **Ece Aktaş**, University of Naples Federico II, Italy
Tin-based perovskite solar cell performances with self-assembled monolayer in dms-free solvent system

09:45 10:00 5° PERSEPHONE Speaker **Yu Wang**, Linköping University, Sweden
Evaluation of multifunctional ion migration in perovskite LEDs

10:00 10:15 6° PERSEPHONE Speaker **Isabella Antony Kalluvila Justin**, University of Valencia, Spain
Effect of coevaporated dopants on the photoemission of lead halide perovskites

10:15 10:30 7° PERSEPHONE Speaker **David Otto Tiede**, Institute of Materials Science of Seville, Spain
Slow Charge Carrier Cooling in Ligand-free Quantum Dot Solids - Elucidating the Influence of Interparticle Interaction

10:30 10:50

COFFEE BREAK

10:50 11:05 8° PERSEPHONE Speaker **Amit Kumar**, University of Oxford, United Kingdom
Ethanol Based Solvent System for FAPbI₃ p-i-n solar cells

11:05 11:20 9° PERSEPHONE Speaker **Teresa Stefanini**, Istituto Italiano di Tecnologia, Italy
Flexible photodetector based on CsPbBr₃ perovskite-polymer composite film

11:20 11:35 10° PERSEPHONE Speaker **Federico Fabrizi**, AMO GmbH, Germany
Scalable Patterning Technique for Metal Halide Perovskites Integration On-Chip Devices

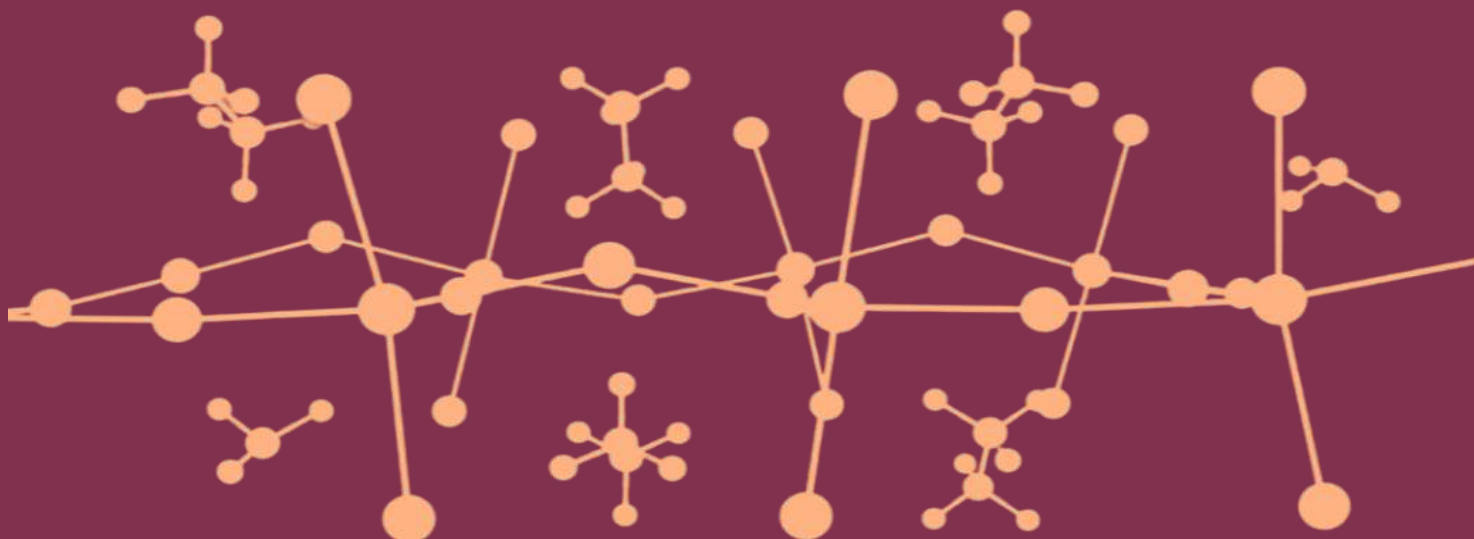
11:35 11:50 11° PERSEPHONE Speaker **Virginia Oddi**, IBM, ETH, Switzerland
Perovskite quantum dots in a tunable microcavity

11:50 12:05 12° PERSEPHONE Speaker **Aditya Bhardwaj**, DECTRIS, Switzerland
Re-assessment of Bismuth Halide based hard radiation detectors

12:05 12:20 13° PERSEPHONE Speaker **Shaoni Kar**, Helio Display Materials, University of Oxford, United Kingdom
Dimethylammonium-incorporated perovskite nanocrystals for bright and efficient red LEDs

12:20 13:30

REGISTRATION & LIGHT BUFFET LUNCH



AMPLIFIED SPONTANEOUS EMISSION PROPERTIES OF METAL CATION TWODIMENSIONAL PEROVSKITES

Yarong He,¹Laine Wong,¹ Annamaria Petrozza,¹ Daniele Cortecchia^{1,2}

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Metal halide perovskites have rapidly emerged as excellent optical gain media with the potential in laser technology. In 2014, room temperature laser emission was first achieved using 3D perovskite materials, underscoring their promise [1] [2]. Additionally, reducing the thickness of halide perovskites enhances the binding energy of excitons, leading to strong light emission even at high temperatures. Specifically, 2D halide perovskites are ideal candidates for highly compact and ultra-low threshold lasers due to their large exciton binding energy, efficient radiative recombination, and excellent environmental stability.

Previous studies have reported that mechanically exfoliated 2D lead-based perovskites ($n > 1$) can achieve optically pumped laser emission in the visible light region without the need for an external resonant cavity [3]. However, the laser properties of 2D lead-based perovskites have only been observed in bulk crystals or under external cavity conditions [4]. Recent research has also shown that 2D tin-based perovskite films exhibit excellent spontaneous emission amplification properties [5], although this behavior has not been observed in corresponding 2D lead-based perovskites. There is still controversy regarding the intrinsic properties of the optical gain medium material itself, generally thinking that 2D lead-based perovskite films have inherent limitations that make spontaneous emission amplification very difficult to achieve, even at low temperatures. Similarly, achieving a stable output ASE signal at room temperature in tin-based perovskite films remains a big challenge.

To address these challenges and better understand the properties of two-dimensional perovskites as optical gain media, we selected the commonly used material PEA_2XI_4 ($X = \text{Pb}, \text{Sn}$) and employed pulsed lasers for optical pumping. This approach aims to reveal the underlying mechanisms of the spontaneous emission signal, and we have made some progress in this endeavor.

[1] A.B. Author, *Journal Title* **Year**, Vol, pages (Times New Roman, 10 pts, justified).

[2] A.B. Author, *Book Title* **Year**, Editor(s), City, pages.

STIMULATED EMISSION IN PEROVSKITE: DEFECTS MANAGEMENT AND THIN-FILM STOICHIOMETRY

Chun-Sheng Jack Wu,^{1,2} Heyong Wang,¹ E. Laine Wong,¹ Hui Li,¹ Andrea Olivati,^{1,2} Giulia Folpini,^{1,3} Annamaria Petrozza^{2*}

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In this study, we explore the intricate interplay between thin film stoichiometry and defect management in perovskite materials to achieve low-threshold and air-stable near-infrared lasers. By optimizing the composition of our FAPbI₃-based perovskite thin films with excess FAI salt, we facilitate the passivation of both deep and shallow carrier trap states. This leads to the formation of multi-dimensional phases that enhance photoluminescence efficiency. However, while these features have been reported to improve the performance of light-emitting diodes, they do not necessarily translate to ideal conditions for lasing applications.

We also demonstrate the origin of stimulated emission in 3D perovskites through microscopic experiments, revealing how stimulated emission evolves in perovskite thin films. It is observed that stimulated emission originates from grain boundaries and defect states.

Such important finding of this work is the identification of shallow energy states and defect levels as crucial for achieving a low threshold and stable laser operation. This understanding of the origin of stimulated emission prompts a re-evaluation of the design of perovskite laser diodes for electrical operation.

FROM ESR TO INDUSTRY: A TALE OF TWO WORLDS

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Transitioning from an ESR role in academia to a professional position in an industrial R&D team presents a unique set of challenges and opportunities. This demanding journey gives proof of the versatility and adaptability of skills acquired during the PERSEPHONE program.

The initial challenge lies in navigating the shift from the academic environment mindset, characterized by intellectual freedom and flexible timelines, to the fast-paced, result-oriented industrial setting. However, the skills developed during the ESR journey, such as critical thinking, problem-solving, and the ability to learn quickly, are highly transferable and valued in the industry. The rigorous research methodology equips one with the ability to approach problems systematically and innovatively. Furthermore, the resilience built through the process of academic research is an asset in overcoming industry challenges.

In conclusion, the transition from academia to industry, while challenging, is a rewarding journey that allows for the application of academic skills in practical, real-world scenarios, ultimately leading to personal growth and professional development.

TIN-BASED PEROVSKITE SOLAR CELLS AND LIGHT EMITTING DIODES

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Tin (Sn)-based perovskites have emerged as promising materials for optoelectronic applications, particularly in solar cells and light-emitting diodes (LEDs), due to their exceptional optoelectronic properties and lower toxicity compared to their lead-based counterparts.¹ Despite challenges such as Sn oxidation and film instability, advancements in material engineering and device architecture have led to remarkable improvements in stability and efficiency. Sn-based perovskite solar cells have gathered noteworthy interest owing to their low bandgap, high charge-carrier mobility, and reduced exciton binding energy.² In the realm of light-emitting diodes, Sn-based perovskites offer tuneable emission spectra, high photoluminescence quantum yields, and solution-processability, making them attractive for next-generation display and lighting technologies.³ Progress in Sn-based perovskite LEDs has been driven by innovations in perovskite composition like mixed-halide and low-dimensional Sn-perovskites, device structure, leading to important enhancements in external quantum efficiency and operational stability with reduced non-radiative recombination losses.⁴ In this study, we investigate the influence of additives on the growth and performance of 2D tin-based perovskite thin films in nonoxidative solvent. By systematically varying the processing parameters, including the amount of additive and the deposition conditions, we gain insights into the underlying mechanisms governing the film formation and properties. As a result, 2D tin-based perovskite LED device had a low turn-on voltage of 2 V, and maximum external quantum efficiency of ~2.2%. Moreover, we demonstrate our nonoxidative solvent system ensures highly reproducible and hysteresis-free solar cells, with the best recorded power conversion efficiency of 5.8% for MeO-2PACz and 8.7% for PEDOT-complex, respectively. Ongoing research focusing on overcoming material and device challenges is expected to further elevate their performance and commercial viability, paving the way for eco-friendly and efficient solar energy conversion and light emission technologies.

Acknowledgements: Ece Aktas acknowledges the European Union's Horizon 2020 research and innovation program under the Marie Skłodowska-Curie grant agreement No 956270 (PERSEPHONE).

[1] E. Aktas, N. Rajamanickam, J. Pascual, S. Hu, M. H. Aldamasy, D. D. Girolamo, W. Li, G. Nasti, E. Martínez-Ferrero, A. Wakamiya, E. Palomares, and A. Abate. *Communications Materials*, 2022, 3, 104.

[2] L. Xu, X. Feng, W. Jia, W. Lv, A. Mei, Y. Zhou, Q. Zhang, R. Chen and W. Huang, *Energy Environmental Science* 2021 14, 4292.

[3] Y. Xing, H. He, Z. Cui, Z. Fu, S. Qin, W. Zhang, S. Mei, and R. Guo. *Adv. Optical Mater.* 2024, 12, 2302679.

[4] F. Yuan, G. Folpini, T. Liu, U. Singh, A. Treglia, J. Wei, M. Lim, J. Klarbring, S. I. Simak, I. A. Abrikosov, T. C. Sum, A. Petrozza, and F. Gao. *Nat. Photon.* 2024, 18, 170.

EVALUATION OF MULTIFUNCTIONAL ION MIGRATION IN PEROVSKITE LEDs

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Halide perovskites, with their remarkable chemical adaptability and exceptional optoelectronic properties, have garnered significant attention for the next generation of semiconductor devices. However, the persistent issue of uncontrollable ion migration casts a shadow over their widespread commercial adoption. This phenomenon is especially problematic in perovskite light-emitting diodes (LEDs), where the presence of intense electric fields can trigger substantial movement of these charged ions. More importantly, the role of mobile ions has been believed to be versatile besides their intrinsic feature of space charges, such as traps and dopants.

While considerable research has been dedicated to elucidating the underlying mechanisms and the potential impact of ion migration in perovskite materials, a knowledge gap persists regarding the manifestation of these complex processes within the device architecture and the utilization of such phenomena during the device operation. Herein, I intend to present our understandings on the impact of versatile roles of mobile ions in the perovskite LEDs and the potential strategies to make best use of this complex process for the future device optimization and innovation.

STRONG GRAIN BOUNDARY PASSIVATION EFFECT OF COEVAPORATED DOPANTS ENHANCE THE PHOTOEMISSION OF LEAD HALIDE PEROVSKITES

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Lead halide perovskites (LHP) have emerged over the past decade as a new family of semiconducting materials with great potential to be incorporated into highly efficient optoelectronic devices. Beyond having become the fastest growing photovoltaic technology, LHP are being explored as active components for light emitting devices, x-ray detectors or memristors^[1]. As for any semiconductor, the presence of structural defects strongly determines the performance of this material in any device and thus compromises its future commercial use. While, due to the peculiar nature of LHP^[2], structural defects are commonly considered as benign, a proper understanding of their nature and role in their photophysical properties is still under debate^[3]. Herein we demonstrate that co-evaporation of the perovskite with the dopants (DPEPO) provide a means to passivate buried interfacial defects occurring at perovskite grain boundaries in evaporated perovskite thin films, thus giving rise to an unprecedentedly enhanced photoluminescence. On the other hand, the presence of an excessive amount of organic dopant can lead to a barrier for carrier diffusion, hence the passivation process demands a proper balance between the two effects. Our analysis allows to discern the role of the dopant under different excitation regimes, which permits evaluating the performance of the material under conditions more adapted for photovoltaic or light emitting applications. This approach taken herein provides a screening method to evaluate the suitability of a passivating strategy prior to its incorporation into a device.

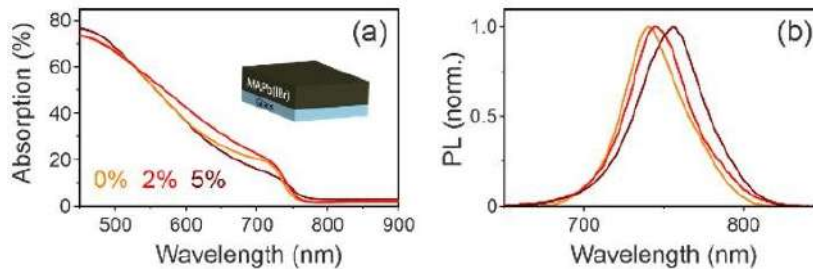


Figure 1: (a) Absorption and (b) PL spectra for LHP films co-evaporated with different amounts of DPEPO

[1] Park, Y.; Lee, J.-S. Metal Halide Perovskite-Based Memristors for Emerging Memory Applications. *J. Phys. Chem. Lett.* **2022**, *13*, 5638–5647.

[2] Egger, D. A.; Bera, A.; Cahen, D.; Hodes, G.; Kirchartz, T.; Kronik, L.; Lovrincic, R.; Rappe, A. M.; Reichman, D. R.; Yaffe, O. What Remains Unexplained About the Properties of Halide Perovskites. *Adv. Mater.* **2018**, *30* (20), 1800691.

[3] Kim, G.-W.; Petrozza, A. Defect Tolerance and Intolerance in Metal-Halide Perovskites. *Adv. Energy Mater.* **2020**, *10*, 2001959.

SLOW CHARGE CARRIER COOLING IN LIGAND-FREE QUANTUM DOT SOLIDS – ELUCIDATING THE INFLUENCE OF INTERPARTICLE INTERACTION

David O. Tiede,¹ **Carlos Romero Pérez**,¹ **Katherine A. Koch**,² **Mauricio E. Calvo**,¹ **Juan F. Galisteo-López**,¹ **Ajay R. S. Kandada**,² **Hernán Míguez**¹

¹*Institute of Materials Science of Seville, Spanish National Research Council (CSIC -US), Spain*

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Charge carrier cooling mechanisms describe the relaxation of above-gap electrons and holes to their respective band edges through energy transfer to lattice vibrations. Tuning the carrier cooling mechanisms is of fundamental interest, as long carrier relaxation times are required for applications such as hot carrier solar cells in order to avoid energy loss associated with these carriers. On the other hand, light-emitting applications require fast carrier cooling. Extended charge carrier cooling times have in particular been demonstrated for confined semiconductor structures [1]. However, the precise origin of slow charge carrier cooling remains to be fully understood.

Herein, we employ a system of ligand-free quantum dot solids with tunable interparticle spacing as a testbed to analyse the effects of interparticle electronic coupling on charge carrier cooling mechanisms in confined systems [2]. We find that Auger processes can strongly contribute to charge reheating effects and analyse the effect of the local environment on the charge cooling pathways [3]. In particular, the effect of the phonon landscape is addressed in greater detail. With this work we emphasize that not only confinement effects, but also coupling to neighbouring QDs fundamentally contributes to charge carrier relaxation processes. This finding is particularly relevant for optoelectronic devices based on QD solids, as charge injection and extraction requires electronic coupling.

[1] J.W.M Lim, *J. Am. Chem. Soc.* **2024**, *146.1*,437-449.

[2] D.O. Tiede, *ACS Nano* **2024**, *18*, 2325-2334.

[3] D.O. Tiede, *Submitted 2024*.

ETHANOL BASED SOLVENT SYSTEM FOR FAPbI₃ P-I-N SOLAR CELLS

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Laboratory-scale power conversion efficiencies (PCE) of ABX₃ type perovskite solar cells have surpassed 26%. However, the typical solution-processed methods, involving spin-casting, antisolvents, or gas quenching, and using N,N-Dimethylformamide (DMF) and Dimethyl sulfoxide (DMSO) solvent systems, pose scalability challenges. To address this, we optimized a DMF/DMSO and antisolvent-free solvent system for 1.51eV FAPbI₃-based p-i-n architecture solar cells using 2-methoxyethanol. We incorporated N-Methylpyrrolidone (NMP), a non-volatile and Pb²⁺ coordinating additive, to inhibit non-perovskite phase formation during room-temperature deposition. Unlike common Pb²⁺ coordinating agents such as DMSO, DMPU, or DMAc, our method showed no precipitation at any concentration. With high reproducibility, we achieved a stable maximum power point tracking (MPPT) of 22.00% for a 25mm² area, attributed to enhanced photoluminescence quantum efficiencies (~8%), compact and pinhole-free morphology, and a highly oriented crystal structure. This technique is easily scalable for larger areas. Despite these efficiency gains, stability remains crucial for commercial viability. Our study investigates the high stability of optimal bandgap FAPbI₃ perovskite using in-situ 2D XRD. We stressed thin films at 130°C and 50% RH for 9 hours, noting that DMF films turned yellow, while 2-ME films retained their black phase, indicating higher stability. Temperature ramping showed that DMF films first developed a strong yellow phase before converting, whereas 2-ME films showed a weak phase transition. Optoelectronic response tests revealed ~no degradation in 2-ME films, following ISOS-D2 and ISOS-L3 protocol. Loss quantification using half-stack PLQE measurements identified the perovskite/C60 interface as the performance limiter.

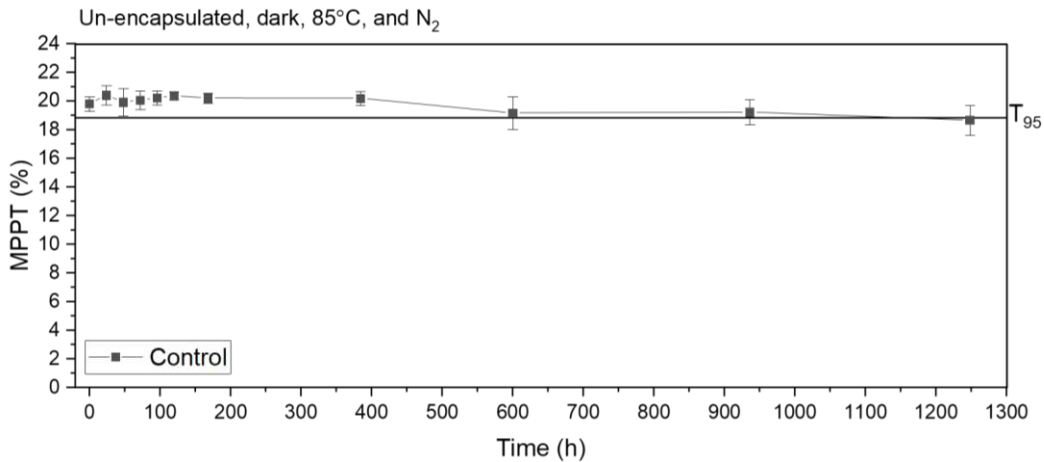


Figure 1: The maximum power point tracking of 8 devices of p-i-n architecture perovskite solar cells

SOLUTION PROCESSED FLEXIBLE UV-Vis-PHOTODETECTOR BASED ON CsPbBr₃ PEROVSKITE-POLYMER COMPOSITE FILM

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²*Politecnico di Milano, Italy*

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This study presents the development and characterization of a flexible, solution-processed UV-vis photodetector employing a composite film of CsPbBr₃ perovskite merged with PVP polymer and covered by a PCBM layer. The device is fabricated with scalable and cost-effective methods adaptable both on rigid and flexible substrates. The active layers are obtained through a facile solution-based deposition on top of ink-jet printed interdigitated electrodes. The presence of the polymer and of the PCBM layer in the composite film improves its surface coverage, surface passivation, light absorption and stability. The optimized CsPbBr₃-polymer based photodetector has a photo-to-dark current ratio of 3.5×10^3 at 5 V applied bias, a peak responsivity $> 1 \text{ AW}^{-1}$ across the whole visible range, with a peak of 34.3 AW^{-1} at 370 nm and the specific detectivity can be estimated to reach 3.2×10^{12} Jones. The detector, which is symmetric, works along a photoconduction regime, though shows reasonably short rise and fall times of 657 and 835 μs , respectively. The performances of the device are stable over 4 weeks under ambient environmental conditions.

The scalability and compatibility of the solution-processing method hold promise for large-scale manufacturing of cost-effective and flexible UV-vis photodetector devices and opens avenues for the integration of perovskite materials into diverse optoelectronic applications.

VERSATILE AND SCALABLE PATTERNING TECHNIQUE FOR ON-CHIP INTEGRATION OF METAL HALIDE PEROVSKITES

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Introduction: Solution-processed metal halide perovskites (MHPs) are promising semiconductors for integrating electrically electro-optic devices into photonic circuits [1,2]. Typically, the functional layers of MHP-based optoelectronic devices are deposited sequentially, while the device area is defined by shadow-mask evaporation of top contacts. However, integrated micro- and nanometer-scale perovskite devices require efficient and scalable top-down patterning processes [3]. Several methods have been developed, including nanoimprint patterning [4], gas-assisted focused ion beam etching [5], and laser writing [6]. Here, we introduce a versatile top-down patterning technique using conventional photolithography and reactive ion etching (RIE) specifically tailored for perovskite layers that is applicable independent of their composition and dimensionality (3D, 2D, and 0D).

Fabrication: Cesium lead bromide (3D-CsPbBr₃), methylammonium lead iodide (3D-MAPbI₃), phenethylammonium/methylammonium lead bromide (Quasi 2D-PEA₂(MAPbBr₃)_n-PbBr₄), and formamidium lead bromide (0D-FAPbBr₃) perovskite thin films were spin-coated onto Si/SiO₂ substrates and then covered with polymethyl methacrylate (PMMA) and AZ MIR701 positive photoresist. (Figure 1. a-c). The PMMA protects the perovskites against polar solvents, which typically degrade them during photolithography. It enables the deposition and patterning with standard contact lithography using AZ MIR701. Next, chlorine-based RIE was used to etch the AZ MIR701 pattern into the PMMA and the perovskite layers. PMMA was then dissolved in an organic solvent, lifting off the AZ MIR701. This resulted in perovskite features down to 1 μm, limited only by the resolution of our contact lithography tool (Figure 1 d-f).

Results. The surface roughness of the perovskite thin films was analyzed using Atomic Force Microscopy (AFM, Figure 2a, details to be shown in the talk). The data indicate minimal variation before and after patterning. Optical properties of the perovskites were investigated via ultraviolet-visible (UV-Vis) and photoluminescence (PL) spectroscopy before and after the etching process (Figures 2b-e). The absorption and PL spectra show almost no change in peak positions before and after etching, except for the nanocrystal (NC) thin films, demonstrating that the optical properties and phase purity of the perovskites are largely maintained in the patterning process. However, we observed a small shift of approximately 8 nm in the NC films, which may be attributed to particle redistribution during the PMMA layer spin-coating. Furthermore, the confocal microscopy images (insets of Figure 3) confirm that the perovskite's emission remains consistent with the optical spectroscopy results, regardless of chemical composition and morphology. Cross-sectional scanning electron microscopy (SEM) of the various etched perovskite layers shows sidewall angles of more than 80° which is desired for achieving high-precision vertical structures. (Figures 3 a-d).

Conclusions. We have developed a top-down etching process for integrating perovskites into semiconductor technology. It enables the deterministic, micrometer-scale patterning of perovskites while maintaining the optical properties of the pristine (as deposited) perovskite thin films. This work contributes to closing the crucial gap between exploratory research and manufacturability of halide perovskites.

Acknowledgements. The authors acknowledge funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 951774, the Marie Skłodowska-Curie grant agreement No 956270, and the Deutsche Forschungsgemeinschaft (DFG) under project number 502102 (Hiper-Lase).

[1] P. J. Cegielski et al., *Opt. Express*, 25 (2017) 13199-13206. [2] Neda Pourdavoud et al., *Adv. Material* 31 (2019) 1903717.

[3] M. Saliba et al., *Adv. Material* 28 (2016) 923-929.

[4] A. Mayer et al., *Appl. Phys. A* 128 (2022) 399.

[5] M. S. Alias et al., *Phys. Chem. Lett.* 7 (2016) 137-142.

[6] J. Chen et al., *Adv. Mater. Technology* 2 (2017) 1700132.

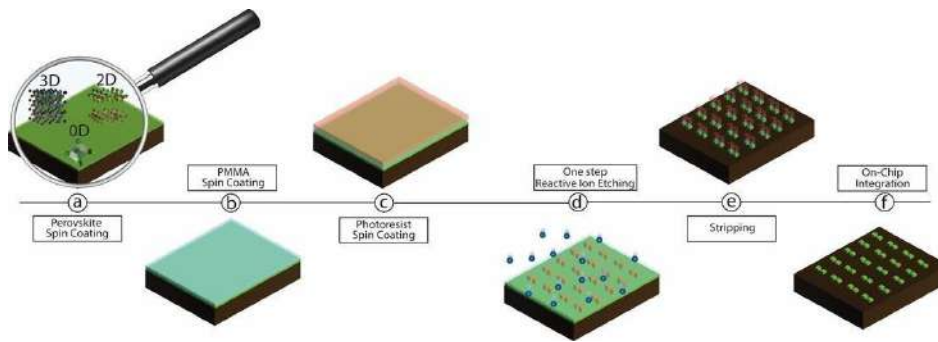


Figure 1. Fabrication process flow: (a) Deposition of the perovskite thin film (b) Deposition of the PMMA layer (c) Deposition of the top photoactive resist layer (d) Development of the resist layer and pattern transfer into the perovskite layer by reactive ion etching (e) Resist stripping by dissolving the PMMA layer and lifting the top layer (f) Perovskite layer monolithically integrated on-chip.

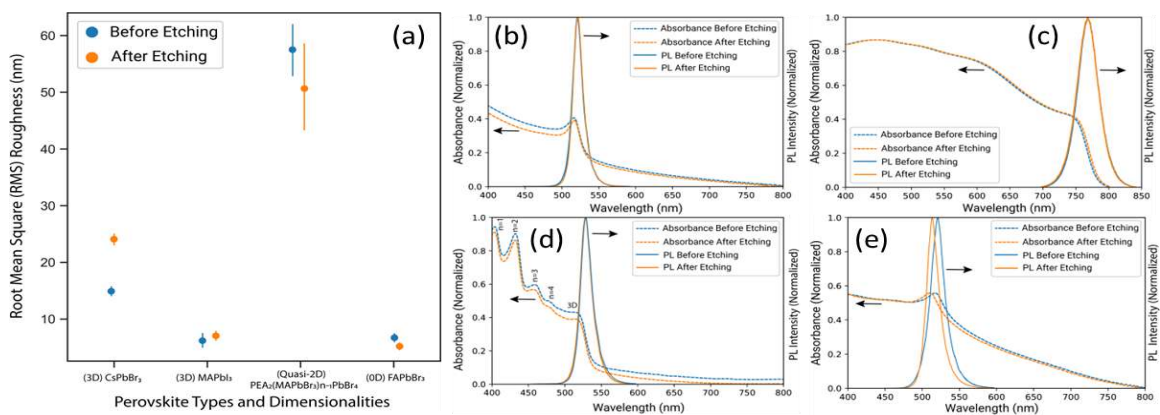


Figure 2. (a) Root mean square (RMS) values before and after the etching process for all the perovskite thin films. The inserts show the AFM scans after the stripping of the photoresist. Absorption and PL spectra before and after the etching process of (b) 3D-CsPbBr₃ (c) 3D-MAPbI₃ (d) Quasi 2D-PEA₂(MAPbBr₃)_{n-1}PbBr₄ (e) 0D-FAPbBr₃ NCs thin films.

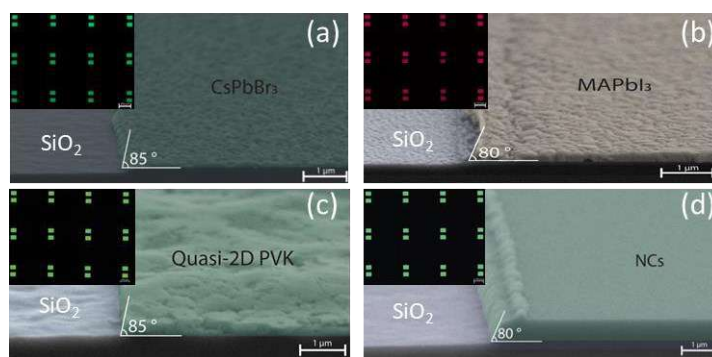


Figure 3. SEM lateral view of the etched structure. (a) 3D-CsPbBr₃ (b) 3D-MAPbI₃ (c) Quasi 2D-PEA₂(MAPbBr₃)_{n-1}PbBr₄ (d) 0D-FAPbBr₃ NCs thin films. The insets show a confocal microscopy image after the etching process.

PEROVSKITE QUANTUM DOTS EMBEDDED IN A TUNABLE, OPEN MICROCAVITY

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Cesium lead halide perovskite quantum dots (QDs) have recently emerged as promising platform for quantum light sources, showing a photoluminescence quantum yield above 90% and the generation of antibunched light with an ultrafast radiative lifetime and a long coherence time. In this work we investigate the integration of CsPbBr₃ QDs into an optical microcavity to further boost the radiative decay, consequently, improving the photon coherence time. Additionally, the extraction efficiency would be also enhanced thanks to the coupling of the emission into a well-defined cavity mode. By spatially and spectrally coupling a single CsPbBr₃ QD to a cavity mode, the number of electromagnetic modes to which the emitter is coupled can be controlled and, therefore, the Fermi golden rule, which governs the spontaneous emission rate (SE), can be modified. The SE enhancement is quantified by the so called Purcell factor, which is proportional to the ratio Q/V where Q is the quality factor and V the modal volume. To achieve our goal, we use a tunable, open microcavity with a Gaussian-shaped deformation which creates lateral confinement and supports a set of Laguerre-Gaussian modes. Our cavity configuration leads to a high Q and a small V and allows to easily tune the microcavity resonance with respect to the QD emission.

In my presentation, I will report the first preliminary results related to single CsPbBr₃ QDs with 25 nm size embedded in our optical microcavity system at cryogenic temperatures. With the current configuration, we do not observe a significant Purcell enhancement (lower than 2). FDTD simulations corroborate our experimental findings and provide information to further improve our system for the achievement of larger Purcell factors, ideally in a range between 20 and 30.

RE-EVALUATION OF THE AIR-MEDIATED RESPONSE IN Bi-BASED PEROVSKITE X-RAY DETECTORS

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The Metal halides perovskites such as CsPbBr₃ and MAPbI₃ have gained significant attention for X-ray detection application over a decade.^[1] Recently Pb-free alternatives, particularly A₃B₂X₉ metal halide family has been considered as environmentally greener alternatives to CdTe and CsPbBr₃. Our systematic investigation demonstrates that a surprisingly high figure of merits reported in literature with these A₃B₂X₉ materials^[2] as X-ray detectors do not correspond to inherent properties of the material but rather originate from air-ionization due to ill-characterization measurement employed. With the help of a specifically constructed chamber for measurements, we instantiate that the X-ray detection response is extremely dependent on the chamber-environment used during the measurement i.e. air, Ar or vacuum. After carefully eliminating the plausible deleterious effects of crystallographic orientation, crystal quality, and metallization interface, more than 1000-fold higher X-ray response could be generated using an Argon-filled environment with minimum metal-contact area. In our work, not only we exemplified by decoupling the X-ray photocurrent contribution of ionized-air from the true intrinsic material response but also aimed to lay down important standard experiment parameters to be considered in order to report trustworthy X-ray detection.

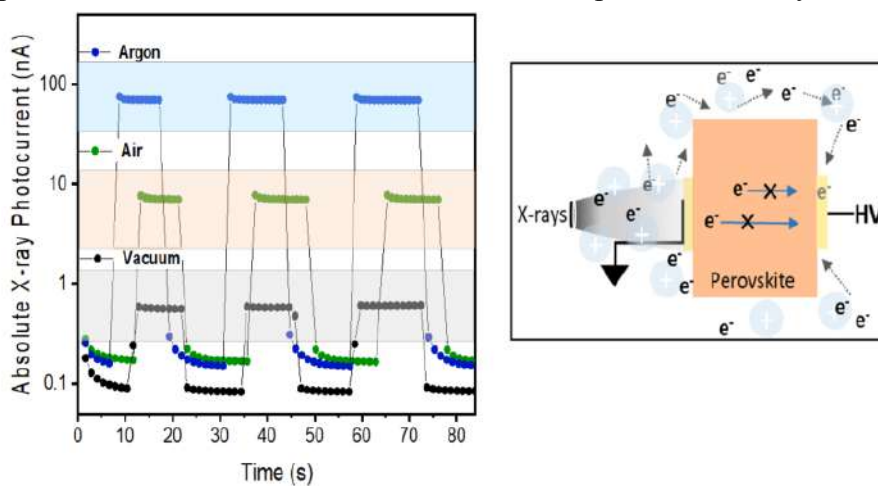


Figure 1: Depicts a 100-fold increase in absolute X-ray photocurrent obtained with the Cs₃Bi₂I₉ single crystal when measured under vacuum, air, and argon filled chamber environment. The samples was biased at 150V and 22keV X-ray was turned on after 20-30 seconds leading to increased photocurrent. The schematic depicts the collection of charged ions on the contacts externally instead of photo-generated carrier from the perovskite sensor.

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DIMETHYLAMMONIUM-INCORPORATED MIXED HALIDE PEROVSKITE NANOCRYSTALS FOR STABILIZED RED EMISSION

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All-inorganic perovskite nanocrystals are attractive candidates for light emission applications. Of these, cesium lead iodide (CsPbI₃) nanocrystals have been shown to be promising but their device application is still inhibited by their inherent ambient instability due to rapid conversion of the metastable black perovskite γ -phase into the yellow δ -phase at room temperature [1]. With addition of bromine (Br), CsPbI_xBr_{3-x} nanocrystals are formed with ideal bandgaps for emission within the Rec 2020 colour gamut. Furthermore, in contrast to the pure-iodide compositions that require high temperature-based (hot injection) processes to form the perovskite phase, mixed-halide nanocrystals afford facile synthesis through room-temperature ligand assisted reprecipitation (LARP). However, these materials are still plagued by phase separation under optical or electrical excitations of intensities typical in a working device [2].

In this work, we alloy the A-site of the pure-red emitting CsPbI₂Br with dimethylammonium (DMA) to improve its phase stability under excitation while retaining high photoluminescence quantum yields. DMA, among other organic cations, has recently been shown to alloy successfully with Cs in 3D perovskite thin films and lend it stability under operational conditions [3]. To our knowledge, this is the first study of DMA-alloying in perovskite nanocrystals through facile LARP synthesis techniques. We propose a novel synthetic route at room temperature and then study the crystal structure and morphology as a function of different DMA contents through an interplay of crystallographic and optical data. We report higher ambient stability even under intense optical excitation. We further probe the crystal lattice through solid-state NMR and high-resolution STEM-EDX to understand the mechanism and extent of DMA incorporation. We also use X-ray photoelectron spectroscopy (XPS) to investigate the DMA-contents. Finally, we fabricate light emitting diodes (LEDs) using these materials and show improved brightness, efficiency and operational stability in DMA-incorporated NC-based devices as compared to the pristine reference samples.

These findings are currently being compiled into a manuscript.

Acknowledgements: S.K. acknowledges funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement no. 956270 and from a Viperlab grant for access to STEM-EDX and XPS/UPS in HZB, Berlin and Fraunhofer, Centre for Silicon Photovoltaics, Halle respectively.

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13:30 13:45

OPENING CEREMONY by Prof. Filippo De Angelis

Session 1 - Invited Lectures | Town Hall

Session Chair: *Filippo De Angelis, University of Perugia, Italy*

13:45 14:10 1° INVITED LECTURE - **Michael Graetzel**, EPFL, Switzerland
Catalyzed formation of pure α -FAPbI₃ under ambient conditions for high performance perovskite photovoltaics

14:10 14:35 2° INVITED LECTURE - **Sam Stranks**, University of Cambridge, United Kingdom
Operando Studies of Halide Perovskite Devices

14:35 15:00 3° INVITED LECTURE - **Jianpu Wang**, Nanjing Tech University, China
Perovskite LEDs for Lighting and Displays

15:00 15:25 4° INVITED LECTURE - **Stefan Glunz**, Fraunhofer ISE, University of Freiburg, Germany
Characterization and simulation of perovskite-silicon tandem solar cells and modules

15:25 15:50 5° INVITED LECTURE - **Kai Zhu**, National Renewable Energy Laboratory, United States
Towards outdoor operation of perovskite solar cells

15:50 15:55 HALOCELL (5 mins)

15:55 15:58 WVELABS (3 mins)

15:58 16:25 COFFEE BREAK

Session Chair: *Maksym Kovalenko, ETH Zurich, Switzerland*

16:25 16:50 6° INVITED LECTURE - **Jinsong Huang**, University of North Carolina, Chapel Hill, United States
Understanding the Multiple-Facet Degradation Pathways in Metal Halide Perovskite Solar Cells

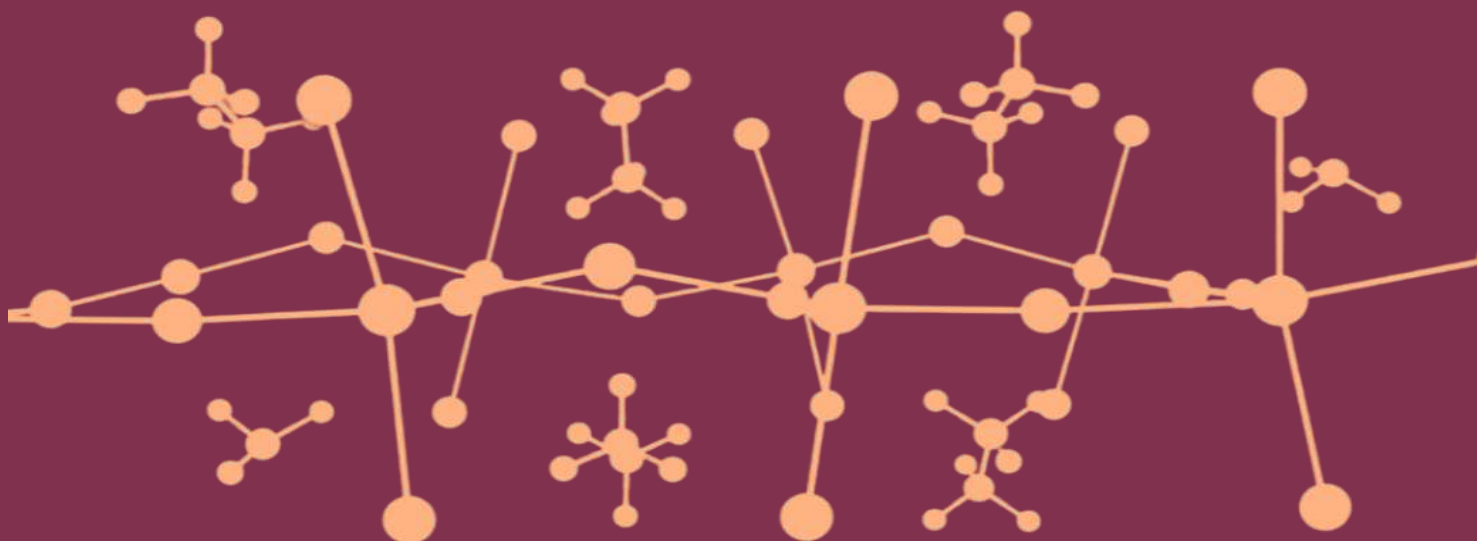
16:50 17:15 7° INVITED LECTURE - **Aldo Di Carlo**, ISM-CNR, Italy
Large area halide perovskite modules and panels: from interface engineering with two-dimensional materials to outdoor testing

17:15 17:40 8° INVITED LECTURE - **Marina Leite**, UC Davis, United States
Machine learning driven analysis of halide perovskites

17:40 18:05 9° INVITED LECTURE - **Lorenzo Malavasi**, University of Pavia, INSTM, Italy
Metal halide perovskites: a materials chemistry perspective from design to applications

18:05 18:30 10° INVITED LECTURE - **Annalisa Bruno**, NTU, Singapore
Advanced Device Customization and Quantum Confinement Using Thermal Evaporation of Metal-Halide Perovskites

18:30 18:37 COMFORT BREAK



CATALYZED FORMATION OF PURE α -FAPbI₃ UNDER AMBIENT CONDITIONS FOR HIGH PERFORMANCE PEROVSKITE PHOTOVOLTAICS

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Owing to their high photovoltaic performance, formamidinium lead iodide (FAPbI₃) based perovskite solar cells (PSCs) hold great promise as a revolutionary future PV technology. Its narrow bandgap and superior opto-electronic properties allows the power conversion efficiency (PCE) of PSCs to approach the Shockley–Queisser (S-Q) limit. However, the high temperature annealing and inert atmosphere required during the FAPbI₃ film preparation by solution processing remains an obstacle for wide spread future applications. Fabricating pure α -FAPbI₃ films at ambient conditions and at high throughput rates is essential for large scale production but implies major challenges. We prepared pure α -FAPbI₃ films via a two-step sequential deposition using an ionic liquid to dissolve the PbI₂ in the presence of a molecular catalyst, enabling the complete conversion of PbI₂ into phase-pure α -FAPbI₃ at room temperature within just 6 seconds. The conversion remains quantitative even under relative humidity levels exceeding 90%, allowing cell fabrication in ambient air at high humidity. Our pure α -FAPbI₃ based PSCs obtain a power conversion efficiencies (PCEs) of 26.3% (certified at 26.1%) and 22.4% for a laboratory cell and mini-module, respectively showed excellent long-term operational stability.

OPERANDO STUDIES OF HALIDE PEROVSKITE DEVICES

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Halide perovskites are generating enormous excitement for next-generation optoelectronic devices, but understanding about performance and stability on different length scales is limited – in turn limiting improvements in these parameters. Here, I will present recent work from our group in which we utilise operando macro- and micro-scale techniques to study operating perovskite solar cells, LEDs and X-ray detectors. We identify how phase impurities and chemical inhomogeneities, even in trace amounts, are problematic as non-radiative recombination centres and sites of degradation. We show how specific passivation and interface control approaches can boost performance and stabilise operation. These platforms provide critical insights into issues currently plaguing the further development of halide perovskite devices.

PEROVSKITE LEDs FOR LIGHTING AND DISPLAYS

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Solution-processed light-emitting diodes (LEDs) are attractive for applications in low-cost, large-area lighting sources and displays. Organometal halide perovskites can be processed from solutions at low temperatures to form crystalline direct-bandgap semiconductors with intriguing optoelectronic properties, such as high photoluminescence yield, good charge mobility and excellent color purity. In this talk, I will present our effort to boost the efficiency of perovskite LEDs to a high level which is comparable to organic LEDs.^[1–9] More importantly, organic LEDs are difficult to maintain high efficiency at high current densities due to their excitonic nature and low charge mobilities. Low temperature solution-processed perovskite LEDs demonstrate remarkably high efficiency at high current densities, suggesting unique potential to achieve large size planar LEDs with high efficiency at high brightness.

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CHARACTERIZATION AND SIMULATION OF PEROVSKITE-SILICON TANDEM SOLAR CELLS AND MODULES

S. W. Glunz^{1,2}, O. Fischer^{1,2}, D. Chojniak¹, C. A. Messmer^{1,2}, O. Er-raji^{1,2}, M. Mahmoud¹, M. Heydarian¹, M. Heydarian^{1,2}, B. P. Kore², T. Rößler¹, V. Nikitina¹, A. Schmid¹, G. Siefert¹, M. Bivour¹, F. Schindler¹, A. Kraft¹, P. S.C. Schulze¹, H. Neuhaus^{1,2}, M. C. Schubert¹, J. Borchert^{1,2}, M. Hermle¹

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Perovskite silicon tandem solar cells have shown promising progress in device performance, i.e. conversion efficiencies, making them an attractive successor to the currently dominant crystalline silicon solar cells. However, there are some important prerequisites before perovskite-silicon tandem cells and modules can replace the mature and well-established silicon photovoltaics:

1. Industrially feasible production processes.
2. Stable device performance comparable to silicon modules.
3. Proper understanding of loss channels and device characteristics.
4. Accurate calibration of cells and modules.

At Fraunhofer ISE and the University Freiburg we are trying to tackle all these tasks, but this talk will focus on the last two points.

Our long-term research on III-V semiconductor-based tandem solar cells led to record efficiencies of 47.6% for quadruple-junction cells under concentration and a deep understanding of the general tandem solar cell physics. In particular, the correct analysis of tandem solar cells, which is by far more complicated than that of single-junction solar cells, is one of the main research fields at Fraunhofer ISE. Based on this know-how we have developed a calibration procedure for perovskite silicon solar cells and set up a large LED-based sun simulator for full-size tandem modules (see Fig. 1).

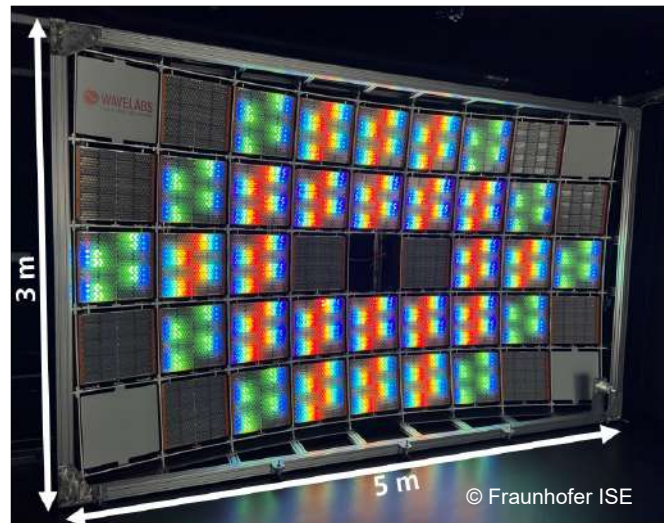


Figure 1: LED-based sun simulator for IV-measurement of tandem modules at Fraunhofer ISE.

Since the IV characteristics of perovskite-based solar cells is strongly influenced by migrating ions, we have set up a comprehensive numerical simulation model to understand the influence of different preconditioning and measurement procedures.

For a targeted technological development of tandem cells, it is important to understand not only the IV characteristics of the complete device but also of the individual sub-cells. As we focus on a monolithic two-terminal device architecture, this is a rather challenging task since it is not possible to contact the sub-cells individually. Therefore, we have developed an advanced set of characterization tools to determine subcell-selective data as photoluminescence-based iVoc images and Suns-Voc.

TOWARDS OUTDOOR OPERATION OF PEROVSKITE SOLAR CELLS

Kai Zhu

Chemistry and Nanoscience Center, National Renewable Energy Laboratory, 15013 Denver West Parkway, Golden, CO 80401

Perovskite solar cells (PSCs) based on halide perovskite light absorbers have skyrocketed the photovoltaic (PV) community as a promising technology for future commercial PV applications. The certified efficiency of single-junction perovskite solar cells (PSCs) has reached 26%. To push PSC technology to the commercialization stage, it is important to develop accelerated aging test protocols and understand their correlation to device operation under outdoor conditions. In this talk, I will first discuss our recent studies on perovskite surface engineering to improve device stability under indoor operational conditions. Using molecules/structures based on bulky organic cations to improve the surface/interface properties has become a promising strategy to enhance PSC efficiency and stability. I will highlight a few strategies on suppressing defect formation, improving bulk and surface morphology, and reducing transport barriers for better extraction. Then, I will focus on our recent progress toward understanding the correlation between indoor accelerated tests and outdoor operational tests. I will show the importance of understanding the thermally activated degradation mechanism and kinetics on improving device reliability under real-world outdoor conditions where multiple stress factors (e.g., light, heat, humidity) coexist. Understanding the link between indoor and outdoor behaviors is necessary to help identify accelerated indoor testing protocols to quickly guide PSC development.

Understanding the Multiple-Facet Degradation Pathways in Metal Halide Perovskite Solar Cells

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The efficiencies of perovskite solar cells demonstrated in lab are so high that they can be seriously candidates for commercialization. However, the low longevity of perovskite solar cells and modules remains to be a major roadblock after years of research. Understanding the underlining mechanisms of device degradation is crucial before inventing strategies to enhance their stability. The degradation of perovskites solar cells is much more complicated than silicon and other thin film solar cells. Here I will report our progress in understand the mechanisms of solar cell degradation under stressors including ultraviolet light, visible light, reverse bias and their combinations. Outdoor stability test, which combines all degradation pathways, will be presented.

LARGE AREA HALIDE PEROVSKITE MODULES AND PANELS: FROM INTERFACE ENGINEERING WITH TWO-DIMENSIONAL MATERIALS TO OUTDOOR TESTING

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In this talk, I will present the progress made to scale up both single junction and tandem from small area solar cells to modules and panels up to a dimension > 0.5 sqm. Key to this transition is the use of two-dimensional (2D) materials, such as graphene, MoS₂, MXenes^[1] and 2D perovskite^[2], to tune interface properties, significantly enhancing the stability and efficiency of perovskite solar cells (PSCs) and modules (PSMs). The large-area panels have been tested in a solar farm setup, covering a total area of 4.5 sqm and achieving peak power exceeding 250 W.^[3] Performance analysis over several months highlighted the importance of the lamination process in mitigating degradation due to environmental factors such as high temperatures and moisture. To further enhance the stability of perovskite modules and panels, innovative encapsulation methods have been developed involving the use of a highly viscous liquid encapsulant adhesive, polyisobutylene, that reduces thermomechanical stresses and improves thermal management.^[4] The addition of 2D hexagonal boron nitride flakes into the polymeric matrix enhances the barrier properties and thermal conductivity of the encapsulant. Encapsulated PSCs and PSMs withstood rigorous accelerated aging tests, including ISOS-D2 (85°C, >1000 hours), ISOS-L1 (light soaking, >1000 hours), thermal shock (200 cycles between +85°C and -40°C), and humidity freeze (10 cycles between +85°C and -40°C, including water immersion before freezing), retaining more than 80% of their initial power conversion efficiency. The success of scaling up is also related to the possibility to achieve very high geometrical fill factor (GFF). Advanced laser manufacturing processes have improved the GFF to 99.6%, with interconnection widths reduced to 45 µm and to 19.5 µm with a discontinuous P2 design.^[5] This significant enhancement results in higher overall efficiency and reduced intrinsic losses during the scaling process from cells to modules. Many of the strategies described above have been also used to realize 4 terminal perovskite/tandem modules and panels that are now under outdoor characterization. Modules' manufacture can be successfully transfer out of glove box without compromising efficiency. Specific efforts have been devoted to developing a deposition process in conventional ambient air. Modules with total area of 320 cm² and aperture area 201 cm² have been fabricated in ambient air by hybrid meniscus coating techniques assisted by air and green antisolvent quenching method showing an efficiency of 15% on aperture area (16.13% on active area).^[6]

Acknowledgements: European Union's Horizon 2020 project Graphene Flagship Core 3 (no. 881603), Horizon Europe project DIAMOND (no. 101084124) and Italian project MASE RdS22-24.

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MACHINE LEARNING DRIVEN ANALYSIS OF HALIDE PEROVSKITES

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Machine learning (ML) is a powerful tool to accelerate the development of halide perovskite materials and devices [1,2]. We apply ML models varying from echo state networks to statistical models to classify and predict physical properties such as hole transport layer electrical conductivity [3], halide perovskite photoluminescence response [4], the power conversion efficiency of photovoltaic devices, etc. Specifically, we use *in situ* environmental optical measurements to predict the optical behavior of Cs-FA perovskites for 50+ hours, upon materials' exposure to moisture [5]. Further, we use ML to identify hidden correlations between chemical composition and material's optical response upon its exposure to environmental stressors [6]. Overall, our platform can be extended to diagnose degradation pathways and mechanisms in different perovskite families, including Pb-free options.

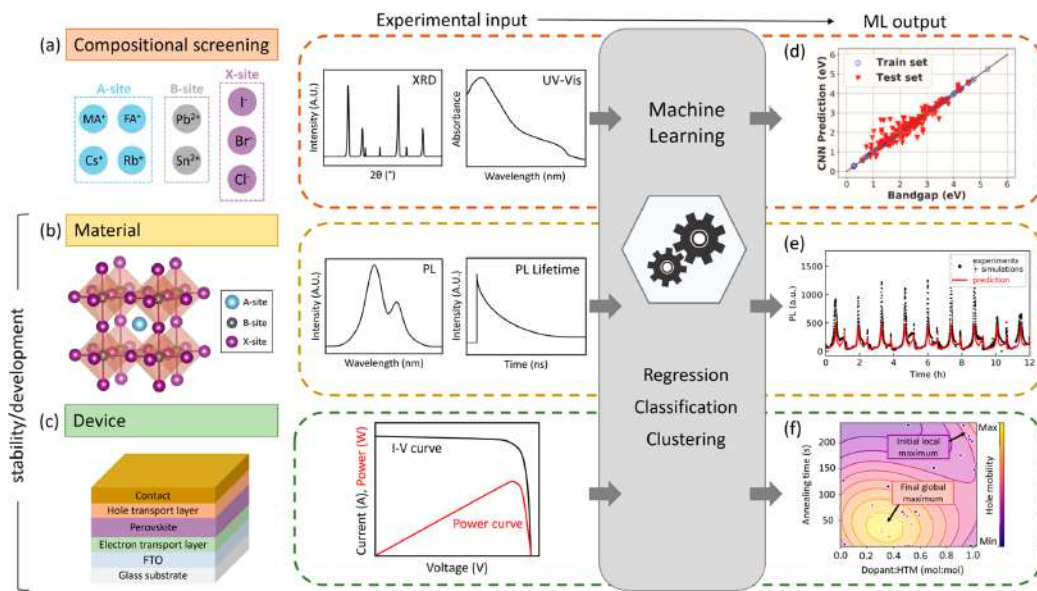


Figure 1: Machine learning for perovskite solar cells. (a) Compositional screening, (b) material, and (c) device development/stability testing. (d–f) Specific examples of model outputs from the literature. Figure from [3].

Acknowledgements: Funding support from DARPA (award #HR00112390144), NSF (ECCS award #2023974), and Sandia National Laboratories.

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METAL HALIDE PEROVSKITES: A MATERIALS CHEMISTRY PERSPECTIVE FROM DESIGN TO APPLICATIONS

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Metal halide perovskites (MHPs) are attracting a huge interest for their potential use in different applicative fields ranging from photovoltaics to photocatalysis. The most investigated MHPs possess the architepal ABX_3 crystal structure, where A= protonated monotopic amine or monovalent inorganic cation, B= Pb, Sn or Ge, and X = Cl⁻, Br⁻, or I⁻. By playing with the nature of the different chemical constituents on the different perovskite sites, it is possible to tune and modulate the optoelectronic properties of the final material and provide materials suitable for different applications. Moreover, by changing the dimensionality of the perovskite structure, *i.e.* moving towards low-dimensional perovskite such as 2D systems, an immense playground for materials chemistry and structural chemistry can be accessed.

In the present contribution, we will present some selected examples in the field of MHPs where, through a rigorous structure-property correlation approach, it was possible to design novel materials with tailored functional properties. This aim requires to devise, synthesise, and characterize rational series of samples to unveil the role of the various chemical degree of freedoms on the optoelectronic properties. We will show how it is possible to design photocatalytically active MHPs to be used in the photogeneration of hydrogen and in the photofixation of nitrogen. This was achieved by selecting suitable amine ligands as well as by understanding the role of central metal ion.^[1-4] The reaction mechanism at the basis of their photocatalytic activity will be also presented, including the role of defect chemistry on the redox activity. A similar materials-design guided approach will be presented for perovskite derivatives used in efficient photodetectors and in the understanding of the chirality transfer mechanisms in chiral perovskite.^[5-6]

Acknowledgements: *This work was supported in part by the Italian Ministry of Foreign Affairs and International Cooperation and by Italian Ministry of University and Research through the program “Dipartimenti di Eccellenza 2023–2027”, PRIN 2022 Grant No 2022F2K7J5 with title Two-dimensional chiral hybrid organic–inorganic perovskites for chiroptoelectronics (MIRROR).*

[1] L. Romani, A. Speltini, F. Ambrosio, E. Mosconi, A. Profumo, M. Marelli, S. Margadonna, A. Milella, F. Fracassi, A. Listorti, F. De Angelis, L. Malavasi, *Angew. Chem. Int. Ed.*, **2021**, *60*, 3611.

[2] L. Romani, A. Speltini, C. N. Dibenedetto, A. Listorti, F. Ambrosio, E. Mosconi, A. Simbula, M. Saba, A. Profumo, P. Quadrelli, F. De Angelis, L. Malavasi, *Adv. Funct. Mater.*, **2021**, *31*, 2214428.

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[4] C. Tedesco, L. Gregori, A. Simbula, F. Pitzalis, A. Speltini, F. Merlo, S. Colella, A. Listorti, E. Mosconi, A. A. Allothman, W. Kaiser, M. Saba, A. Profumo, F. De Angelis, L. Malavasi, *Adv. Energy Sust. Res.*, **2024**, *31*, 2214428.

[5] C. Coccia, M. Morana, A. Mahata, W. Kaiser, M. Moroni, B. Albin, P. Galinetto, G. Folpini, C. Milanese, A. Porta, E. Mosconi, A. Petrozza, F. De Angelis, L. Malavasi, *Angew. Chem. Int. Ed.*, **2024**, 2400040.

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ADVANCED DEVICE CUSTOMIZATION AND QUANTUM CONFINEMENT USING THERMAL EVAPORATION OF METAL-HALIDE PEROVSKITES

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Metal-halide perovskites (MHP) are highly promising optoelectronic materials due to their exceptional properties and versatile fabrication methods [1]. These materials are crucial in applications ranging from solar cells to quantum emitters, harnessing quantum confinement to unlock unique device functionalities.

Thermal evaporation represents a powerful technique for depositing halide perovskite films, offering precise control over layer thickness, composition tuning, stress-free deposition, and surface modification capabilities [2]. This method has revolutionized the perovskite's thin film formation by enabling the creation of ultrathin perovskite layers, forming the basis for constructing different types of multi-quantum well structures as shown in Figure 1.

By manipulating the growth parameters, thermal evaporation enhances the optoelectronic properties of nanoscale thin films, leveraging quantum confinement effects to finely tune photoluminescence characteristics. This capability opens avenues for unconventional optoelectronic functionalities and innovative perovskite applications [3].

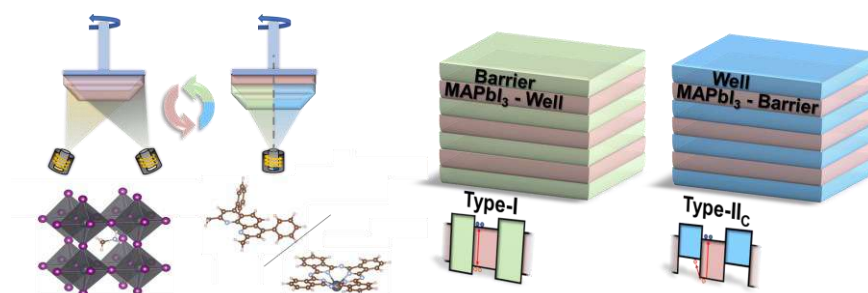


Figure 1: Thermal Evaporation Process for MQW Growth and Schematic Representations of Type I and Type II MQW Structures

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[2] A. Li et al., Joule 2020, 4, 1035; F. Kosasih, 2022 Joule 6(2692); H.A. Dewi et al., Adv. Funct. Mater. 2021, 11, 2100557; J. Li et al., Adv. Funct. Mater. 2021, 11, 2103252;
[3] E. Parrott et al., Nanoscale 2019, 11, 14276; K.J. Lee et al., Nano Letters 2019, 19, 3535; K.J. Lee et al., Advanced Materials 2021, 33, 2005166; T. Antrack et al., Adv. Sci. 2022, 9, 2200379

Poster Pitch Presentations (2 minutes each) | Town Hall

Session Chair: *Daniele Meggiolaro, CNR-SCITEC, Italy*

18:37	18:39	Lorenzo Squillantini , CNR, Italy <i>The role of carbon-based nanomaterials as additives in improving the performance of hybrid perovskite solar cells</i>
18:39	18:41	Selene Matta , University of Cagliari, Italy <i>Space-confined 2D and quasi-2D halide perovskite single crystals</i>
18:41	18:43	Lukasz Przypis , Wroclaw University of Science and Technology, Poland <i>Additive-Assisted Synthesis of Tin(II) Iodide: A Key Factor for Stable Large-Area Lead-Free Perovskite Solar Cells</i>
18:43	18:45	Yassine Raoui , CHOSE, University of Rome Tor Vergata, Italy <i>Efficient Inverted Semi-Transparent Perovskite Solar Cells based on scalable Solution-Processed Hole Transport Layer toward 4T tandem integration</i>
18:45	18:47	Erica Magliano , CHOSE, University of Rome Tor Vergata, Italy <i>Solution-Processed Buffer Layer for Monolithic Perovskite/Silicon Tandem Solar Cells with Unpolished Rear Surface Silicon Heterojunction</i>
18:47	18:49	Shaoni Kar , Helio Display Materials, University of Oxford, United Kingdom <i>Dimethylammonium-incorporated mixed halide perovskite nanocrystals for stabilized red emission</i>
18:49	18:51	David Otto Tiede , Institute of Materials Science of Seville, Spain <i>Revisiting Time Resolved Measurements - How Amplitude Derivatives Reveal Hidden Global Recombination Mechanisms</i>
18:51	18:53	Amin Hasan Husien , University of Milano-Bicocca, Italy <i>Chalcogenide-based hole transport material for stable perovskite solar cells</i>
18:53	18:55	Sam Teale , University of Oxford, United Kingdom <i>Monolithic perovskite tandem photovoltaics optimised for maximum energy yield</i>
18:55	18:57	Elisa Nonni , Solertix s.r.l., Italy <i>Techniques for low-cost upscaling of bifacial 4 terminal perovskite-silicon tandem</i>
18:57	18:59	Rahul Ajit Nambiar , University of Oxford, United Kingdom <i>Interdiffusion control in sequentially evaporated inorganic-organic fully vacuum deposited perovskite solar cells</i>
18:59	19:01	Hadi Rostamzadeh Kalkhoran , Eindhoven University of Technology, Netherlands <i>Characterization of quasi-reversible performance losses in an outdoor perovskite solar cell under partial shading</i>
19:01	19:03	Roland Clausing , Institute for Solar Energy Research Hamelin ISFH, Germany <i>Fast and scalable two-step pin-FAXCs_{1-x}PbI_{3-x}yBr_y formation via gas-transport deposition for single-junction and tandem application</i>
19:03	19:05	Yasuhiro Miura , Hamamatsu University School of Medicine, Japan <i>A Strategy for Fabricating Two-Dimensional Hybrid Perovskite Ultra-Thin Films Utilizing Langmuir-Blodgett and Intercalation Methods</i>
19:05	21:00	POSTER SESSION & BUFFET DINNER



THE ROLE OF CARBON-BASED NANOMATERIALS AS ADDITIVES IN IMPROVING THE PERFORMANCE OF HYBRID PEROVSKITE SOLAR CELLS

Squillantini Lorenzo,¹ De Giorgio Francesca,^{1,2} Natali Marco,¹ Dionigi Chiara,¹ Seri Mirko,¹ Mezzi Alessio,³ Liscio Fabiola,⁴ Tocco Davide,⁵ Fratini Emiliano,⁵ Parisini Andrea,⁴ Ruani Giampiero¹

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Hybrid Perovskite Solar Cells (HPSCs) based on lead halide perovskites as absorbers came to the attention of the material science community thanks to their comparable performances to traditional Si-based inorganic solar cells, combined with low production costs due to solution processability.

However, HPSCs suffer from poor environmental and thermal stability and very often from inadequate quality of the polycrystalline structure in terms of traps and grain boundaries, dramatically affecting the performance of the devices^[1].

To attenuate these undesired effects, a large variety of additives were proposed, including carbon-based nanomaterials such as fullerene derivatives^[2], carbon nanotubes^[3] and carbon quantum dots (CQDs)^[4]. Due to the richness of functional groups on their surfaces, the latter are particularly suited to interact with perovskite grain boundaries, reducing defects and recombination centers.

Here, CQDs synthesized under relatively mild reaction conditions^[5] using cheap and readily available precursors, i.e. citric acid and L-tryptophan, are proposed as additives for Methylammonium PbI₃ (MAPI)-based HPSCs. The CQDs are studied through XRD, TEM and various spectroscopic approaches, while the performances of HPSCs are evaluated by using optoelectronic, electrical and electrochemical techniques. An improvement of HPSCs performances such as the PCE and fill factor is observed, depending also on the composition of the CQDs, i.e. the relative proportions of L-tryptophan and citric acid in the CQDs reaction mixtures.

[1] J.M. Azpiroz, et al., *Energy Environ. Sci.* **2015** 8, 2118-2127

[2] L. Jia, et al., *Nano Today* **2021** 39, 101164

[3] X. Ma, et al., *ACS Appl. Energy Mater.* **2020** 3, 11674-11680

[4] A. Kim, et al., *ACS Appl. Electron. Mater.* **2022** 4, 27-58

[5] X. Zhang, et al., *J. Photochem. Photobiol. A-Chem.* **2019** 372, 71-77

SPACE-CONFINED 2D AND QUASI-2D HALIDE PEROVSKITE SINGLE CRYSTALS

Matta S,¹ Liscia S,¹ Demontis V,¹ Marongiu D,¹ Simbula A,¹ Pitzalis F,¹ Lai S,¹ Pau R,^{1,2} Wu R,¹ Cadeddu E.D,¹ Wu L,¹ Quochi F,^{1,3} Saba M,¹ Mura A,¹ Bongiovanni G¹

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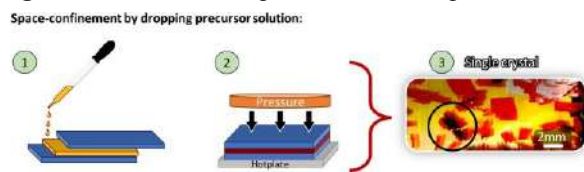
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Photovoltaic research aims to find materials for high-performance devices. Perovskites, especially 3D variants, are promising due to their excellent properties, making them ideal for solar cell applications. Despite their high performance, perovskites face instability issues, which can be mitigated through the passivation with 2D perovskites. Notable for their environmental resilience, 2D perovskites feature inorganic layers interposed between organic spacers. Recent research indicates that both 2D and 3D perovskites are suitable for solar cells due to their abundance of free carriers [1,2]. Although aligning the preferred crystallography orientation of 2D perovskites with the carrier collection direction is necessary for optimal performance, the abundance of free carriers makes them suitable for passivating 3D perovskites without compromising solar cell efficiency. Passivation with 2D layers reduces non-radiative recombination, improves charge carrier lifetimes, and enhances device stability against moisture, which is crucial for long-term performance. For this reason, an optimal interface between 3D and 2D perovskites becomes fundamental not to affect the cell efficiency. Notably, in 2D single crystals the absence of grain boundaries enhances electronic properties, such as charge transport. Achieving ultrathin passivating layers is crucial for device performance too, preventing carrier loss, and ensuring effective light absorption to unlock the full potential of carrier transport. This can be attained by a successful space-confined method, which allows to control the thickness during perovskite preparation.

My work related to space-confined technique will be explained, in which the details of the processes and interfaces between the 2D and 3D perovskites obtained will be explored. By controlling the growth within specific spaces and altering confinement surfaces, we shaped the crystals' size and form. We analysed the samples using techniques like confocal microscopy and XRD to study their thickness, morphology, and orientation.

Figure 1: Process description and the sample obtained.



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ADDITIVE-ASSISTED SYNTHESIS OF TIN(II) IODIDE: A KEY FACTOR FOR STABLE LARGE-AREA LEAD-FREE PEROVSKITE SOLAR CELL

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Despite advancements in perovskites, the quest for stable and high-performance tin-based perovskite solar cells (TPSCs) continues. Various avenues have been explored, including the use of reducing agents, antioxidants, bulky cations, and tailored solvent systems. Our work presents a fresh perspective on the synthesis of SnI₂, unveiling a novel approach based on additive engineering. This innovative strategy not only streamlines the synthesis process but also enhances the stability of precursors against oxidation. The interaction of their functional groups with precursors results in defect suppression, improving device performance and stability. In this research, we briefly summarize the different types of additives applied in our synthesis of SnI₂ to enhance not only efficiency but also long-term stability. We discuss the different mechanisms behind additive engineering and the role of the functional groups of these additives for the synthesis of SnI₂ and tin-based perovskite. Furthermore, our study unveils remarkable reproducibility in the fabrication of large-area (>1 cm²) flexible TPSCs, showcasing enhanced open-circuit voltage compared to those produced from commercial SnI₂. These findings hint at the promising methodology in advancing the field of stable and efficient tin-based perovskite solar cells.

INDUSTRIAL-SCALE FABRICATION METHODS OF HTL AND TCO FILMS FOR EFFICIENT INVERTED SEMI-TRANSPARENT PEROVSKITE SOLAR CELLS AND 4T TANDEM APPLICATIONS

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Efforts to exceed the Shockley-Queisser (SQ) limit in single-junction solar cells have been realized through tandem integration. In this context, semi-transparent inverted wide band gap perovskite solar cells (STPSCs) offer a promising solution due to their low-temperature fabrication process, which is suitable for tandem integration^{[1] [2]}. However, scalable solution processing of the hole transport layer (HTL) and traditional radio frequency (RF) sputtering of transparent conductive oxides (TCOs), such as indium tin oxide (ITO), presents significant challenges. This study introduces a scalable solution processing approach for the HTL using a blade-coating (BC) technique with nickel oxide nanoparticles (NiOx-np). Additionally, the performance of RF and pulsed direct current (DC) sputtering of ITO as the front electrode of STPSCs is compared. As a result, methylammonium (MA)-free STPSCs based on the scalable solution-processed HTL of NiOx-np achieved a champion power conversion efficiency of 18.01% and 18.79% using RF and pulsed DC sputtered ITO, respectively. The present study demonstrates a significant achievement, exceeding an efficiency of 27% for both sputtering techniques of the front TCO electrode in 4T tandem perovskite-silicon solar cells. This innovative approach not only enhances the performance of semi-transparent inverted wide band gap perovskite solar cells but also establishes a low-cost, high-efficiency, and industrially scalable method for the HTL and sputtering of front TCOs electrode, advancing the commercialization of 4T perovskite-silicon tandem solar cells.

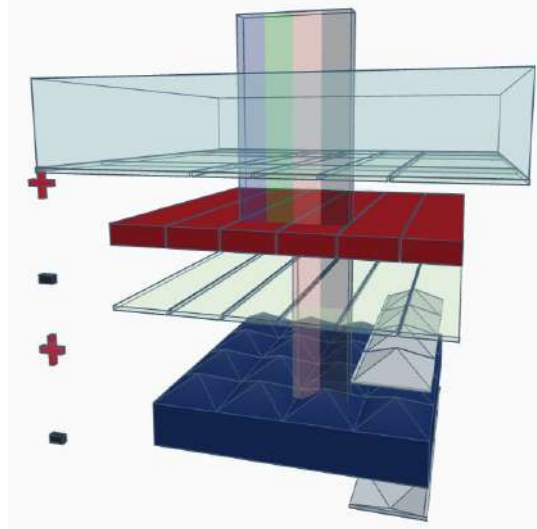


Figure 1: Schematic illustration of the 4T perovskite-Silicon tandem solar cells.

[1] T. Han, et al., *Advanced Functional Materials* (2023) 2311679..

[2] D. Zhang et al. , *Solar RRL* 7 (2023) 2200914.

TWO-STEP HYBRID PEROVSKITE DEPOSITION: ORGANIC CATIONS INTERDIFFUSION THROUGH SPIN-COATING AND BLADE-COATING FOR TANDEM APPLICATIONS

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Perovskite/silicon tandem solar cells represent a promising solution to overcome single junction limit.^[1,2] A conformal deposition of the perovskite top cell on silicon substrates represents a crucial aspect in monolithic tandem architecture. In this context, a two-step hybrid deposition (consisting of evaporation of the inorganic components and subsequent solution-processing of the organic salts solution) can ensure the advantages of vacuum deposition, such as layer conformality, while overcoming the drawbacks encountered in the evaporation of organic cations.^[3,4]

In this work, the two-step hybrid method is employed for perovskite deposition in inverted *p-i-n* solar cells. The inorganic components (PbI₂ and CsBr) are thermally evaporated, whereas the infiltration of the organic cations is performed by either spin-coating or blade-coating. The optimization of the former technique allowed us to achieve a power conversion efficiency (*PCE*) of 19.5% with fill factor (*FF*) around 82%. In order to apply this process to a monolithic tandem solar cell, we developed a simple solution-process buffer layer strategy to sputter ITO without damaging the underlying layers.

The fabrication process was then successfully transferred on fully-flat front-side polished *p*-type silicon-based heterojunction with an efficiency of ~ 18%. The resulting monolithic tandem cells showed an efficiency of ~ 25%, thus achieving a 40% relative efficiency gain as compared to the standalone SHJ. However, spin-coating can hinder film uniformity and scalability. Blade-coating represents a promising alternative approach for organic cations infiltration to meet the demands of large-scale manufacturing. Nonetheless, the control of solvent volatilization kinetics in blade-coating can be more arduous. In order to optimize the solvent evaporation rate, we tuned the blading substrate temperature and gas quenching parameters. An improved crystallization and film morphology was obtained with substrate temperature at 30°C and high-pressure air knife (flow rate of 150 L min⁻¹). Additionally, the optimal solvent and concentration were investigated, resulting in devices with *FF* slightly lower (~ 77.5%) than the spin-coated counterpart.

Future steps will explore the implementation of the optimized evaporation/blade-coating perovskite on Si HJT in tandem configuration. Thus, the present study paves the way for developing highly efficient tandem solar cells.

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[3] M. Roß, M. B. Stutz, and S. Albrecht, *Sol. RRL* **2022**, vol. 6, no. 10.

[4] F. U. Kosasih, et al., *Joule* **2022**, vol. 6, no. 12, pp. 2692–2734.

DIMETHYLAMMONIUM-INCORPORATED MIXED HALIDE PEROVSKITE NANOCRYSTALS FOR STABILIZED RED EMISSION

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All-inorganic perovskite nanocrystals are attractive candidates for light emission applications. Of these, cesium lead iodide (CsPbI₃) nanocrystals have been shown to be promising but their device application is still inhibited by their inherent ambient instability due to rapid conversion of the metastable black perovskite Υ -phase into the yellow δ -phase at room temperature [1]. With addition of bromine (Br), CsPbI_xBr_{3-x} nanocrystals are formed with ideal bandgaps for emission within the Rec 2020 colour gamut. Furthermore, in contrast to the pure-iodide compositions that require high temperature-based (hot injection) processes to form the perovskite phase, mixed-halide nanocrystals afford facile synthesis through room-temperature ligand assisted reprecipitation (LARP). However, these materials are still plagued by phase separation under optical or electrical excitations of intensities typical in a working device [2].

In this work, we alloy the A-site of the pure-red emitting CsPbI₂Br with dimethylammonium (DMA) to improve its phase stability under excitation while retaining high photoluminescence quantum yields. DMA, among other organic cations, has recently been shown to alloy successfully with Cs in 3D perovskite thin films and lend it stability under operational conditions [3]. To our knowledge, this is the first study of DMA-alloying through facile LARP synthesis techniques. We propose a novel synthetic route at room temperature and then study the crystal structure and morphology as a function of different DMA contents through an interplay of crystallographic and optical data. We report higher ambient stability even under intense optical excitation. We further probe the crystal lattice through solid-state NMR and high-resolution STEM-EDX to understand the mechanism and extent of DMA incorporation. We also use X-ray photoelectron spectroscopy (XPS) to investigate the DMA-contents. Finally, we fabricate light emitting diodes (LEDs) using these materials and show improved brightness, efficiency and operational stability in DMA-incorporated NC-based devices as compared to the pristine reference samples.

These findings are currently being compiled into a manuscript.

Acknowledgements: S.K. acknowledges funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement no. 956270 and from a Viperlab grant for access to STEM-EDX and XPS/UPS in HZB, Berlin and Fraunhofer, Centre for Silicon Photovoltaics, Halle respectively.

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[3] A. R. Marshall et al., *Solar RRL* (2021), 5, 1.

REVISITING TIME RESOLVED MEASUREMENTS – HOW AMPLITUDE DERIVATIVES REVEAL HIDDEN GLOBAL RECOMBINATION MECHANISMS

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Charge carrier recombination models such as Shockley-Read-Hall (SRH) are commonly used in the study of semiconductor materials to understand charge carrier recombination and eventually evaluate their performance in an optoelectronic device. A typical experimental approach to imitate the processes predicted by this model is to employ time resolved emission and absorption spectroscopy, where the time evolution of these magnitudes can be associated to that of the charge carrier populations. This approach is, however, often limited to canonic material systems where all charge carrier evolution channels are precisely known. In contrast to that, many novel perovskite morphologies present additional mechanisms such as diffusion or local charge trapping that impedes an unambiguous description within these charge carrier recombination models.

In this presentation, we revise the use of charge carrier recombination models on material systems that do not enter the canonical description associated with SRH. A novel, though universally applicable analysis toolbox, is introduced that considers the derivative representation of time resolved spectroscopic measurements^[1]. This toolbox allows to disentangle overlapping charge carrier dynamics in time resolved photoluminescence and transient absorption measurements, where a distinction between diffusion, carrier cooling and band-to-band recombination processes can be established. We employ this model to a broad range of diverging samples with acknowledged potential for optoelectronic devices. Effects of connectivity are analysed in quantum dot solids^[2], surface passivation effects are discriminated in evaporated thin films and charge carrier transport in device stacks are quantified.

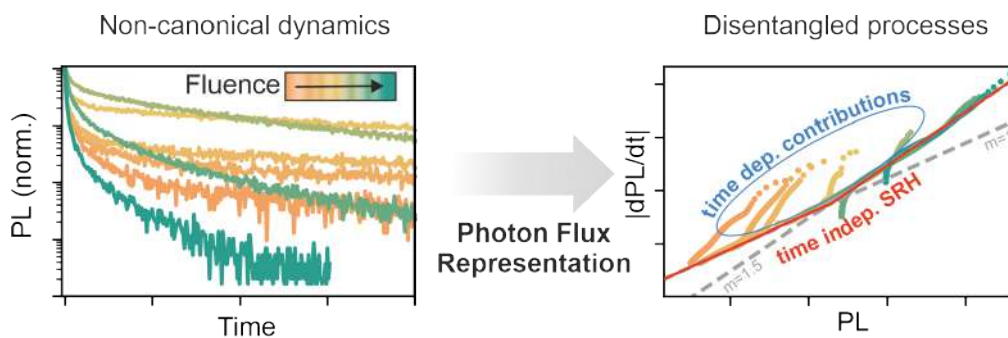


Figure 1: Representation of TRPL data as photon flux vs. its time derivative. Main processes are highlighted.

[1] D.O. Tiede, *in preparation* 2024.

[2] D.O. Tiede, *ACS Nano* 2024, 18, 2325-2334.

CHALCOGENIDE-BASED HOLE TRANSPORT MATERIAL FOR STABLE PEROVSKITE SOLAR CELLS.

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To drive perovskite photovoltaic (PV) toward commercialization is necessary to develop large-area modules with high efficiency, enhance large-scale and low-cost production processes, and achieve long-term operational stability. The solar cells' stability depends upon many factors including the materials employed to produce the hole transporting layer (HTL). Besides, novel hole transport materials (HTMs) are required to achieve a large deployment of sustainable and cost-effective PV devices. $\text{Cu}_2\text{ZnSnS}_4$ (CZTS) can fulfil the targets of cost-effectiveness and sustainability, and here we investigate its impact on PV performance stability when employed as HTM. CZTS is a p-type semiconductor, commonly studied as a light absorber layer in heterojunction solar cells, but lately, it has shown promising results also as HTL in perovskite solar cells (PSCs). Here, we report on the synthesis of CZTS nanoparticles (NPs) employed as HTM in PSCs. The NPs have been synthesized by the hot-injection method, in an oxygen-free environment using a Schlenk line apparatus. CZTS NPs ink has been obtained by dispersing the undried nanoparticles in xylene. The ink was filtered and then spin-coated on the substrate. The resulting film was annealed in air on a hot plate. The resulting 50 nm thick HTL was almost transparent in the visible range of the solar spectrum, and it has been fully characterized by transmittance and scanning electron microscopies, UV-Vis, μ -Raman, and X-ray diffraction spectroscopies. Hole mobility and charge transport have been evaluated in plane and out of plane, ensuring the material feasibility to act as HTL. The preliminary results of the CZTS NPs-based HTM for PSCs in p-i-n architecture are discussed, focusing on the retention of the initial PV performances. The control device (organic-HTL / $\text{CH}_3\text{NH}_3\text{PbI}_3$ / PC_{60}BM -BCP / Ag) loses more than half of the initial efficiency in one month, but the devices employing the CZTS-NPs remain stable, and, in some cases, the PV performances improved with time. The PV parameters evolution with time has been monitored through periodical current/voltage and external quantum efficiency measurements, aided by admittance spectroscopy data analysis and scanning electron microscopy imaging. This work aims to promote a new path to control stability, employing an HTM able to prevent the degradation of the PV performance.

MONOLITHIC PEROVSKITE TANDEM PHOTOVOLTAICS OPTIMISED FOR MAXIMUM ENERGY YIELD

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Photovoltaic cells are generally optimised for operation at 25 °C under the AM1.5 solar spectrum. This is useful for comparing different technologies, but ultimately energy yield (the energy output across a year of operation) is what we aim to maximise. This is generally estimated using the power conversion efficiency (PCE) of a cell at 25 °C and its temperature coefficient (how PCE changes with temperature). For monolithic tandem cells, this method is less accurate as current matching between each sub cell is required for maximum performance. To understand how to optimise tandems for energy yield, we fabricated perovskite/Si (30.8% PCE) and all-perovskite (25.4% PCE) tandems and tested them over a range of temperatures. Opposing temperature dependence with bandgap - perovskite bandgaps tend to widen with increasing temperature, whereas Si narrows - results in a worse temperature coefficient for perovskite/Si (-0.23%/°C) compared to all-perovskite tandems (-0.17%/°C). Thus, we engineered the perovskite structure so that its bandgap does not widen with temperature, resulting in an improved temperature coefficient (-0.19%/°C). Surprisingly, when estimating energy yields using real-world data, this improved temperature coefficient does not translate to increased yields. Instead, we find that the opposing temperature/bandgap correlation of perovskite/Si tandems is an advantage as the solar spectrum is blue-shifted compared to AM1.5 when cells are warmest and operate at their peak power output. Thus, we expect a 1-2.5% increase in energy yield for optimised perovskite/Si tandems compared to other tandem technologies with the same PCE.

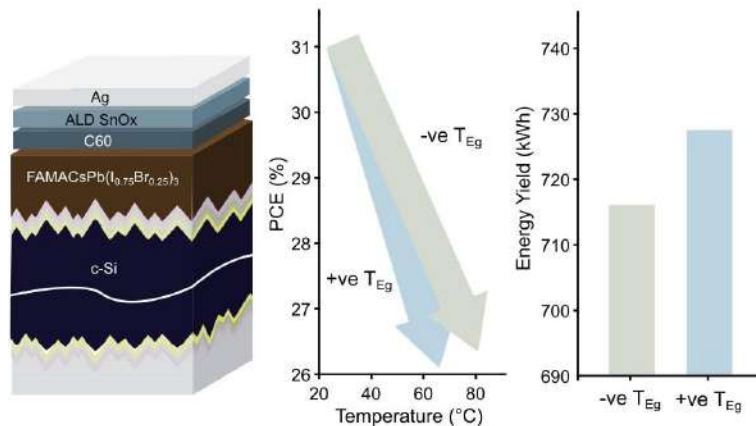


Figure 1: Summary demonstrating that perovskites with negative T_{Eg} (their bandgaps' narrow with temperature, as does Si) have improved temperature coefficients, but this does not translate into higher energy yields.

TECHNIQUES FOR LOW-COST UPSCALING OF BIFACIAL 4 TERMINAL PEROVSKITE-SILICON TANDEM

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Bifacial Four terminal (4T) perovskite-silicon tandem are a promising concept for achieving a high energy yield in PV installation. Solertix is a start-up company born from the CHOSE group of the University of Tor Vergata and is now part of the FuturaSun group. The company is developing highly efficient semitransparent perovskite cells and modules to demonstrate how the 4T tandem technology can be a viable and cost effective method to go beyond the efficiency of conventional Si panel. In this talk, we will discuss the steps taken into the stack optimization to maximize the efficiency of semitransparent perovskite solar cells with efficiency above 20 %. We will discuss the impact of hole transport layers and their modification, as well as the comparison of solution processable vs. PVD+sALD deposition of the electron transport layers compatible with the sputtering of transparent top electrodes, and their impact on device stability. We will also discuss the pathways to deposit a uniform perovskite layer over large area samples. We will examine the impact of the ink chemistry in combination with different deposition and crystallization methods, as well as the evaluation of the impact of the processing environment with a focus on the relative humidity. The morphology and crystallinity of the perovskite films will be analyzed and correlated with the efficiency of semitransparent solar cells and modules for the use in 4T tandem devices with efficiency of 30%.

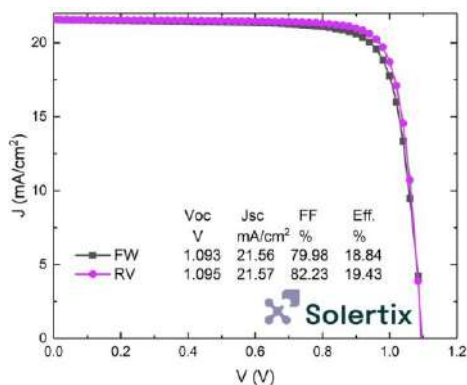


Figure 1: J-V curve of semitransparent perovskite solar cell

INTERDIFFUSION CONTROL IN SEQUENTIALLY EVAPORATED INORGANIC-ORGANIC FULLY VACUUM DEPOSITED PEROVSKITE SOLAR CELLS

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Vacuum deposition emerges as a pivotal method for scaling up perovskite solar cells (PSCs) in commercial applications, offering conformal coatings on various surfaces and precise layer control, aligning with large-scale manufacturing(1). Atmospheric conditions, particularly moisture in the atmosphere, significantly impact perovskite layer quality, requiring controlled environments(2). Through in-situ grazing incidence wide angle x-ray scattering (GIWAX) and 3D time of flight secondary ion mass spectroscopy (ToF-SIMS) we show that annealing in the presence of humidity, is essential for the interdiffusion of inorganic and organic precursors necessary to achieve high quality thermally evaporated perovskite absorbers via sequential deposition. Notably, spectroscopy measurements also indicate a bulk limitation in the absorbers photoluminescence when processed without the presence of any relative humidity, bolstering the importance of interdiffusion for the device's overall performance. This breakthrough has resulted in the development of high-performance perovskite solar cells (PSCs) exclusively processed through vacuum techniques, achieving an impressive power conversion efficiency of 20.45%. Stability tests reveal an initial burn-in phase during accelerated aging at 85°C and 1 sun illumination using full spectrum while holding the device at open circuit condition. Despite this phenomenon, the devices exhibit remarkable stability, remaining functional for an additional 500 hours post the initial challenge. This finding highlights the resilience and potential durability of the newly developed vacuum-processed PSCs, marking a significant advancement in the field of perovskite solar cell technology.

[1]T. Abzieher *et al.*, Vapor phase deposition of perovskite photovoltaics: short track to commercialization? *Energy & Environmental Science*, (2024).

[2]G. E. Eperon *et al.*, The Importance of Moisture in Hybrid Lead Halide Perovskite Thin Film Fabrication. *ACS Nano* **9**, 9380-9393 (2015).

CHARACTERIZATION OF QUASI-REVERSIBLE PERFORMANCE LOSSES IN AN OUTDOOR PEROVSKITE SOLAR CELL UNDER PARTIAL SHADING

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Metal halide perovskite solar cells exhibit intriguing behavior under partial shading conditions, owing to their mixed ionic-electronic properties. When subjected to reverse bias, electrons within the perovskite layer tunnel to the electron transport layer (ETL) due to the higher energy level of the perovskite valence band relative to the ETL conduction band¹. This phenomenon leads to hole generation and tunneling at the ETL/perovskite interface toward the perovskite/HTL (hole transport layer), while hindering electron tunneling at the perovskite/HTL interface due to large injection barrier. Consequently, holes accumulate within the perovskite layer near the HTL, oxidizing the halides and forming neutral halogens, which act as recombination centers. These centers reduce solar cell efficiency under forward bias and necessitate characterization for outdoor performance evaluations.

This study consists of two investigation phases. The initial phase involves characterizing performance loss in a perovskite solar cell under prolonged reverse bias at standard testing conditions, using advanced device modeling. The model integrates the kinetics of three species- iodine atoms, iodide anions, and iodine molecules- affecting iodide chemistry. The effects of shading duration, reverse bias magnitude, iodide anion concentration, and kinetic reaction rates related to halide photo-oxidation and halogen photoreduction on reversible and irreversible performance losses are investigated. The second phase aims to understand iodide anion chemistry in a glass-glass encapsulated perovskite solar cell under outdoor operating conditions. The solar cell's performance losses and recovery under partial shading varying with solar irradiance, incident angle, and ambient temperature can be understood by coupling the developed electrochemical model with optical and thermal models.

The findings indicate that incorporating iodide chemistry into optical, electrical, and thermal modeling of outdoor perovskite solar cells enhances the accuracy of energy yield calculations. The solar cell experiences significant performance losses under partial shading, which remain irrecoverable under prolonged shading, leading to irreversible degradation. Notably, the solar cell exhibits severe hysteresis under shading, with its effects persisting and intensifying over post-shading time, further contributing to irreversible degradation. Consequently, the study recommends reconfiguring the physical properties of the solar cell to mitigate the irreversible degradation effects of shading, while vigilantly monitoring the reversible performance losses.

[1] Bertoluzzi, L.; Patel, J. B.; Bush, K. A.; Boyd, C. C.; Kerner, R. A.; O'Regan, B. C.; McGehee, M. D. Incorporating Electrochemical Halide Oxidation into Drift- Diffusion Models to Explain Performance Losses in Perovskite Solar Cells under Prolonged Reverse Bias. *Advanced Energy Materials* **2021**, *11* (10), 2002614.

FAST AND SCALABLE TWO-STEP PIN - $FA_xCs_{1-x}PbI_{3-x-y}Br_y$ FORMATION VIA GAS-TRANSPORT DEPOSITION FOR SINGLE-JUNCTION AND TANDEM APPLICATION

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For industrial production of perovskite (pk) solar cells or pk-based tandems, a two-step approach for scalable deposition techniques enables easy to control and reproducible processes. Following the approach of Guesnay and Sahli et al. [1,2,3], we developed an ammonia-based gas-transport deposition of the organic component (mainly formamidinium-iodide, FAI) in a quartz tube three-zone-furnace at much higher processing pressure (~1 mbars) than typically needed for physical-vapor deposition.

For compact $Cs_{1-x}PbI_{3-x-y}Br_y$ precursors, Moser et al. [4] showed a rather slow surface-to-bulk conversion. To enable a fast conversion, we therefore form a porous precursor by (co-) evaporation of PbI_2 (and optionally $CsBr$ and $PbBr_2$) to allow fast in-diffusion of FAI. These precursors were evaporated onto glass/ITO-substrates, or onto silicon bottom cells with an ITO recombination layer, after HTL-deposition. Both the precursor process and the conversion step in the furnace are able to conformally coat textured silicon bottom cells as shown in Fig. 1.

In the furnace, a crucible containing an organic salt (e.g. FAI) and the zone with the precursor substrates are heated to their respective processing temperatures. Then, the gas flow direction is inverted, allowing the ammonia to carry the evaporated FAI onto the substrates, starting the conversion. To stop the process, the gas flow is simply reversed again and the zones cooled down to room temperature for subsequent processing steps. As the precursors are converted at ~150 °C, an additional advantage of this technique is the omittable annealing step, causing the resulting pk to already be present in the photoactive α phase. XRD measurements indicate a complete conversion after 15 min (no resolvable remaining PbI_2 peak). This is an important step towards an industrially relevant processing speed. The first pk single junction cells show an efficiency of 13.1%. By fine-tuning temperatures, gas flow rates and passivating additives, we aim to improve the electronic absorber quality (especially the voltage) significantly further until the conference.

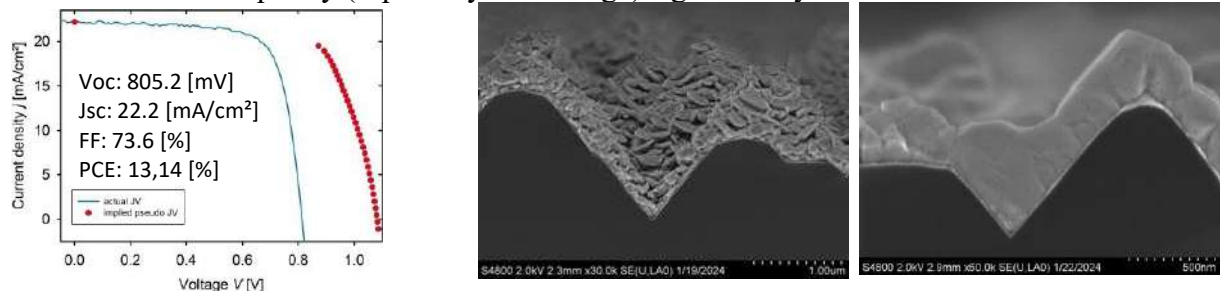


Figure 1: JV-curve (blue) of the current record FAPBI₃-SJ cell and implied pseudo-JV-curve (red) from intensity-dependent absolute photoluminescence (left), SEM-images of porous PbI_2 -precursor (middle) and converted pk (right) on textured silicon bottom cells.

Acknowledgements: The authors would like to thank C. Marquardt, A. Raugewitz, J. Strey (all ISFH). This work was carried out in the project APERO funded by the Federal Ministry for Economic Affairs and Climate Action under grant no 03EE1113B.

[1] Q. Guesnay et al., *APL Mater.* **2021** 9, 100703, <https://doi.org/10.1063/5.0060642>

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[3] Q. Guesnay et al., *Adv. Energy Mater.* **2024** 14, 2303423. <https://doi.org/10.1002/aenm.202303423>

[4] T. Moser et al., *Front. Energy Res.* **2022** 10:883882. <https://doi.org/10.3389/fenrg.2022.883882>

A STRATEGY FOR FABRICATING TWO-DIMENSIONAL HYBRID PEROVSKITE ULTRA-THIN FILMS UTILIZING LANGMUIR-BLODGETT AND INTERCALATION METHODS

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Thin film fabrication of 2D layered hybrid perovskites (LHPs) attracts significant attention, from both the standpoint of basic research and practical applications.^[1] Here we demonstrate the fabrication of well-organized ultra-thin films of 2D LHPs simply by immersing octadecyl amine (ODA) Langmuir–Blodgett (LB) films in the PbX_2/HX ($\text{X} = \text{Cl}, \text{Br}, \text{I}$) aqueous solutions.^[2]

Figure 1(a) shows UV-visible absorption spectra of ODA LB films (3–21 layers) after immersing in the PbI_2/HI solution. The films exhibit a sharp band at 486 nm (2.55 eV), which is due to the excitonic absorption. The peak absorbance increases with the number of layers proportionally, indicating successful layer-by-layer fabrication. The film exhibits a bright green emission under ultraviolet light at room temperature. The photoluminescence spectrum has a distinct peak at 497 nm (2.49 eV) and is a mirror image of the absorption spectrum. Figure 1(b) illustrates a distinct fluorescent contrast at the nanometer-scale step-like structure of the film in the micrograph, indicating precise layer-by-layer fabrication. The XRD analyses reveal that the film has a bilayer-like structure with a d -spacing of 6.4 nm, which is equal to that of a $(\text{C}_{18}\text{H}_{37}\text{NH}_3)_2\text{PbI}_4$ perovskite single crystal with a quantum well structure. Only intense peaks of the $(0\ 0\ l)$ ($l = 2, 4, 6, 8, 10, 12, 14, 16, 18, 20, 22,$ and 24) reflections are observed in the out-of-plane XRD pattern, indicating that the c -axis is vertically oriented with respect to the substrate surface with a remarkably high order. We will further discuss our recent success in the fabrication of various lead-halide-based 2D LHP films. Because of the versatility of the present technique, which allows us to fabricate 2D LHP films with various compositions while controlling thicknesses at the nanometer scale, we believe that the proposed technique will contribute to the development of highly efficient 2D LHP materials.

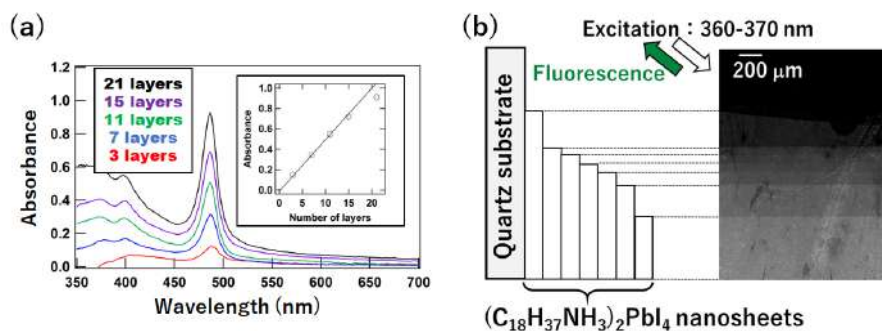


Figure 1. (a) UV-visible absorption spectra of the ODA LB film with various numbers of layers after immersing in the PbI_2/HI aq. solution for 50 min. The inset shows the absorbance at 486 nm plotted against the number of layers; (b) a fluorescent micrograph observed at the nanometer-scale step-like structure.

[1] L. Mao, C. C. Stoumpos, and M. G. Kanatzidis, *J. Am. Chem. Soc.* **2019**, 141, 1171-1190.

[2] Y. F. Miura, Y. Akagi, D. Hishida, and Y. Takeoka, *ACS Omega* **2022**, 7, 47812-47820.

Day 2 - Tuesday, September 17th, 2024

Session Chair:		Lorenzo Malavasi, University of Pavia, INSTM, Italy
08:30	08:55	11° INVITED LECTURE - Henry Snaith , University of Oxford, United Kingdom <i>Improving stability and efficiency of metal halide perovskite solar cells</i>
08:55	09:20	12° INVITED LECTURE - Monica Lira Cantu , ICN2, Spain <i>Indoor and outdoor stability studies of perovskite solar cells</i>
09:20	09:45	13° INVITED LECTURE - Edoardo Mosconi , CNR-SCITEC Perugia, Italy <i>Computational modeling of perovskite for photovoltaics and photocatalysis</i>
09:45	10:10	14° INVITED LECTURE - Maria Antonietta Loi , University of Groningen, Netherlands <i>Scalable deposition of lead-tin perovskite solar</i>
10:10	10:13	NIREOS (3 mins)
10:13	10:16	GREATCELL SOLAR (3 mins)
10:16	10:50	COFFEE BREAK
Session Chair:		Monica Lira Cantu, ICN2, Spain
10:50	11:15	15° INVITED LECTURE - Prashant Kamat , University of Notre Dame, France <i>Impact of ion migration on perovskite solar cell performance</i>
11:15	11:40	16° INVITED LECTURE - Xiaodan Zhang , Nankai University, China <i>Inorganic perovskite solar cells and its application in tandem solar cells</i>
11:40	12:05	17° INVITED LECTURE - Maksym Kovalenko , ETH Zurich, Switzerland <i>Engineering perovskite nanocrystals as quantum light sources</i>
12:05	12:08	MBRAUN (3 mins)
12:08	12:11	SOLAVENI (3 mins)
12:11	13:35	LIGHT BUFFET LUNCH
Special Session - Management of lead use in perovskite photovoltaics		
13:35	13:50	Markus Lenz , FHNW, Switzerland <i>Management of Lead Use in Perovskite Photovoltaics</i>
13:50	14:00	Johannes Sutter , Karlsruher Institut für Technologie, Germany <i>Green Solvents for Inkjet-Printed Perovskite-Based Photovoltaics</i>
14:00	14:10	Dalila Rocco , University of Applied Sciences and Arts North-western Switzerland, Switzerland <i>Indium and silver recovery from thin film solar cell waste by means of nanofiltration</i>
14:10	14:20	Bastien Vallat , University of Applied Sciences Northwestern Switzerland, Switzerland <i>Assessing lead leaching from perovskite solar cells more realistically</i>
14:20	14:30	Jonas Hanisch , Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg (ZSW), Germany <i>Slot-die coating of flexible perovskite solar cells with green solvents</i>



IMPROVING THE STABILITY AND EFFICIENCY OF METAL HALIDE PEROVSKITE SOLAR CELLS

Henry J. Snaith,¹

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When we first started working with metal halide perovskites more than a decade ago, they immediately worked efficiently as absorbers in solar cells and seemed to possess almost perfect optoelectronic quality, despite being very simply processed. Nevertheless, as “defect tolerant” as perovskites are, they still require controlled growth and passivation in order to reach peak performance, and suppressing losses at interfaces has been and remains critical to continuously improving the efficiency. Understanding degradation pathways and maximising the long-term operation stability is arguably the most important challenge for perovskite solar cells. In this talk I will present some of our recent work advancing the efficiency of multi-junction perovskite solar cells and understanding and suppressing degradation pathways in these devices.

INDOOR AND OUTDOOR STABILITY STUDIES OF PEROVSKITE SOLAR CELLS

Prof. Monica Lira-Cantu¹

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The industrialization of Perovskite Solar Cells (PSCs) can only be possible if device stability and module reliability is further enhanced. In this work, we present our most recent work related to the enhancement of perovskite solar cells stability. The studies were carried out following the ISOS protocols for dark storage (ISOS-D), indoor (ISOS-L) and outdoor (ISOS-O) analysis. We have modified the halide perovskite absorber, the transport layers and the device interfaces via several methods such as additive engineering and the application of novel electron and hole transport layers (like MXenes, novel organic hole transport materials, etc). For example, we use the 2D Ti_3C_2 MXene in normal PSC configuration of the type: FTO / c-TiO₂ / m-TiO₂ / halide perovskite (HP) / MXene / Spiro-OMeTAD / Au. We employed the quadruple halide perovskite (HP) $\text{Rb}_{0.05}\text{Cs}_{0.05}\text{MA}_{0.15}\text{FA}_{0.75}\text{Pb}(\text{I}_{0.95}\text{Br}_{0.05})_3$ as the absorber, and the MXene ($\text{Ti}_3\text{C}_2\text{-T}_x$) at the interface of HP and the hole transport layer (HTL) to fabricate HP/MXene heterojunctions. Our champion solar cells resulted in 21.95% PCE, in comparison with the 20.56 % obtained for the reference PSC. Both indoor stability studies under ISOS-L protocol (continuous MPP tracking under N₂ atmosphere for 1000 h) and outdoor stability analyses under the ISOS-O protocol (MPP tracking, encapsulated devices) demonstrated the superior stability of PSCs when the MXene is employed, especially under high humidity (60-85%) conditions where the PSCs showed excellent recovery after a rainy day. Thermal admittance spectroscopy (TAS) revealed that the use of MXene:H3pp results in the decrease of deep and shallow trap state densities. This report provides pioneering study of additive engineering for adaptable bulk passivation and interface passivation through MXene nanosheets. Other examples include the application of novel organic HTL or the use of Machine Learning to understand the correlation of indoor and outdoor stability.

[1] Kouroudis, I.; et al., Lira-Cantu, M.; Gagliardi, *ACS Energy Letters* **2024**, 9 (4), 1581-1586,

[2] Karimipour, M.; et al., Lira-Cantu, M. *Advanced Energy Materials* **2023**, 13 (44),

[3] Haibing Xie, et al., Monica Lira-Cantu. *Joule*, **5**, **2021**, 1-21.

[4] Khenkin, M.V., et al., Lira-Cantu, M. *Nature Energy* **2020**, 5, 35-49.

COMPUTATIONAL MODELING OF PEROVSKITE FOR PHOTOVOLTAICS AND PHOTOCATALYSIS

Edoardo Mosconi¹

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Hybrid AMX_3 perovskites (A=Cs, CH_3NH_3 ; M=Sn, Pb; X=halide) have in the last years revolutionized the scenario of photovoltaic technologies. Despite the extremely fast progress, the materials electronic properties which are key to the performance are relatively little understood. A series of computational simulation carried out using Car-Parrinello molecular dynamics have been performed investigating the nature of the perovskites/ TiO_2 interface, the role of moisture in the perovskite degradation process and the effect of the defect on the device working mechanism. Finally, a series of different strategies will be reported to increase the device stability and efficiency.[1] While instability in aqueous environment has long impeded employment of metal halide perovskites for heterogeneous photocatalysis, recent reports have shown that some particular tin halide perovskites (THPs) can be water-stable and active in photocatalytic hydrogen production. To unravel the mechanistic details underlying the photocatalytic activity of THPs, we compare the reactivity of the water-stable and active $DMASnBr_3$ (DMA = dimethylammonium) perovskite against prototypical $MASnI_3$ and $MASnBr_3$ compounds (MA = methylammonium), employing advanced electronic-structure calculations, see Figure 1. We find that the binding energy of electron polarons at the surface of THPs, driven by the conduction band energetics, is cardinal for photocatalytic hydrogen reduction.[2]

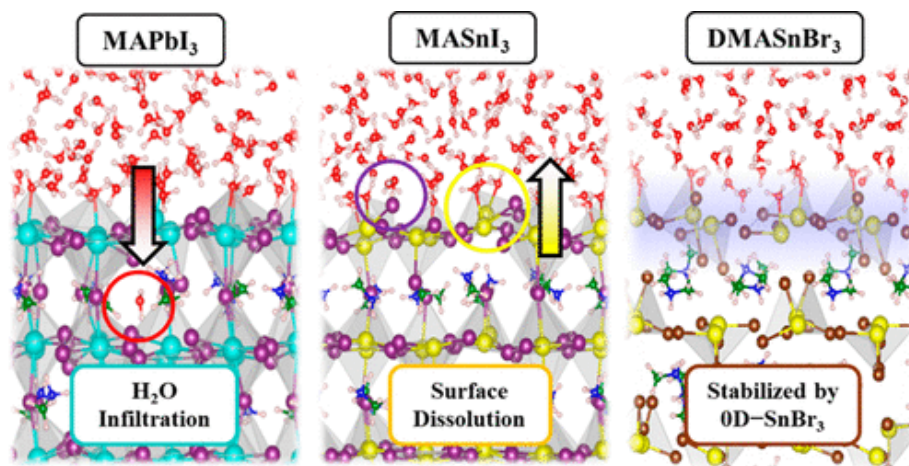


Figure 1: *Ab initio* molecular dynamics (AIMD) simulations of THP/water interfaces

[1] Yang, S.; Chen, S.; Mosconi, E.; Fang, Y.; Xiao, X.; Wang, C.; Zhou, Y.; Yu, Z.; Zhao, J.; Gao, Y.; De Angelis, F.; Huang, J. Stabilizing halide perovskite surfaces for solar cell operation with wide-bandgap lead oxysalts *Science* **2019**, *365*, 473.

[2] Kaiser W.; Ricciarelli D.; Mosconi E.; Althman A. A.; Ambrosio F.; De Angelis F. "Stability of Tin- versus Lead-Halide Perovskites: Ab Initio Molecular Dynamics Simulations of Perovskite/Water Interfaces" *J. Phys. Chem. Lett.*, **2022**, *13*, 2321.

SCALABLE DEPOSITION OF LEAD-TIN PEROVSKITE SOLAR

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Lead-tin (Pb-Sn) perovskites are a highly promising composition for single-junction and all-perovskite tandem solar cells due to their narrower bandgap. While the use of quasi-two-dimensional (quasi-2D) Ruddlesden-Popper phases has resulted in superior stability towards the environment and large improvement in the crystallization with respect to the 3D compositions, very little work has been done towards their deposition with scalable techniques. Here, I will report the fabrication of quasi-2D Pb-Sn perovskite solar cells by a two-step blade coating process. By changing the solvent of the second step from isopropanol to 2-methyl-2-butanol and 3-pentanol we increase the efficiency of the devices from about 12.5% till above 16%.

Furthermore, I will show that films which are treated with tin (II) acetate (SnAc_2) along with N,N-dimethylselenourea (DMS) exhibit a reduced number of surface traps and enhanced surface crystallization, owing to the in-situ formation of tin selenide (SnSe)^[1]. More importantly, the hydrophobic SnSe significantly protects the active layer from the environment. These devices retain 91% of the original PCE after 10 days in ambient air (30%-40% humidity) without encapsulation, and nearly no-degradation of the PCE is detected after over a month of storage in inert atmosphere, and under continuous MPP tracking for 15 hours.

[1] L. Chen, E. K. Tekelenburg, K. Gahlot, M. Pitaro, J. Xi, A. Lasorsa, G. Feraco, L. Protesescu, P.C.A. van der Wel, G. Portale, P. Rudolf, Christoph J. Brabec, M. A. Loi, *Energy Environ. Sci.*, 2023,16, 5315-5324.

IMPACT OF ION MIGRATION ON PEROVSKITE SOLAR CELL PERFORMANCE

Prashant V. Kamat

Times New Roman, 12 pts, centred, principal author underlined, typed in single spacing

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Ion migration in metal halide perovskites is one of the key factors determining long term stability of metal halide perovskite solar cells. Photoinduced phase segregation in mixed halide perovskites (MHP) to form bromide rich and iodide-rich domains can act as charge carrier traps and lower the efficiency of perovskite-based devices.[1,2] The thermodynamic and redox properties of halide perovskites provide a strong driving force for hole trapping and oxidation of iodide species. The iodine formed during the hole trapping process either can escape or complex with hole transport layer (e.g, spiroOMETAD). Thus, the mobility of halides and their susceptibility to hole-induced oxidation play a crucial role in determining the long-term stability of metal halide perovskite solar cells.

Ruddlesden-Popper 2D mixed-halide perovskite films with spacer cations such as butylammonium are introduced into three-dimensional (3D) perovskite films to stabilize against moisture-induced degradation at room temperature. While such passivation of 3D perovskites using 2D perovskites has been reported widely, the instability of the 2D/3D interface during long term solar cell operation can be problematic.[3,4] The cation migration under light and heat can significantly alter the 2D/3D interface, thus affecting the solar cell performance. Thus, suppression of halide ion migration as well as cation migration remains a key factor in achieving long term stability and improving efficiency of perovskite solar cells and light emitting devices.

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[3] Chakkamalayath, J.; Hiott, N.; Kamat, P. V. How Stable Is the 2D/3D Interface of Metal Halide Perovskite under Light and Heat?, *ACS Energy Letters* 2023, 8, 169-171.

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INORGANIC PEROVSKITE SOLAR CELLS AND ITS APPLICATION IN TANDEM SOLAR CELLS

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Inorganic perovskite solar cells (IPSCs) have attracted much attention due to their excellent thermal stability and suitable bandgap (~1.7 eV), and absence of light-induced phase separation, making them an ideal top-cell material candidate for silicon tandem solar cells. However, inorganic perovskites have a faster crystallization rate, which means higher defect densities and phase instability in humid environments, and energy level mismatch make the preparation of efficient and stable inverted IPSCs still challenging. One of the effective strategies to address the issues of interface energy level arrangement and charge extraction is to adopt effective interface control strategy.

Firstly, an innovative in-situ-etching (ISE) treatment method is proposed to reduce surface defects through methanol without additional passivator.^[1] Due to the insoluble property of PbI_2 in methanol, a small excess of PbI_2 nanosheets are left on the surface, besides passivating the trap states in grain boundaries, also bending the energy level downward because of the large work function of PbI_2 , successfully regulates energy level alignment. As a result, the efficiency of inverted IPSC is enhanced from 16.00% to 19.34%.

Secondly, a method by reconfiguring the surface properties of $\text{CsPbI}_{2.85}\text{Br}_{0.15}$ film with 2-amino-5-bromobenzamide (ABA) is developed.^[2] The carbonyl and amino in ABA effectively passivate Pb^{2+} -related defects, and the Br on the benzene ring fills the halide vacancies and suppresses the formation of Pb_0 , effectively passivating the defective top surface. As a result, a champion efficiency of 20.38% is achieved. Furthermore, the successful fabrication of a pin-type monolithic inorganic perovskite/silicon tandem solar cells (TSCs) with an efficiency of 25.31% for the first time in the world is demonstrated.

Thirdly, the use of 3-amino-5-bromopyridine-2-formamide (ABF) in methanol is dynamically spin-coated on the surface of $\text{CsPbI}_{2.85}\text{Br}_{0.15}$ film, which facilitates the limited etching of defect-rich subsurface layer, resulting in the formation of vertical PbI_2 nanosheet structures.^[3] This enabled localized contacts between the perovskite film and the electron transport layer, suppress the recombination of electron-hole and beneficial to electron extraction. Eventually, the efficiency of pin-type IPSCs is improved to 20.80% (certified efficiency of 20.02%), which is the highest certification efficiency of pin-type IPSCs ever reported to date. Based on this, we successfully fabricated pin-type monolithic inorganic perovskite/silicon TSCs with an efficiency of 26.26%, which is currently the highest efficiency values reported.

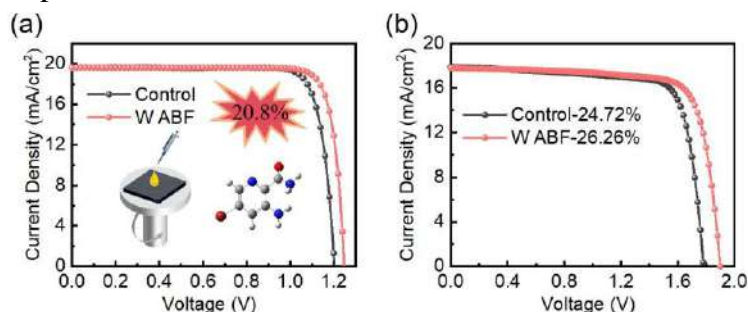


Figure 1: *J-V curves of the devices. (a) single junction IPSCs; (b) inorganic perovskite TSCs.*

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ENGINEERING PEROVSKITE NANOCRYSTALS AS QUANTUM LIGHT SOURCES

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In my talk, I will cover our latest work on the synthesis, self-organization and optical properties of colloidal lead halide perovskite nanocrystals (LHP NCs), including unpublished work. LHP NCs are of broad interest as classical light sources (LED/LCD displays) and as quantum light sources (quantum sensing and imaging, quantum communication, optical quantum computing). The current development in LHP NC surface chemistry, using designer phospholipid capping ligands, allows for their increased stability down to single particle level [1]. The brightness of such a quantum emitter is ultimately described by Fermi's golden rule, where a radiative rate proportional to its oscillator strength (intrinsic emitter property) and the local density of photonic states (photonic engineering, *i.e.* cavity). With perovskite NCs, we present a record-low sub-100 ps radiative decay time for CsPb(Br/Cl)₃, almost as short as the reported exciton coherence time, by the NC size increase to 30 nm [2]. The characteristic dependence of radiative rates on QD size, composition, and temperature suggests the formation of giant transition dipoles, as confirmed by effective-mass calculations for the case of the giant oscillator strength. Importantly, the fast radiative rate is achieved along with the single-photon emission despite the NC size being ten times larger than the exciton Bohr radius. When such bright and coherent QDs are assembled into superlattices, collective properties emerge, such as superradiant emission from the inter-NC coupling [3]. In the most recent work [4], the functionality of the second SL component can give rise to the enhancement of the LHP NCs properties or the emergence of new collective effects. We present the formation of multicomponent SLs made from the CsPbBr₃ NCs of two different sizes. The diversity of obtained SLs encompassed the binary ABO₆-, ABO₃-, and NaCl-type structures, all of which contained orientationally and positionally confined NCs. For the selected model system, the ABO₆-type SL, we observed efficient NC coupling and Förster-like energy transfer from strongly confined 5.3 nm CsPbBr₃ NCs to weakly confined 17.6 nm CsPbBr₃ NCs. Exciton spatiotemporal dynamics measurements reveal that binary SLs exhibit enhanced exciton diffusivity compared to one-component SLs across the entire temperature range (from 5 K to 298 K). Observed incoherent NC coupling and controllable excitonic transport within the solid NC SLs hold promise for potential applications in optoelectronic devices.

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[2] C. Zhu, S.C. Boehme, L.G. Feld, A. Moskalenko, D.N. Dirin, R.F. Mahrt, T. Stöferle, M.I. Bodnarchuk, A.L. Efros, P.C. Sercel, M.V. Kovalenko, G. Rainò. *Nature*, **2024**, 626, 535–541

[3] I. Cherniukh, G. Rainò, T. Stöferle, M. Burian, A. Travasset, D. Naumenko, H. Amenitsch, R. Erni, R.F. Mahrt, M.I. Bodnarchuk & M.V. Kovalenko. *Nature* **2021**, 593, 535–542

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Day 2 - Tuesday, September 17th, 2024

Session Chair:		Lorenzo Malavasi, University of Pavia, INSTM, Italy
08:30	08:55	11° INVITED LECTURE - Henry Snaith , University of Oxford, United Kingdom <i>Improving stability and efficiency of metal halide perovskite solar cells</i>
08:55	09:20	12° INVITED LECTURE - Monica Lira Cantu , ICN2, Spain <i>Indoor and outdoor stability studies of perovskite solar cells</i>
09:20	09:45	13° INVITED LECTURE - Edoardo Mosconi , CNR-SCITEC Perugia, Italy <i>Computational modeling of perovskite for photovoltaics and photocatalysis</i>
09:45	10:10	14° INVITED LECTURE - Maria Antonietta Loi , University of Groningen, Netherlands <i>Scalable deposition of lead-tin perovskite solar</i>
10:10	10:13	NIREOS (3 mins)
10:13	10:16	GREATCELL SOLAR (3 mins)
10:16	10:50	COFFEE BREAK
Session Chair:		Monica Lira Cantu, ICN2, Spain
10:50	11:15	15° INVITED LECTURE - Prashant Kamat , University of Notre Dame, France <i>Impact of ion migration on perovskite solar cell performance</i>
11:15	11:40	16° INVITED LECTURE - Xiaodan Zhang , Nankai University, China <i>Inorganic perovskite solar cells and its application in tandem solar cells</i>
11:40	12:05	17° INVITED LECTURE - Maksym Kovalenko , ETH Zurich, Switzerland <i>Engineering perovskite nanocrystals as quantum light sources</i>
12:05	12:08	MBRAUN (3 mins)
12:08	12:11	SOLAVENI (3 mins)
12:11	13:35	LIGHT BUFFET LUNCH
Special Session - Management of lead use in perovskite photovoltaics		
13:35	14:00	Markus Lenz , FHNW, Switzerland <i>Management of Lead Use in Perovskite Photovoltaics</i>
14:00	14:10	Johannes Sutter , Karlsruher Institut für Technologie, Germany <i>Green Solvents for Inkjet-Printed Perovskite-Based Photovoltaics</i>
14:10	14:20	Dalila Rocco , University of Applied Sciences and Arts North-western Switzerland, Switzerland <i>Indium and silver recovery from thin film solar cell waste by means of nanofiltration</i>
14:20	14:30	Bastien Vallat , University of Applied Sciences Northwestern Switzerland, Switzerland <i>Assessing lead leaching from perovskite solar cells more realistically</i>



MANAGEMENT OF LEAD USE IN PEROVSKITE PHOTOVOLTAICS

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Perovskite photovoltaics have emerged as a promising technology for high-efficiency, low-cost solar energy conversion. However, the use of lead (Pb) in perovskite materials raises concerns regarding possible environmental impacts and social acceptance. This session will explore if there are actual grounds for these concerns and discuss strategies to mitigate them. In addition to addressing Pb, the session will explore other materials that impact sustainability and how their replacement could enhance the overall environmental performance of perovskite photovoltaics. The talks will cover the entire lifecycle of perovskite photovoltaics, from the use of green solvents in production to lead leakage risks during the operational phase, as well as sustainable recycling approaches at end-of-life.

The key questions addressed include: How significant is the environmental and health risk posed by Pb in perovskite PVs? What are the potential impacts of Pb and other materials during production, use, and end-of-life phases? How can we minimize risks and impacts during the life phase?

This session aims to provide a balanced view of the opportunities and challenges posed by perovskite PVs and offer insights into sustainable development pathways for this rapidly advancing technology.

GREEN SOLVENTS FOR INKJET-PRINTED PEROVSKITE-BASED PHOTOVOLTAICS

Johannes Sutter,¹ Raphael Pesch,¹ Uma Danguubiyam,¹ Helge Eggers¹ and Ulrich W. Paetzold¹

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In recent years, perovskite single junction solar cells and perovskite-based tandem solar cells have made significant strides in laboratory-scale power conversion efficiency^[1]. However, the transition to commercial viability presents several obstacles. The primary challenges include upscaling without compromising performance, high process expenses, and the use of hazardous materials. Specifically, solvent-based material deposition techniques, such as coating and printing, encounter difficulties when applied to larger areas due to increased solvent consumption and potential hazards associated with toxic solvents, raising safety and environmental concerns^[2]. Addressing these challenges is crucial for realizing the full potential of perovskite solar cell technology in practical applications.

In our study, we explore the feasibility of using non-hazardous and environmentally friendly solvents, commonly known as “green solvents”, for the commercialization of perovskite-based photovoltaics. We outline specific criteria that such solvents must meet to enable cost-effective and safe scaling processes while maintaining the efficiency of solar cell performance. Our research proposes two fundamental approaches to address these challenges, using inkjet printing technology. A one-step perovskite deposition process with an adapted solvent system and processing parameters and a hybrid two-step perovskite deposition. The first method aims at developing a one-step perovskite inkjet process using green solvents with good stability and convenient operation. In the second method, inkjet printing is used to introduce organic cation precursor materials into evaporated lead iodide thin films. This strategy aims to overcome upscaling obstacles by ensuring film conformity, which is crucial for fabricating efficient solar cell devices.

Our most recent findings have resulted in one-step inkjet-printed perovskite layers with good optoelectronic properties and the creation of perovskite solar cells that exhibit a power conversion efficiency exceeding 18% with the two-step route. These cells also demonstrate remarkable reproducibility and maintain high conformity even on textured surfaces. Importantly, both of our fundamental approaches eliminate the need for toxic solvents, such as dimethylformamide. We are confident that our research provides valuable insights and practical strategies for a safer and more environmentally friendly scalable production of efficient perovskite photovoltaics.

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[2] Rosario Vidal, *Nat Sustain* **2021** *4*, 277–285.

INDIUM AND SILVER RECOVERY FROM THIN FILM SOLAR CELL WASTE BY MEANS OF NANOFILTRATION

Rocco Dalila,¹ Amrein Meret,^{1,2} Hengevoss Dirk,¹ Meier Ursina,¹ Thomann Michael,¹ Nüesch Frank,^{2,3} Lenz Markus^{1,4}

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Due to low material use and easy processing, new generation thin film solar cells represent a promising alternative to commonly used crystalline silicon solar cells.^[1] Among those, perovskite solar cells have made large improvements in power conversion efficiency and are currently standing at the edge of market entry.^[2] However, the electrodes of the most efficient and stable perovskite solar cells contain indium and silver. Whereas indium is already considered a critical raw material suffering from supply risks, insufficient silver supply is expected to limit PV deployment at the TW scale. Therefore, it is crucial to find energy efficient and scalable recycling solutions.^[3] Here, we demonstrate an environmentally benign recycling process for lead, indium and silver from end-of-life perovskite solar cells. It consists of mechanical dismantling (milling), aqueous extraction / purification of PbI₂, as well as acid extraction and purification of indium and silver by nanofiltration. After quantitative recovery of Pb as PbI₂,^[4] indium and silver were quantitatively dissolved by using nitric acid. LCA calculations were used to determine optimal conditions (5% HNO₃, 1L/m² solar cell, 5h, 80°C) in terms of a minimal environmental impact per gram of extracted element. After acid extraction, nanofiltration using both custom-made layer-by-layer membranes and commercially available acid resistant membranes were used to separate indium from silver. Using an optimized design, indium could be quantitatively retained using a PES(PAH/PSS)₄ membrane, resulting in a retention of 96.9 ± 0.4% over 50% permeate recovery. Hence, twofold concentration of indium was achieved over the course of the filtration. In contrast, silver was not retained, resulting in a low retention of -7.6 ± 6.3% and hence a 50% removal of Ag from the feed. Retention by commercial membranes (flatsheet AMS 3012 NF) was similar compared to layer-by-layer membranes, however at the expense of considerably higher operating pressure (25 bars for commercial membranes vs 5 bars) and lower flux (6 L/m²h vs 30 L/m²h). In summary, LbL membrane filtration has proven to be superior in terms of energy consumption for the filtration process.

Acknowledgements: This work has received funding from the Swiss State Secretariat for Education, Research and innovation (SERI) and from the European Union. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or RIA. Neither the European Union nor the granting authority can be held responsible for them. NEXUS and PEARL projects have received funding from the European Union's Horizon Europe research and innovation program under grant agreements No. 101075330 and 101122283, resp.

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ASSESSING LEAD LEACHING FROM PEROVSKITE SOLAR CELLS MORE REALISTICALLY

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While offering many advantages over other photovoltaic technologies already in widespread use, the lead (Pb) content in perovskites solar cells (PSCs) may be perceived as a challenge in commercialization due to environmental concerns and social acceptance. Despite the low Pb concentrations used, Pb may enter the environment for example during the use-phase when modules break or at the end-of-life-phase when inappropriately disposed of.

Currently, laboratory-based metal leaching tests have been conducted to assess the potential Pb release during use-phase.^[1-3] However, these often represent simplified systems and lack real outdoor stressors as well as temporal effects (intermittent rain, diurnal temperature cycles, biofilm formation, ...).^[4] It may thus be doubted that leaching kinetics observed in laboratory directly transfer to the field. To address these limitations, outdoor PSC leaching tests were conducted. Pb was quantified down to low $\mu\text{g/L}$ range using triple-quadrupole Inductively Coupled Plasma Mass Spectrometry (qqq-ICP-MS), deriving closer to application Pb leachate concentrations. These trace concentrations need to be put into perspective by environmental risk assessment. In this regard, an open access web application is presented that allows the user (both public and professionals) to determine Pb leachate concentrations interactively (based on e.g. type of PSC, roof coverage, climate, etc.). Then, a context menu puts these Pb concentrations into perspective in terms of actual risks. With this we provide the scientific community with realistic Pb concentrations for risk assessment as well as a mean to proactively counter possible social concerns on PSCs.

Acknowledgements:

This work has received funding from the Swiss State Secretariat for Education, Research and innovation (SERI) and from the European Union. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or RIA. Neither the European Union nor the granting authority can be held responsible for them. NEXUS and PEARL projects have received funding from the European Union's Horizon Europe research and innovation program under grant agreements No. 101075330 and 101122283, resp.

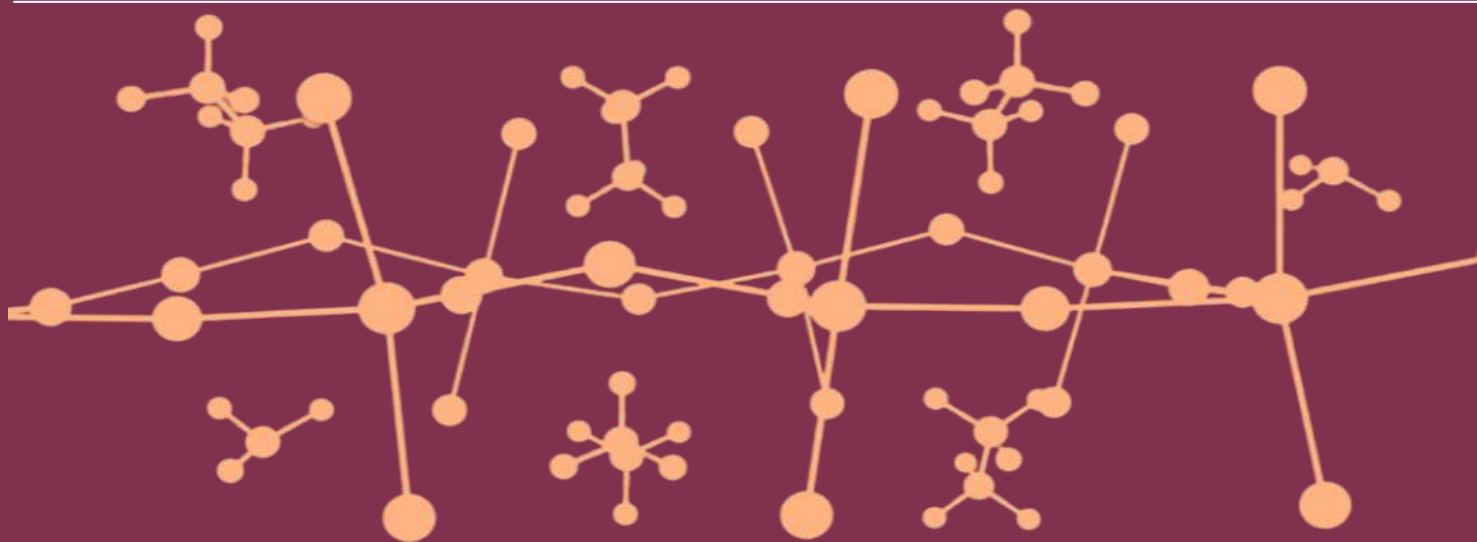
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14:30	14:35	COMFORT BREAK	
		Session 1A Town Hall	Session 1B Trumpet
Session Chair:		Ute Cappel , Uppsala University, Sweden	Sam Stranks , University of Cambridge, United Kingdom
Session Title:		Phase Stability	Tandem PV
14:35	14:47	Jiajia Suo , Uppsala University, Sweden <i>Multifunctional sulfonium-based treatment for perovskite solar cells with a non-degraded 4500-h operational stability</i>	Melissa Fitzsimmons , University of Cambridge, United Kingdom <i>All-perovskite tandem solar cells with optimised interconnecting layer</i>
14:47	14:59	Tino Lukas , University of Oxford, United Kingdom <i>Using the synergies: Carbon-Based Electrodes and ALD-SnOx for Efficient Inverted Perovskite Solar Cells</i>	Oussama Er-raji , Fraunhofer ISE, Germany <i>Fully-textured perovskite silicon tandems: from groundwork to efficient solar cells</i>
14:59	15:11	Simon Ternes , CHOSE, University of Rome Tor Vergata, Italy <i>Toward feedback-controlled solution printing of perovskite photovoltaics</i>	Wiktor Żuraw , Saule Research Institute, Poland <i>Large-area flexible all-perovskite tandem solar modules obtained by solvent engineering</i>
15:11	15:23	Riccardo Pau , University of Cagliari, Italy <i>Solution-Processed Cul as hole transport layer for improved efficiency and stability</i>	Paola Delli Veneri , ENEA, Italy <i>Dopant-free c-Si Heterojunction for silicon/perovskite tandem solar cells</i>
15:23	15:35	David McMeekin , University of Oxford, United Kingdom <i>Intermediate-phase engineering via dimethylammonium cation additive for stable perovskite solar cells</i>	Seongrok Seo , University of Oxford, United Kingdom <i>Efficient Charge Carrier and Light Management for Perovskite-Silicon Tandem Solar Cell Through Controlling Electron Transporting Contact</i>
15:35	15:47	Bowen Yang , Uppsala University, Sweden <i>From solution chemistry to device fabrication: a universal additive for high efficiency and stability perovskite solar cells</i>	Fabio Matteocci , University of Rome Tor Vergata, Italy <i>Strategies to manipulate AVT and PCE in wide bandgap perovskite solar cells for semitransparent two-terminal PSC-OPV tandem modules</i>
15:47	15:59	Susana Ramos Terron , University of Cordoba, Spain <i>Modulation of stability and efficiency in 2d/3d perovskite solar devices by the molecular geometry of bulky diammonium cation</i>	Dong Zhang , Swift Solar, United States <i>Endeavors on commercialization of perovskite-silicon tandem photovoltaics at Swift Solar</i>
15:59	16:11	Viktor Škorjanc , HZB GmbH, Germany <i>Simple templating step improves uniformity and increases efficiency of co-evaporated wide band gap perovskite solar cells</i>	Mohammad Gholipoor , Karlsruhe Institute of Technology, Germany <i>Highly-efficient textured three-terminal perovskite/silicon tandem solar cells</i>
16:11	16:23	Hashini Perera , University of Surrey, United Kingdom <i>Improving Stability of Perovskite Solar Cells on Self Assembled Monolayers by Surface Modification</i>	Marcel Roß , Helmholtz-Zentrum Berlin (HZB), Germany <i>Impact of high deposition rates on co-evaporated perovskite-absorbers for monolithic silicon tandem solar cells</i>
16:23	16:53	COFFEE BREAK	



MULTIFUNCTIONAL SULFONIUM-BASED TREATMENT FOR PEROVSKITE SOLAR CELLS WITH A NON-DEGRADED 4500-H OPERATIONAL STABILITY

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The stabilization of grain boundaries and surfaces of the perovskite layer is critical to extend the durability of perovskite solar cells. In our recent work,^[1] we introduced a sulfonium-based molecule, dimethylphenethylsulfonium iodide (DMPEI, **Fig a**), for the post-deposition treatment of formamidinium lead iodide perovskite films. As shown in **Fig b-f**, the treated films show improved stability upon light soaking and remains in the black α phase after two years ageing under ambient condition. The DMPEI-treated perovskite solar cells show less than 1% performance loss after more than 4,500 h at maximum power point tracking (**Fig g**), yielding a theoretical T_{80} of over nine years under continuous 1-sun illumination. The result makes our device among the most stable, high-efficiency PSCs reported to date, as illustrated in **Fig h**. In my presentation, I will systematically introduce the unique chemical properties of sulfonium salts in comparison with widely used ammonium salts and reveal the stabilization mechanism of the sulfonium treatment.

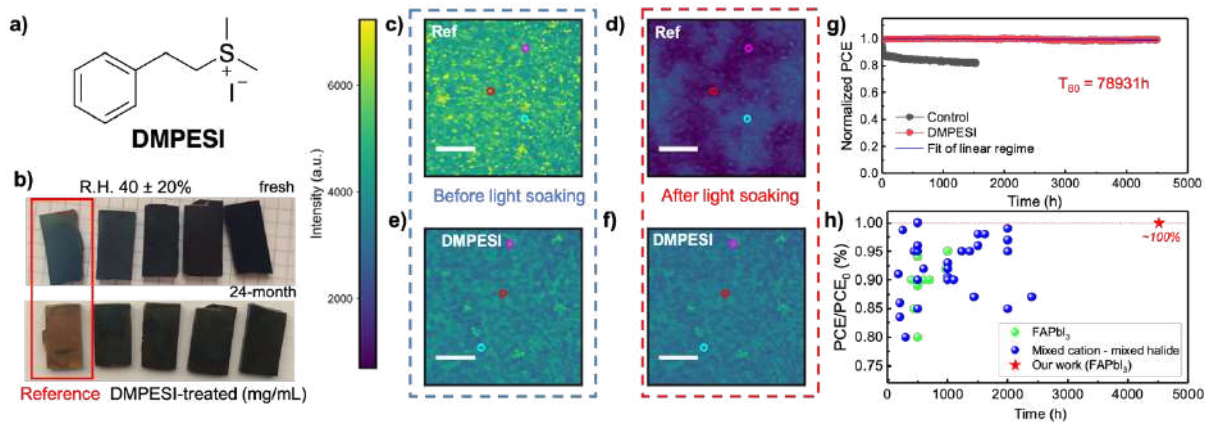


Figure: a) Chemical structure of DMPEI; b) Photographs of fresh and 24-month aged perovskite film without and with DMPEI treatment in ambient air; c-f) Photoluminescence (PL) map of reference and DMPEI treated perovskite film before and after light soaking; g) MPPT stability test of PSCs; h) Operational stability of state-of-the-art highly efficient (PCE > 22%) PSCs extracted from literature.

Acknowledgements: We acknowledge Swiss National Science Foundation for financial support with project number 200020_185041 and from the Horizon Europe framework programme for research and innovation under grant agreement number 101084124–DIAMOND.

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ALL-PEROVSKITE TANDEM SOLAR CELLS WITH OPTIMISED INTERCONNECTING LAYER

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All-perovskite tandem solar cells have achieved a certified record power conversion efficiency (PCE) of 28.0%,^[1] surpassing that of single-junction perovskite solar cells (PSCs). In a two-terminal tandem device, sub-cells are connected by an interconnecting layer (ICL), with state-of-the-art ICLs commonly consisting of SnO₂/Au/PEDOT:PSS.^[1-3] This ICL architecture suffers from significant optical losses, primarily due to parasitic absorption in the Au and PEDOT:PSS layers. In this study, we explore a novel ICL composed of SnO₂ and a thin layer of Graphene Oxide (GO). The inclusion of GO facilitates the replacement of PEDOT:PSS with [2-(9H-carbazol-9-yl)ethyl] phosphonic acid (2PACz) as the hole transporting layer (HTL) in the lead-tin sub-cell. We investigate three device architectures with distinct ICLs: SnO₂/Au/PEDOT:PSS, SnO₂/GO/PEDOT:PSS, and SnO₂/GO/2PACz. We observe reduced parasitic absorption when Au is replaced by GO, with further reductions when PEDOT:PSS is substituted with 2PACz. This reduction translates to increased J_{SC} in the lead-tin sub-cell. Additionally, devices incorporating a GO interlayer exhibit increased open-circuit voltage (V_{oc}), attributed to enhanced quasi-Fermi level splitting (QFLS) in the lead-tin sub-cell. As a result, we find that the novel ICL architecture containing GO results in an improvement of both PCE and stability, with further improvements observed when the PEDOT:PSS HTL is replaced with 2PACz.

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USING THE SYNERGIES: CARBON-BASED ELECTRODES AND ALD-SnO_x FOR EFFICIENT INVERTED PEROVSKITE SOLAR CELLS

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In recent years, Perovskite solar cells (PSCs) have reached high power conversion efficiencies (PCE). However, record efficiencies rely on the evaporation of metals as electrode materials¹. This slow process increases the cost of the devices and lowers their stability. All metal electrodes, including gold, react with the perovskite layer^{2,3}.

Strong candidates to replace evaporated metal electrodes are carbon-based materials like graphite-based pastes deposited via solution processes such as blade coating, stencil or screen printing. This promises cheaper, faster fabricated, and more stable electrodes⁴. However, the application processes of carbon pastes result frequently in problems such as solvent incompatibility to the top transport layer. Most PSCs with carbon electrodes are in the regular n-i-p structure or the hole-transport-layer-free architecture. We found the incompatibility of carbon blade coating with most of the commonly used electron transport layers in p-i-n devices like PCBM and BCP as a possible reason for this gap in the literature. To overcome the mentioned processing issues we show an innovative approach of combining the ambient blade coating process of carbon pastes with an SnO_x electron transport layer deposited by atomic layer deposition (ALD). This way we demonstrate the first perovskite solar cells with the more stable p-i-n architecture and without any evaporation processes. ALD is quicker than evaporation and is compatible with higher throughput processes like spatial ALD. Further, the ALD layer protects the underlying layers during the carbon blade coating. Finally, both SnO_x and carbon are inert to the halides. All other layers besides the tin oxide in our p-i-n carbon devices were solution-processed.

We encountered challenges in the electrical connection between tin oxide and carbon, which we overcame by altering the interface to be more conductive and less n-type. By increasing the conductivity at the SnO_x/C interface we reached reproducibly higher performance. This way we reached a stabilised performance of 16.6% and maintained 94% of the initial performance aged outdoors for 500h (T80 of 1200h). These results are an important step towards more stable, significantly cheaper, and industrially viable PSC.

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[2] Domanski, K et al., *ACS Nano* **2016**, 6306–6314

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[4] Bogachuk, D. Z. *Energy & Environmental Science*, **2020**

FULLY-TEXTURED PEROVSKITE SILICON TANDEM: FROM GROUNDWORK TO EFFICIENT SOLAR CELLS

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Fully-textured perovskite silicon tandem solar cells are compatible with industrial-grade silicon substrates and offer enhanced light-trapping. For a conformal perovskite growth on textured silicon with $> 1 \mu\text{m}$ -sized pyramids, the hybrid evaporation/spincoating method is typically employed. It involves the reaction between thermally evaporated inorganic precursors (e.g., PbI_2 & CsI) and subsequently wet-chemically deposited organic precursors (e.g., FAI & FABr) during an annealing step.^[1] Recently, multiple reports focused on improving the perovskite absorber quality via additive engineering, which led to a high 31.25% power conversion efficiency.^[2]

Herein, we report a new method to control the perovskite growth with the hybrid route: it is based on tuning the surface polarity of the substrate material. Particularly, we demonstrate that mixing a commonly used self-assembled monolayer (Me-4PACz) with a hydrophobic molecule increases the hydrophobicity of the formed hole transport layer (HTL) (Fig. 1-f). This induces a higher degree of porosity and orientation in the evaporated inorganic scaffold (Fig. 1-a,c,e). As a result, the subsequent organohalide solution infiltration is improved, and the obtained perovskite absorber is homogeneous (Fig. 1-b,d). The reduced residual PbI_2 at the perovskite/HTL interface reduces series resistance, which increases the FF of the target device (Fig. 1-g). Building on the insights from the formation of perovskite absorbers on different substrate materials, a basic crystallization model for hybrid route-processed perovskite thin films is suggested.

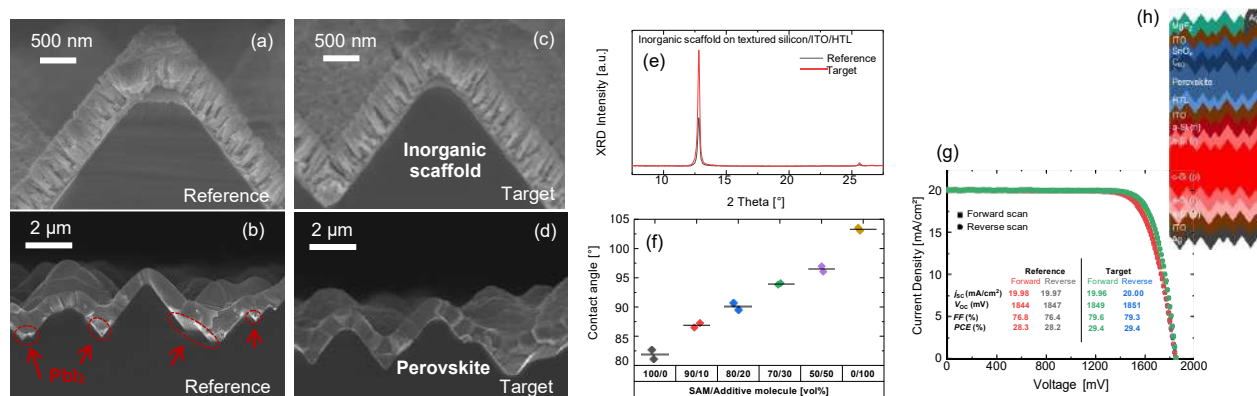


Figure 1: SEM images of the inorganic scaffold and the perovskite absorber on (a), (b) reference SAM (Me-4PACz) and (c), (d) target mixture of SAM with a hydrophobic molecule. (e) X-ray diffraction (XRD) patterns of the inorganic scaffold deposited on either the reference or the target underlying HTL. (f) Contact angle measurements carried out on glass/ITO/HTL substrates with HTL being mixtures between Me-4PACz and a hydrophobic molecule. (g), (h) Tandem solar cell design schematic and jV measurements of reference vs target device.

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TOWARD FEEDBACK-CONTROLLED SOLUTION PRINTING OF PEROVSKITE PHOTOVOLTAICS

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The solution processing route of perovskite photovoltaic (PV) fabrication has a very high potential for commercialization of the emerging technology. The reason is that, analogous to photographic film production, roll-to-roll coating of perovskite PVs would enable very cost-effective scaling relying on comparatively simple equipment. Nevertheless, to date, it is rather unclear if solution processing of perovskite PVs can reach reliable yield and performance output. Consequently, analogous to the industrial fabrication of organic LEDs, the thermal evaporation route might be more attractive for fabricating homogeneous perovskite thin-films on large scales. One of the major drawbacks of roll-to-roll perovskite printing machines is the fact that the perovskite morphology formation from solution is very sensitive to the environment and process parameters such as humidity, temperatures, solvent loading, etc... putting consistent yield at risk. A very promising solution, already applied in industrial fabrication of other thin film technologies, is the implementation of short feedback cycles that ensure a consistent output by continuously adjusting the processing parameters. Rapid, non-invasive and inexpensive feedback can be generated by in-line optical probing (also known as optical in situ characterization), such as reflectance, absorption, photoluminescence and Raman spectroscopy, available in one-point as well as in one-line or imaging modes.

The work presented here assesses the feasibility and potential of the most common optical characterization methods for achieving feedback fabrication. In addition, a proof-of-principle, complete feedback cycle is presented for the first time in a pilot experiment of large-scale perovskite solution printing. In this way, the potential for shorting feedback loops will be effectively demonstrated by assessing the resilience of the process against drifts in the environment and process parameters, enabling improvements in process control as compared to classical fabrication with constant processing parameters.

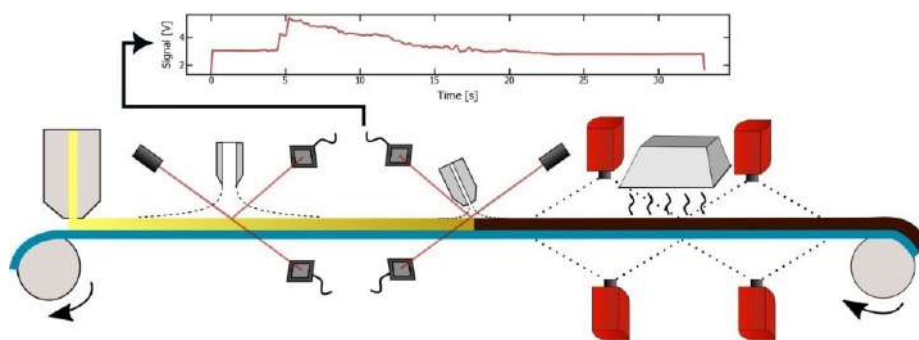


Figure 1: Symbolized perovskite roll-to-roll printing line with added optical in situ characterization and feedback controlled fabrication. A pre-drying step and an additional gas quenching step are employed and monitored by one-point probes, while an infrared annealing step is monitored by continuous imaging. An exemplary one-point reflectance measured on a coated perovskite thin-film is depicted above.

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LARGE-AREA FLEXIBLE ALL-PEROVSKITE TANDEM SOLAR MODULES OBTAINED BY SOLVENT ENGINEERING

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Metal halide perovskites have gained huge attention over the past decade due to their promise in optoelectronic and photovoltaic applications. Perovskite solar cells have achieved more than 26% power conversion efficiency for single-junction devices. The performance can be further improved by combining two perovskite layers into a tandem solar cell. Multijunction all-perovskite architectures offer a route towards high efficiencies (exceeding 30%) with all the beneficial properties of perovskites, including low processing cost, high throughput fabrication, and compatibility with flexible substrates.

The narrow-bandgap (NBG) perovskite junctions (1.2-1.3 eV) pose the largest technical challenge in the commercialization of all-perovskite tandem photovoltaics. Despite achieving high efficiencies for small cells manufactured on a laboratory scale, successful implementation of the technology requires the development of large-scale production methods that can reduce production costs without losing efficiency parameters. Currently, the large-area NBG perovskite devices lag behind the small-area counterparts, showing a significant decline in efficiency as device size increases. This is primarily related to the difficulty in controlling the uniformity of layers over a large surface using scalable wet deposition techniques (presence of defects, discontinuities in the deposited layers).

In this work, we developed NBG perovskite precursor formulation enabling good control over the layer's crystallization dynamics in the blade-coating process on flexible substrates. A key focus of our study was the optimization of the solvent system. Here, we employed a novel approach for synthesizing precursor solution, which involved a dimethylformamide-free composition, the selection of appropriate additives, and meticulous attention to the processing conditions during the deposition step. When combined with carefully selected materials in the device stack and a scaled-up process of interface modification treatments, we obtained flexible NBG perovskite module efficiency (device area > 100 cm²) exceeding 16%.

Moreover, we will present a robust encapsulation protocol, enabling promising results of flexible NBG modules in accelerated aging tests (damp heat tests). Furthermore, based on optimized narrow-bandgap and wide-bandgap perovskite processing, we developed a fabrication protocol for flexible monolithic all-perovskite tandem solar modules.

Acknowledgements: *This work has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement No 101075605 (SuPerTandem).*

SOLUTION-PROCESSED CUI AS HOLE TRANSPORT LAYER FOR IMPROVED EFFICIENCY AND STABILITY OF SN-PB PEROVSKITE SOLAR CELLS

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Over recent years, the remarkable advancement in power conversion efficiency using metal halide perovskites (MHP) as the active material in single junction solar cells has been accompanied by a growing apprehension regarding their environmental repercussions. This concern primarily arises from the significant presence of water-soluble, toxic lead in the active material. To confront this challenge, tin (Sn)-based and mixed tin-lead (Sn-Pb) perovskites are emerging as promising substitutes for the extensively researched lead (Pb)-based perovskites, and due to their smaller bandgap, these materials can be implemented as narrow energy gap material in all-perovskite tandem with an efficiency expected to overcome 30%.

However, this thriving solution presents new obstacles to surmount, such as the introduction of intrinsic Sn-defects and the Sn(II) oxidation to Sn(IV), both of which contribute to the ongoing challenge of achieving photovoltaic performance levels that still remain considerably inferior of those exhibited by lead-based counterparts. In this framework, the best Sn-Pb based devices are fabricated in the inverted planar configuration with PEDOT:PSS (poly(3,4-ethylenedioxythiophene) polystyrene sulfonate) as the most widely used hole transport layer. However, the acidic and hygroscopic nature of this polymer can cause degradation and reduce the device stability over time. Despite the limited number of materials with high optical transmittance and electrical conductivity suitable for perovskite-based devices, in the last years new HTLs gathered substantial attention, such as SAMs (self-assembled monolayers) and the low-cost solution-processed copper iodide (CuI).

Here we present the application of an undoped CuI as hole transport layer deposited from solution for the fabrication of methylammonium (MA)-free half Sn-half Pb perovskite solar cells with power conversion efficiency of over 20% and enhanced stability.

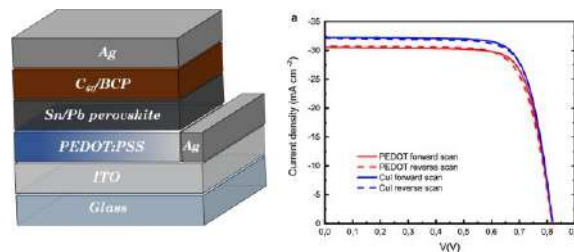


Figure 1: Device structure of the fabricated p-i-n perovskite solar cell and current density-voltage (J-V)

DOPANT-FREE SILICON/PEROVSKITE TANDEM SOLAR CELLS

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Tandem solar cells that combine silicon with a metal halide perovskite are demonstrating to be a promising option for surpassing the efficiency limitations of single-junction solar technologies at reasonable cost. Among the different possible tandem configurations, the monolithically integrated 2-terminal tandem design, in which the perovskite top cell is directly deposited onto the silicon bottom cell, may offer significant benefits in terms of device performance, reliability, and cost. For the silicon cell component, the silicon heterojunction (SHJ) cell technology is currently the preferred choice to construct monolithic perovskite/silicon tandems. Carrier selectivity at the contacts is here traditionally achieved by depositing doped silicon layers after passivation, using Plasma-Enhanced Chemical Vapor Deposition (PECVD). This process requires a capital-intensive system with mandatory safety schemes considering the flammable and toxic gas precursors. To address these issues, recent research focuses on developing alternative dopant-free materials for charge extraction within the silicon cell. This approach typically utilizes low temperature, low-cost fabrication techniques. Moreover, the use of different carrier-selective materials opens for a wider optical and electrical parameter space.

This work explores the integration of various charge-selective materials into monolithic silicon-perovskite tandem architectures. SHJ solar cells based on n-type wafer were fabricated with both front-emitter and back-emitter design (hole collector on the front or on the back side, respectively). Fully dopant-free SHJ cells with front MoO_x/TCO, as hole collector, and back LiF/Al, as electron collector, were developed with V_{oc} around 700 mV. For cells with dopant-free MoO_x/Ag (hole collector) at the rear side, V_{oc} up to 720 mV was achieved. FF was in the range 70-75% in all the cases. Other selective contacts are under investigation, such as CeF/Al, LiF/Ti, and stacks with organic self-assembled monolayers (2PACz). Depending on the bottom cell layout, pin or nip perovskite top cells were deposited using a Cs_{0.05}(I_{0.85}Br_{0.15})_{0.95}Pb(I_{0.85}Br_{0.15})₃ perovskite absorbing layer. IZO, ITO, and AZO were tested as front electrode for the tandem.

We have evaluated the effectiveness of these dopant-free approaches for the bottom cell component through detailed optoelectronic characterization. The results provide valuable insights into optimizing charge extraction, carrier transport, and interfacial energetics. Ultimately, this research aims to develop an approach based on innovative, sustainable, and low-cost materials for the silicon/perovskite tandem solar cell technology.

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INTERMEDIATE-PHASE ENGINEERING VIA DIMETHYLAMMONIUM CATION ADDITIVE FOR STABLE PEROVSKITE SOLAR CELLS

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Achieving the long-term stability of perovskite solar cells is arguably the most important challenge required to enable widespread commercialization. Understanding the perovskite crystallization process and its direct impact on device stability is critical to achieving this goal. The commonly employed dimethyl-formamide/dimethyl-sulfoxide solvent preparation method results in a poor crystal quality and microstructure of the polycrystalline perovskite films. In this work, we introduce a high-temperature dimethylsulfoxide-free processing method that utilizes dimethylammonium chloride as an additive to control the perovskite intermediate precursor phases. By controlling the crystallization sequence, we tune the grain size, texturing, orientation (corner-up versus face-up) and crystallinity of the formamidinium (FA)/caesium (FA)_yCs_{1-y}Pb(I_xBr_{1-x})₃ perovskite system. A population of encapsulated devices showed improved operational stability, with a median T₈₀ lifetime (the time over which the device power conversion efficiency decreases to 80% of its initial value) for the steady-state power conversion efficiency of 1,190 hours, and a champion device showed a T₈₀ of 1,410 hours, under simulated sunlight at 65 °C in air, under open-circuit conditions. This work highlights the importance of material quality in achieving the long-term operational stability of perovskite optoelectronic devices.

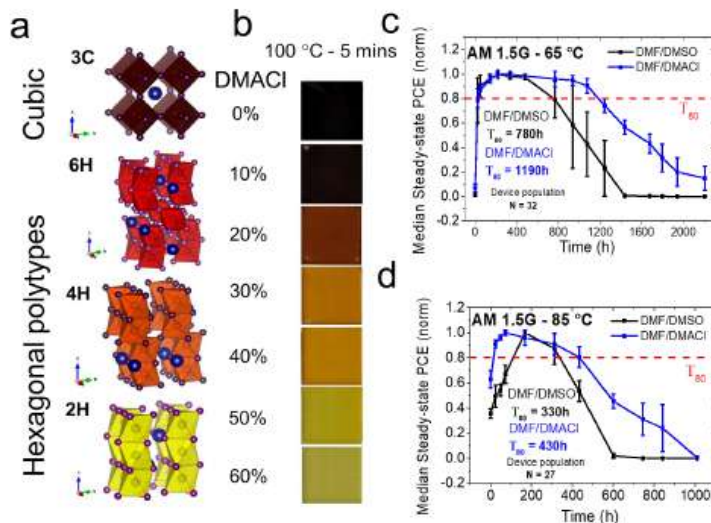


Figure 1: A) Crystal structure of a unit cell of the hexagonal lead halide perovskite polytypes—2H, 4H and 6H—showing PbI₆ octahedra connectivity, along with a 3C cubic perovskite structure. B) A series of photographs of DMACl(FA_{0.83}Cs_{0.17})_{1-x}Pb(Br_{0.21}I_{0.8})₃Cl_x perovskite films spin-coated with various amounts of DMACl additive, where percentages are expressed in excess amounts with respect to lead. C, D) Evolution of normalized (norm.) steady-state PCE, measured at its peak efficiency, between two statistical populations of encapsulated devices of DMF/DMSO and DMF/DMACl designs, aged under simulated sunlight at 65 °C and 85 °C.)

EFFICIENT CHARGE CARRIER AND LIGHT MANAGEMENT FOR PEROVSKITE-SILICON TANDEM SOLAR CELL THROUGH CONTROLLING ELECTRON TRANSPORTING CONTACT

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Over the last eight years, the photo conversion efficiency (PCE) of halide perovskite on silicon tandem solar cells has improved from 23.6% to 33.9% on small area (1cm²), surpassing the theoretical PCE of 29% barrier for silicon single junction solar cells. [1] The p-i-n configuration in perovskite solar cells offers notable benefits over the traditional n-i-p configuration, such as less hysteresis current-voltage characteristics, a low-temperature fabricating process, and with better stability. However, The efficiency of perovskite solar cells with an p-i-n configuration is still constrained by non-radiative recombination occurring at the electron transporting interface, which also limit PCE of p-i-n perovskite-silicon tandem solar cells. Common electron transporting layer for this configuration is fullerene (C60). When in contact with the underlying halide perovskite, C60 significantly quenches photoluminescence. Furthermore, C60 has a high extinction coefficient above its bandgap (approximately 2 eV), leading to parasitic absorption that adversely affects the performance of perovskite-silicon tandem solar cells. Here, we propose the introduction of a molecular self-assembled monolayer (M-SAM) at the perovskite/C60 interface to minimize non-radiative recombination, enable reduced parasitic absorption, achieved by decreasing the overall thickness of C60. Through analysis using X-ray photoelectron spectroscopy and Kelvin probe force microscopy, we have determined that ultra- thin M-SAM is conformally coated on the surface of halide perovskite, resulting in improved charge extraction behaviour from the perovskite/M-SAM/C60 (5nm) interface compared to the traditional perovskite/C60 (15nm) interface. These advancements have enabled 1.68-electron- volt single junction perovskite solar cells to achieve a remarkably high open-circuit voltage of 1.31 volts and an improved fill factor exceeding 84%, combined with synergistic additional surface treatments. As a result, we fabricated highly efficient perovskite-silicon tandem solar cells achieving an open-circuit voltage of 2 volts and a photocurrent of 20.8 mA/cm², facilitated by enhanced charge carrier and light management. Additionally, we compared solar cells with controlled contacts and control ones under light illuminated conditions at 85°C to demonstrate that the contact modification in perovskite solar cells significantly enhances the efficiency and stability of perovskite-silicon tandem solar cells.

[1] NREL, Best Research-Cell Efficiency Chart (2024).

FROM SOLUTION CHEMISTRY TO DEVICE FABRICATION: A UNIVERSAL ADDITIVE FOR HIGH EFFICIENCY AND STABILITY PEROVSKITE SOLAR CELLS

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Chemical environment and precursor-coordinating molecular interactions within a perovskite precursor solution can lead to important implications in structural defects and crystallization kinetics of a perovskite film. Thus, the opto-electronic quality of such films can be boosted by carefully fine-tuning the coordination chemistry of perovskite precursors via controllable introduction of additives, capable of forming intermediate complexes. In this work, we employed a new type of ligand, namely 1-phenylguanidine (PGua), which coordinates strongly with the PbI_2 complexes in the perovskite precursor, forming new intermediate species. These strong interactions effectively retard the perovskite crystallization process and form homogeneous films with enlarged grain sizes and reduced density of defects. In combination with an interfacial treatment, the resulted champion devices exhibit a 24.6% efficiency with outstanding operational stability. Unprecedentedly, PGua can be applied in various PSCs with different perovskite compositions and even in both configurations: n-i-p and p-i-n, highlighting the universality of this ligand.^[1]

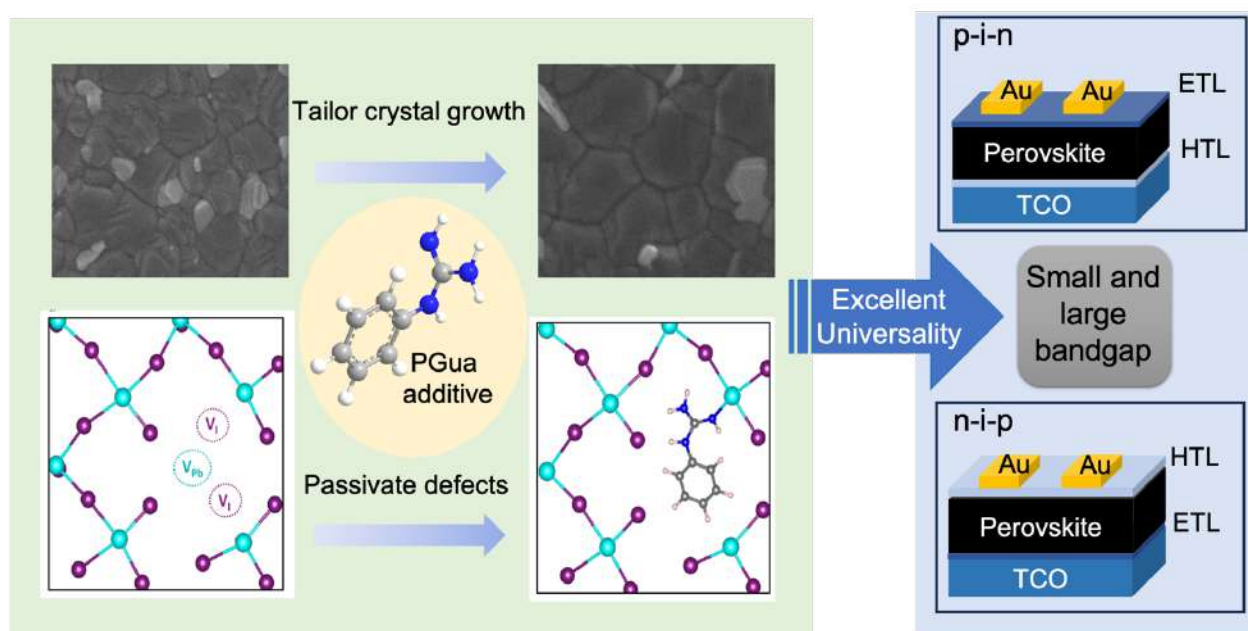


Figure: Effect of PGua in perovskite film and universality in various device configurations

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STRATEGIES TO MANIPULATE AVT AND PCE IN WIDE BANDGAP PEROVSKITE SOLAR CELLS FOR SEMITRANSSPARENT TWO-TERMINAL PSC-OPV TANDEM MODULES

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Building Integrated Photovoltaics (BIPV) consists in the replacement of traditional architectural elements with materials incorporating solar modules and it is one of the most attractive research topic to enable a capillary adoption of photovoltaics towards smart and self-sustaining cities. In this context, perovskite solar cells (PSCs) have attracted huge attention owing to their large absorption coefficient as and the tunability of their bandgap.

Here, we report on a class of mixed halide perovskite named $\text{FAPb}(\text{Br}_{1-x}\text{Cl}_x)_3$ with a tunable bandgap beyond 2.3eV, and we discuss strategy to maximize the key metrics for transparent photovoltaics on rigid^[1] and flexible^[2] substrates: Power Conversion Efficiency (PCE), Average Visible Transmittance (AVT) and Light Utilization Efficiency (LUE). In particular, we demonstrate a passivation strategy to achieve an Open Circuit Voltage (Voc) beyond 1.7V and PCE beyond 8% in 1cm² transparent perovskite solar cells processed from an industrial compatible solvent-antisolvent system. Advanced light management strategies including anti reflective coatings and micropatterning through laser ablation is discussed as a tool to push the AVT beyond 70%, for a LUE exceeding 5.7. Aspects such as the bifaciality of devices and performances with indoor lighting are discussed to estimate the energy yield of the solar cells in operative condition. Up-scaling to development of transparent modules have been achieved showing PCE up to 7% on 100cm² aperture area. The modules have been connected in two-terminal mechanically stacked tandem configuration with opaque and semi-transparent OPV modules in order to increase the PCE up to 14.9%^[3] and 12%, respectively.

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MODULATION OF STABILITY AND EFFICIENCY IN 2D/3D PEROVSKITE SOLAR DEVICES BY THE MOLECULAR GEOMETRY OF BULKY DIAMMONIUM CATION

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Perovskite-derived two-dimensional (2D) materials are emerging as excellent candidates to complement three-dimensional (3D) metal halide perovskites enhancing their stability. In this 2D/3D hybrid approach, bulky ammonium organic cations are deposited atop the 3D perovskite active layer, forming a very thin coating of a low-dimensional 2D perovskite.^[1] 2D/3D inverted perovskite solar cells (PSCs) have demonstrated exceptional stability, retaining over 95% of their initial efficiency values after exposure to damp-heat conditions (85 °C and 85% RH) for more than 1000 hours, with reported power conversion efficiencies (PCE) exceeding 25%.^[2]

In this work, we investigate the deposition of two diammonium spacers with similar chemical composition (4,4'-Dithiodianiline, 2S, and 4,4'-ethylenedianiline, ET) but with a totally different molecular geometry on top of a 3D perovskite with $\text{Cs}_{0.09}\text{FA}_{0.91}\text{PbI}_3$ formula to manipulate the efficiency and stability of the PSCs. Our results demonstrate an improved PCE of 21% when using the 2S spacer in opposition to an inferior PCE of 16% in the cells covered with the ET spacer. The stability tests display no loss in the PCE upon constant illumination at RT at the maximum power point tracking (MPPT) when using the 2S spacer vs. a significant drop in the PCE for the cells with the ET spacer. This divergent behavior is ascribed to the formation of a parallel oriented layer of a 2D perovskite with the 2S spacer that facilitates the charge extraction in the PSC in opposition to the isotropically layer of a 1D perovskite detected upon addition the ET spacer.

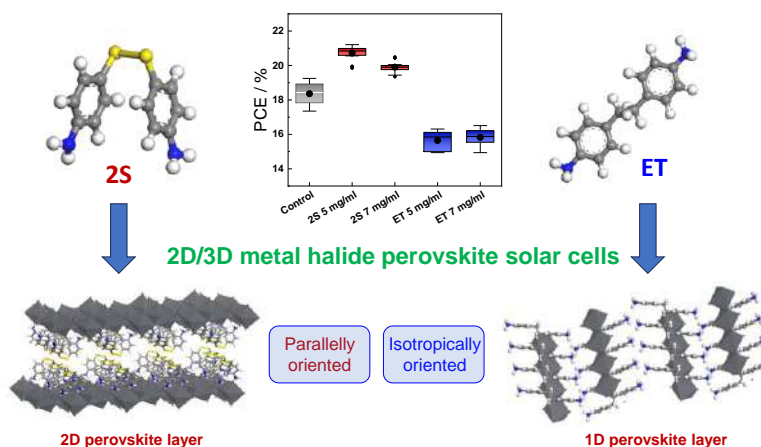


Figure 1: General scheme.

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ENDEAVORS ON COMMERCIALIZATION OF PEROVSKITE-SILICON TANDEM PHOTOVOLTAICS AT SWIFT SOLAR

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As the cost fraction of balance of system (BOS) increases, the photovoltaic (PV) power conversion efficiency (PCE) has become the main driver for cost reduction of the whole PV system. With crystalline silicon (c-Si), the predominant PV technology, nearing its practical PCE ceiling after years of development, tandem technology, particularly perovskite-c-Si tandems, presents a breakthrough opportunity. These tandems leverage perovskite's unique attributes, including defect tolerance, low-cost processing, and tunable bandgap, for a cost-effective solution to surpass single-junction c-Si PCE limitations. Notably, a recent achievement of 33.9% record PCE in perovskite-Si tandems signals a significant milestone towards high-performance PV systems.

However, the path to commercialization extends beyond PCE improvements, encompassing challenges related to stability, scalability, reproducibility, and throughput. At Swift Solar, we are pioneering efforts to address these hurdles, focusing not only on optimizing performance but also on enhancing the heat and light stability of perovskite and scaling up to commercial wafers. Our commitment to developing high-throughput deposition techniques and advancing processing reliability underscores our holistic approach to realizing the full potential of perovskite-Si tandem technology.

This presentation will discuss Swift Solar's progress in making perovskite-Si tandem PV a viable, scalable, and efficient solution for the future of solar energy.

SIMPLE TEMPLATING STEP IMPROVES UNIFORMITY AND INCREASES EFFICIENCY OF CO-EVAPORATED WIDE BAND GAP PEROVSKITE SOLAR CELLS

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Growth of co-evaporated perovskites is strongly impacted by the surface properties of the substrate on which the film is grown. The initial stage of the growth is crucial for the final properties of the deposited film.^[1] In this work, four compounds, namely PbI₂, PbCl₂, CsI and CsCl, chosen for their simple structure and accessibility, are used as templating agents for regulating growth of 4-source co-evaporated wide band gap Cs_xFA_yPb(I_zBr_q)₃ perovskite films with the aim of improving the film quality, reducing the substrate dependence and preventing phase segregation, indicated by multiple peaks in the photoluminescence spectra. It is shown that a 10 nm thin layer of a template has a determining impact on the optoelectronic properties of several hundreds of nanometers thick perovskite films deposited atop. X-ray photoemission spectroscopy (XPS) analysis of the surface of films of various thicknesses reveals the strong influence of the templating agents on the perovskite film composition at different points of the film growth. CsCl is highlighted for preventing phase segregation, regulating the band gap, boosting fill factor, open circuit voltage, and overall PCE, while also minimizing data variance compared to reference solar cell devices. Co-evaporated single junction p-i-n devices with CsCl as the templating agent reached over 18 % PCE with the optimal band gap for perovskite – silicon tandem application (1.68 eV).

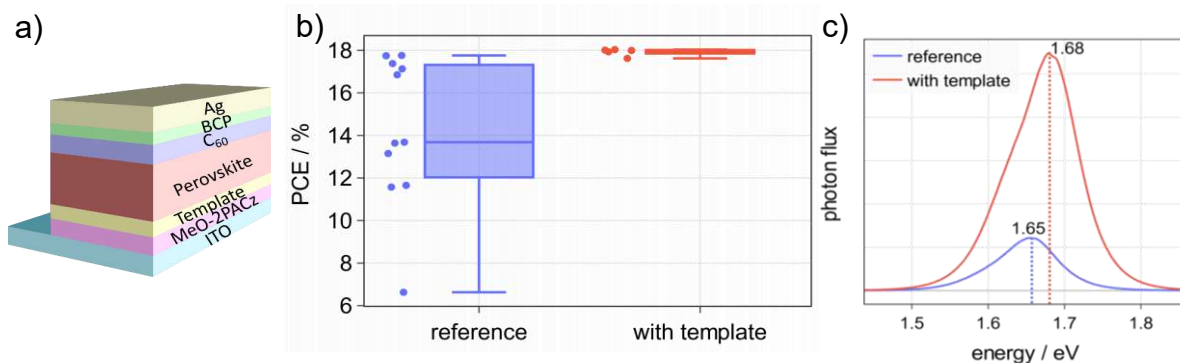


Figure 1: a) Schematic representation of a solar cell device stack with a templating material. b) Comparison of power conversion efficiency of reference and templated PSCs, fabricated in the same deposition run. The PSCs with a template show reduced variance as well as a higher overall PCE. c) Photoluminescence spectra of films with and without the templating material. The templating material regulates the band gap and increases the photoluminescence quantum yield.

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HIGHLY-EFFICIENT TEXTURED THREE-TERMINAL PEROVSKITE/SILICON TANDEM SOLAR CELLS

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Monolithic two-terminal (2T) perovskite/silicon tandem solar cells have demonstrated impressive performance improvements during the last decade,^[1,2] achieving a certified power conversion efficiency (PCE) of 33.9%.^[3] Under real-world conditions, the 2T architecture suffers from limitations such as current mismatch and performance variations with illumination conditions.^[4,5] Three-terminal (3T) perovskite/silicon tandem solar cells have been suggested as an alternative route to circumvent these losses by combining the advantages of 2T (reduced complexity and low optical losses) and four-terminal (4T) (availability of a wider range of perovskite bandgaps) configurations,^[6,7,8] and PCEs up to ~29% have been reported.^[9,10] Still, a more detailed experimental investigation of the device architecture and different perovskite bandgaps in textured 3T tandem solar cells is timely. In this research, we study 3T perovskite/Si tandem solar cells employing nano-textured POLO²-interdigitated back-contact (IBC) Si bottom cells with pyramid sizes of ~0.5-1 μm . To accomplish a conformal growth of perovskite thin films on the nano-textured substrates, we optimize perovskite spin-coating parameters and precursor solution concentration for each bandgap. We will present highly-efficient 3T perovskite/Si tandem solar cells in the architecture textured Si/ITO/SAM-HTL/perovskite/passivation/C₆₀/SnO₂/TCO/ARC at the conference. We develop an optimal top cell bandgap together with device stack optimization and will show that the 3T perovskite/Si tandem cells can noticeably outperform their 2T counterparts that employ POLO Si bottom cells. Furthermore, the cells are examined under various illumination conditions, revealing a stable performance against spectral variations by extra current being injected into or extracted from the third terminal.

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IMPROVING STABILITY OF PEROVSKITE SOLAR CELLS ON SELF ASSEMBLED MONOLAYERS BY SURFACE MODIFICATION

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The use of self-assembled monolayers (SAMs), particularly as hole selective contact modifiers, is now a popular choice for realising high efficiency perovskite devices. These SAMs, when directly coated on either transparent conducting oxides or on charge selective metal oxides (e.g. nickel oxide), have led to single junction efficiencies approaching 27% as well as high performing tandem devices.^[1,2] Among the numerous SAMs developed, the carbazole based methyl substituted SAM, [4-(3,6-Dimethyl-9H-carbazol-9-yl)butyl]phosphonic Acid (Me-4PACz) is widely used in the above high efficiency devices. While its widespread adoption was initially plagued by numerous challenges including the poor wettability of the perovskite on the non-polar Me-4PACz surface, multiple routes have now been developed to address this challenge. These include the formation of a field-enhancing, insulating metal oxide nano contact modifier as well as the co-deposition of organic additives with Me-4PACz.^[3-5]

In this work, we discuss the influence of sequentially deposited contact modifiers on the efficiency, and more importantly, on the stability of perovskite photovoltaics. While demonstrating the use of metal oxides as a universal approach towards realising high efficiencies (>23%), we also show that the adoption of organic contact modifiers can negatively impact the crystallization of the perovskite absorber, leading to an accelerated degradation of the devices. Based on these insights, we show routes by which both efficiency and stability can be improved using metal oxide contact modifiers, particularly under harsh ISOS stability tests including ISOS-LC-3, ISOS-T1 and ISOS-D3. Finally, we also present preliminary results from outdoor testing carried out on these modified cells in Surrey, UK.

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IMPACT OF HIGH DEPOSITION RATES ON CO-EVAPORATED PEROVSKITE-ABSORBERS FOR MONOLITHIC SILICON TANDEM SOLAR CELLS

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Today, most metal halide perovskite solar cells (PSCs) are prepared by solution-based deposition methods, which are known for their high deposition speed and versatility in terms of composition. However, these methods do not allow conformal coverage of textured surfaces, highly relevant for monolithic perovskite/silicon tandem solar cells. Vacuum-based deposition techniques such as sequential or co-evaporation present a solution to this challenge.^[1] However, the application of thermal evaporation processes is currently severely limited by their low deposition rates.^[2] In this work, we focus on the co-evaporation of PbI_2 , PbBr_2 , FAI and CsI from four different sources, to form absorbers with band gaps optimized for perovskite silicon tandem solar cells. Starting from a baseline process with a deposition time of ~90 min for 550 nm thick films, we test the limits of the established co-evaporation process in terms of process speed by increasing the deposition rates by a factor of five. Using *in situ* mass spectrometry, we analyse the atmosphere during the evaporation processes, and correlate the evaporation conditions with the absorber properties of the resulting films, studied by x-ray diffraction, electron microscopy and photoluminescence spectroscopy. We observe that even doubling the rates, leads to differences in phase composition and morphology of the resulting perovskite films. This indicates that the reaction kinetics of perovskite formation changes significantly with increasing deposition rates. By adapting the evaporation process, we are able to speed up the deposition by a factor of five without considerably affecting the optoelectronic properties of the resulting perovskite films (Figure 1b).

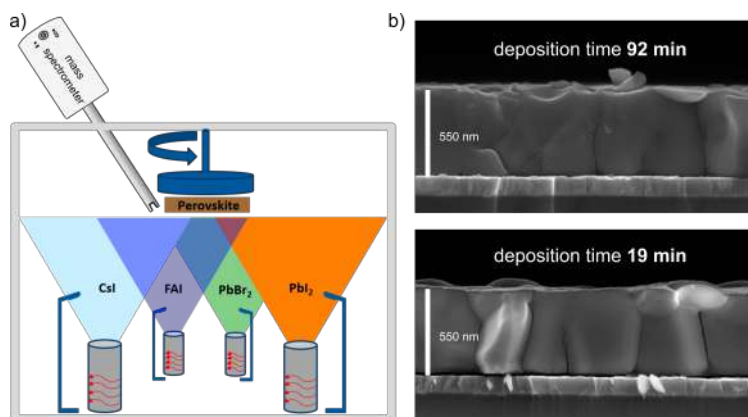
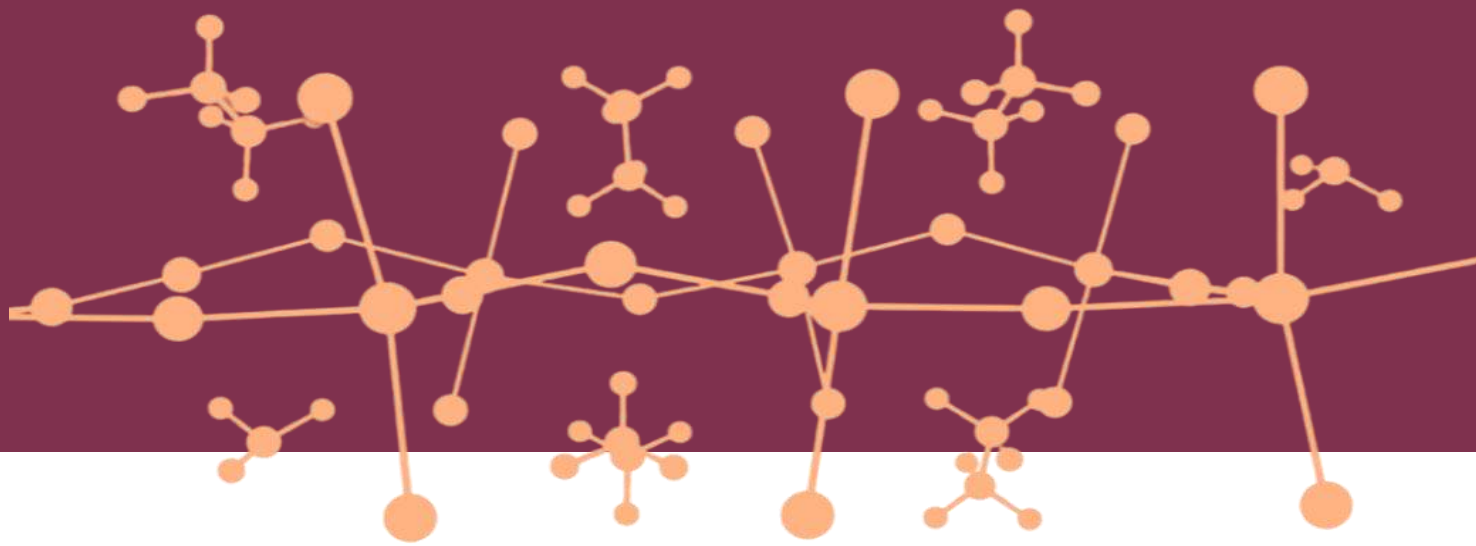


Figure 1: a) Schematic representation of the co-evaporation process with *in situ* mass spectrometry. b) Comparison of morphology analysed by scanning electron microscopy for two different perovskite films prepared with normal and five times faster deposition speed.

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		Session 2A Town Hall	Session 2B Trumpet
Session Chair:		Aldo Di Carlo, ISM-CNR, Italy	Annalisa Bruno, NTU, Singapore
Session Title:		Material processing & optoelectronic properties	Materials' device and their stability
16:53	17:05	Vikram , University of Oxford, United Kingdom <i>Atomistic insights into silanes as effective passivating agents for halide perovskite surfaces</i>	Feng Wang , Linköping University, Sweden <i>Improve the stability of doped spiro-OMeTAD</i>
17:05	17:17	Hayley Gilbert , University of Cambridge, United Kingdom <i>Linking Chemical and Optoelectronic Properties of Alloyed Perovskites using Optical and X-ray Spectro-microscopy</i>	Joost Herps , Eternal Sun, Netherlands <i>Towards full-size perovskite modules: characterization challenges</i>
17:17	17:29	Valentino Romano , Politecnico di Milano, Italy <i>Spin relaxation in layered perovskites: a time-resolved faraday rotation study</i>	Yuttapoom Puttisong , Linköping University, Sweden <i>Spin-Active Center Vanadium V⁴⁺ Complexes in Halide Double Perovskites Cs₂NaInCl₆ bulk crystals</i>
17:29	17:41	Fanny Baumann , Inst Catala De Nanociencia & Nanotecnologia (ICN2), Spain <i>In-situ characterization on operating perovskite solar cells under accelerated stress – expansive strain related to initial degradation</i>	Heyong Wang , Istituto Italiano di Tecnologia, Italy <i>Advancing Perovskites in Optoelectronic Technologies through Carrier Dynamics-Informed Optimization Strategies</i>
17:41	17:53	Cristian Adrian Villalobos Meza , imec, Belgium <i>A versatile perovskite deposition method for efficient and stable perovskite solar cells across a wide range of compositions</i>	Fengning Yang , University of Oxford, United Kingdom <i>Unveiling the impact of electronic and material degradation for inverted perovskite solar cell via inhomogeneous buried interface</i>
17:53	18:05	Valerio Stacchini , Helmholtz-Zentrum Berlin (HZB), Germany <i>Selective Monolayer Improves Buried Interface in DMSO-free Tin Perovskite Solar Cells</i>	Sara Covella , University of Bari, Italy <i>Plasma-driven engineering of metal halide perovskite interfaces for photovoltaic applications</i>
18:05	18:17	Dane deQuillettes , Optigon, Inc., United States <i>Non-contact characterization of perovskites: relating material properties to device performance</i>	Shivam Singh , TU Dresden, Germany <i>Impact of buried interface texture on ion migration in perovskite solar cells</i>
18:17	18:29	Paul Fassl , Karlsruhe Institute of Technology, Germany <i>Thermally evaporated perovskites: conceptual advantages and challenges to accelerate absorber deposition</i>	Gerrit Boshloo , Uppsala University, Sweden <i>Charge trapping at the SnO₂ / perovskite interface and its implementations for solar cells</i>
18:29	18:41	Sofia Chozas Barrientos , University of Valencia, Spain <i>Vacuum deposited perovskites single junction and tandem photovoltaic</i>	Matthew Leyden , Helmholtz-Zentrum Berlin, Germany <i>Modified hole transport layers for improved efficiency in evaporated perovskite solar cells</i>
18:41	20:00	POSTER SESSION - SOCIAL APERITIVO	
20:00	22:00	SOCIAL DINNER	



ATOMISTIC INSIGHTS INTO SILANES AS EFFECTIVE PASSIVATING AGENTS FOR HALIDE PEROVSKITE SURFACES

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Metal-halide perovskites require careful growth and defect passivation strategies to reach the highest efficiency and exhibit improved long-term operational stability in optoelectronic devices. Non-radiative defect-mediated charge-carrier recombination can be inhibited by modifying perovskites with molecular compounds as passivating agents. Recently, silanes are found to be a new generation of passivating agents. Amino-silane treated FAPbI₃ based perovskite solar cells have been shown to maintain 95 per cent of their initial efficiency for more than 1,500 hours when subjected to simulated full-spectrum simulated sunlight at 85°C, under open-circuit conditions in ambient air.^[1] However, the structures and interactions of these silane molecules at the perovskite surfaces are not fully understood at the atomic level. Our density functional theory and ab initio molecular dynamics simulations reveal atomic-scale details of strong passivator binding of the amino-silane molecules on the defective perovskite surface. Since the surface Pb ions adjacent to iodide vacancies are severely undercoordinated, the amino-silane adsorption through both N-Pb and O-Pb bonds acts by increasing the Pb coordination and eliminating the effects of surface vacancy defects, thereby effectively passivating the perovskite surface. Overall, these ab-initio simulation results also agree with our experimental findings and provide new structural and mechanistic insights at the atomic level.

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IMPROVE THE STABILITY OF DOPED SPIRO-OMeTAD

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A key challenge for the practical applications of perovskite solar cells lies in the low stability of the devices, which depends not only on the perovskite materials³ but also on the charge transport layers.^[1,2] Currently, all high-performance perovskite solar cells (PSCs) with > 24% PCE are based on the bench-mark hole transport layer Spiro-OMeTAD, which is doped with lithium bis(trifluoromethane)sulfonimide (LiTFSI) and 4-tert-butylpyridine (tBP), which harms the stability of the devices.^[3] In addition, the complex in situ oxidation processes make it difficult to understand the mechanism of conventional spiro-OMeTAD doping and further limit the development of stable HTLs with high PCEs.

We have developed a clean and free post-oxidation doping for spiro-OMeTAD by using stable organic radicals as the dopant and ionic salts as the dopant modulator (termed ion-modulated (IM) radical doping).^[4] The doped Spiro-OMeTAD based on our IM radical doping strategy provided a high PCE of over 25% and excellent stability (T80 for ~ 1200 h under 70±5% relative humidity and T80 for ~ 800 h under 70±3 °C without encapsulation), minimizing the trade-off between efficiency and stability of PSCs. In this doping strategy, the radicals provide hole polarons that immediately increase the conductivity and work function, and the ionic salts further modulate the work function by affecting the energetics of the hole polarons. By modifying the dopants, we can further increase the thermal stability of the Spiro-OMeTAD layer, which can survive at 80 °C for more than 2000 hours (Unpublished results).

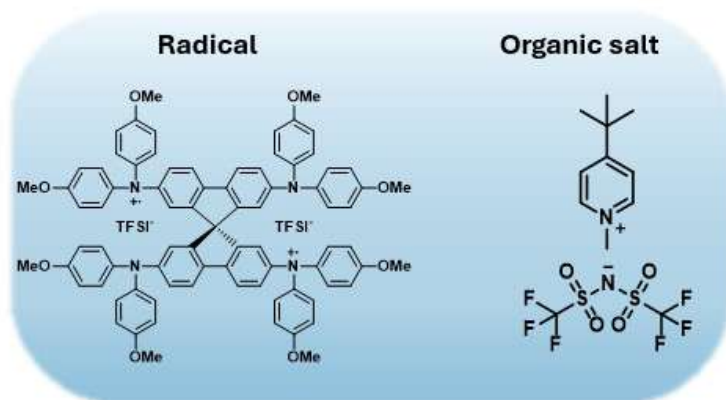


Figure 1: The involved radical and salt for ion-modulated radical doping strategy

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LINKING CHEMICAL AND OPTOELECTRONIC PROPERTIES OF ALLOYED PEROVSKITES USING OPTICAL AND X-RAY SPECTRO-MICROSCOPY

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Mixed composition lead halide perovskites have emerged as a successful material in the development of solar cell devices. For example, state-of-the-art triple cation ($\text{Cs}_{0.05}\text{MA}_{0.17}\text{FA}_{0.78}\text{Pb}(\text{I}_{0.83}\text{Br}_{0.17})_3$) perovskite solar cells have displayed higher power conversion efficiencies (PCEs) and reproducibility than their single cation counterparts^[1]. The tunability of the band gap (E_g) of these materials through compositional engineering is highly desirable for tandem devices, having enabled these devices to exceed PCEs of 30%^[2]. However, the alloyed nature of these materials creates chemical and structural heterogeneities which reduce device performance and long-term stability^[3,4], creating a bottleneck in the development of perovskites into commercial devices. Additionally, increasing the E_g (by increasing the bromide content) has been shown to be beneficial only up to a threshold of $\sim 1.75\text{eV}$ ^[5]. This is a result of halide segregation occurring upon light irradiation^[3,6], which reduces the open circuit voltage and PCEs of devices^[5,7]. Currently, the mechanism behind halide segregation is not fully understood^[8,9]. To elucidate the mechanism of halide segregation and the heterogeneous nature of alloyed perovskites thin films, we used correlative hyperspectral photoluminescence (PL) microscopy and synchrotron X-ray mapping techniques. Techniques including X-ray fluorescence (XRF), X-ray diffraction (XRD), and X-ray absorption near edge spectroscopy (XANES) are used as a chemical probe into localised regions across the film and provide insight into chemical structure, environment, and compositional distribution. Such X-ray techniques are seldom used at the microscale in the halide perovskite field despite their ability to provide unique insight into parameters not commonly explored in literature. Through correlation with PL microscopy, which provides spatially resolved information on the optoelectronic performance, ion migration, and charge carrier trapping, a deeper understanding into key properties such as performance and longevity can be gained. These correlations enable a deeper mechanistic insight into these highly important materials that PL and X-ray spectro-microscopy techniques could not deliver on their own. Performing these experiments in the ‘ground state’ and under *operando* (illumination) conditions will shed light on halide segregation mechanisms and give a full description on how these materials behave and evolve under conditions relevant for eventual use in the field.

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SPIN RELAXATION IN LAYERED PEROVSKITES: A TIME-RESOLVED FARADAY ROTATION STUDY.

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Layered metal halide perovskites (L-MHPs) exhibit a quantum well structure made up by an alternating sequence of metal halide layers and organic cations.^[1] The presence of heavy elements causes a large spin-orbit coupling that, together with the lack of an inversion symmetry point, causes a Rashba splitting of the electronic energy bands that lifts the spin degeneracy.^[2] As a result, spin polarization can be induced into these materials through optical excitation with circularly polarized light.^[3] However, because of quantum confinement effects, photoexcitation leads to the formation of stable excitons in L-MHPs with binding energies reaching values as high as 500 meV, depending on the specific chemical composition.^[4] In this study, time-resolved Faraday rotation spectroscopy (performed using circularly polarized light pulses) is exploited to analyse the processes behind the spin depolarization of excitons in several L-MHPs samples: (Hexa)₂FAPb₂I₇, (Hexa)₂MAPb₂I₇ and (Hexa)₂CsPb₂I₇ (where BA: Butylammonium; Hexa: Hexylammonium; FA: Formamidinium; MA: Methylammonium). By performing a thorough temperature dependence (in the range 4-300 K) and pump wavelength analysis, we have been able to identify an energy-activated process that hinders the loss of spin polarization in these materials. Indeed, the spin relaxation lifetime increases with increasing temperature and increasing pump wavelength. Because of the polar and soft nature of L-MHPs, we suggest that the process governing this behaviour involves the formation of polarons that prevents spin depolarization by shielding the excitons from the surrounding environment. These results, in agreement with those obtained previously,^[5] contribute to a better understanding of exciton-polaron interactions in L-MHPs, with emphasis on their role into spin depolarization processes and their engineering by proper choice of the chemical composition.

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SPIN-ACTIVE CENTER VANADIUM V⁴⁺ COMPLEXES IN HALIDE DOUBLE PEROVSKITES Cs₂NaInCl₆ BULK CRYSTALS

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Metal doping Halide double perovskite (HDP) has recently emerged as new revenue for modifying the physical properties of the HDP, highlighting target application in optoelectronics and magnetic functionalized semiconductors. Incorporating first-row transition metals such as Fe, Cr, and V into a B'-site of A₂B(+1)B'(+3)X₆ HDP host has led to many interesting properties such as bandgap tuning [1,2], highly efficient broadband near-infrared emission [3], and magnetic response [4]. However, introducing metal ions into the HDP might also lead to the formation of thermodynamical stable point defects that would alter the target application. In this study, we show that doping Vanadium (V) into Cs₂NaInCl₆ not only leads to a target V³⁺ isoelectronic In substitution but also promotes the formation of V⁴⁺ tetragonal complex [5]. The existence of V⁴⁺ tetragonal complex was concluded from single crystal electron spin resonance (ESR) spectra that exhibited S = 1/2, I = 7/2 (100% natural abundance), with g_x=g_y=1.973, g_z=1.945, A_x=A_y=180 MHz and A_z=504 MHz. The tetragonal distortion was found to be along <001> principal axis. The controlled growth of V-doped Cs₂NaInCl₆ in an oxygen-free environment is shown to suppress the V⁴⁺ EPR signal. The defect model is suggested to have a VOCl₅ octahedral coordination, that is V⁴⁺ tetragonal complex to V⁴⁺-O²⁻ at the B' site octahedral lattice, where one of Cl⁻¹ is replaced by O²⁻. We highlight the importance of complex defects in HDP that hold a new potential application both for optoelectronics, spintronics and quantum spin qubits. We will also shortly present our ongoing study of other transition metal doping (i.e., Fe and Cr) into Cs₂Na(Ag)InCl₆, with a highlight target application in light-emitting and spin-related functionality.

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IN-SITU CHARACTERIZATION ON OPERATING PEROVSKITE SOLAR CELLS UNDER ACCELERATED STRESS – EXPANSIVE STRAIN RELATED TO INITIAL DEGRADATION

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In light of recent improvements of perovskite solar cell (PSC) stability, evaluation of life expectancy can become costly as T80 could surpass 1000s of hours. ^[1] Accelerated testing could offer a solution by reducing resources needed to advance in preventing the initial stages of degradation, especially if properly related to long-term studies and by use of semi-automated analysis. Additionally, by suitable experiments, it becomes feasible to track physical phenomena occurring during the application of stress, and consequences for stability of reversible processes such as ion migration. ^[2] We have developed *in-situ* characterization methods to be applied in line with or parallel to ISOS-grade indoor and outdoor operational testing. These include X-ray diffraction (XRD), electrochemical impedance spectroscopy (EIS) and photoluminescence. I aim to present implementations of accelerated stress tests on PSCs under operando conditions, among others applying continuous light irradiation and bias-voltage. We followed device response with time under bias via *in-situ* XRD analyses in conjunction with quasi *in-situ* EIS. Our results demonstrate a clear relation between halide perovskite lattice expansion/constriction, increased ionic conductivity, current decay with time and device stability. ^[3] EIS analyses revealed a threshold where some of these bias-induced degradation mechanisms become irreversible. By a combination of detailed characterization, we could elucidate mechanisms of actuation when using additive engineering to passivate shallow defects. ^[3-5]

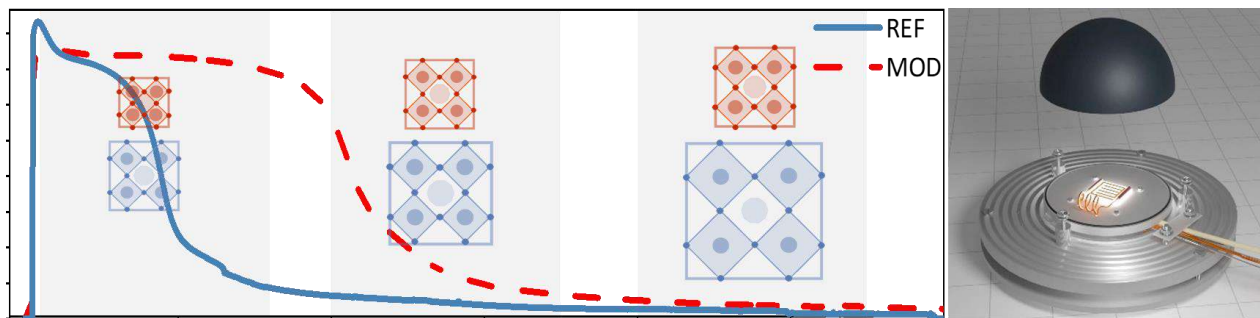


Figure 1: Left: Schematic of current evolution and visualization of lattice expansion during accelerated stress test. Right: *in-situ* XRD sample mount.

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ADVANCING PEROVSKITES IN OPTOELECTRONIC TECHNOLOGIES THROUGH CARRIER DYNAMICS-INFORMED OPTIMIZATION STRATEGIES

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In recent years, significant progress has been achieved in metal halide perovskites, particularly in solar cells, LEDs, and solid-state lasers. However, distinct optimization approaches are evident across these applications. This study reexamines the stoichiometry strategy from the perspective of carrier dynamics, elucidating its profound impact on device performance. Using Cs/FAPbI₃ as a model system, we investigate how precursor stoichiometry influences carrier relaxation and recombination processes, guiding customized optimization paths for perovskite components in various optoelectronic scenarios. Furthermore, employing additive engineering to target carrier radiative recombination yields impressive results, as demonstrated by highly efficient LEDs (24.5%) with exceptional stability (LT90=147h). These findings reinforce the fundamental principles governing perovskite behavior and highlight the effectiveness of carrier dynamics-informed strategies in advancing perovskite-based optoelectronic technologies.

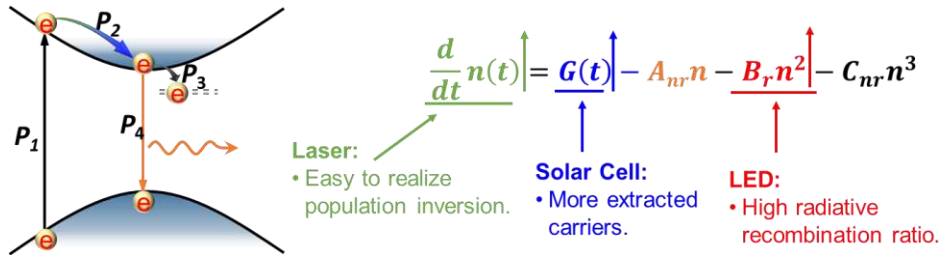


Figure 1: Carrier dynamics-informed optoelectronic technologies.

A VERSATILE PEROVSKITE DEPOSITION METHOD FOR EFFICIENT AND STABLE PEROVSKITE SOLAR CELLS ACROSS A WIDE RANGE OF COMPOSITIONS

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A sequential 2-step hybrid deposition method, comprising thermal co-evaporation of inorganic halides, followed by solution coating of organic halides has been employed to produce perovskite thin films with bandgaps ranging from 1.55 eV to 1.80 eV. Applications such as top cell in a perovskite-silicon tandem cell (1.65-1.70 eV), and middle (1.50-1.60 eV) and top cells (≥ 1.80 eV) in a perovskite-perovskite-silicon triple-junction cell lie within the developed bandgap range. High efficiency and stability have been realized with multiple perovskite compositions. On the narrower bandgap side, a 1.55 eV FAPbI₃-based perovskite has been implemented in p-i-n perovskite solar cells and mini-modules. At the present stage of development, champion efficiencies of 22.9% for 0.125 cm² cells, and 20.7% for 4 cm² minimodules have been achieved. Moreover, a novel perovskite surface treatment allowed for excellent thermal stability, maintaining 94.8% of the initial efficiency after 3250 hours of thermal ageing test at 85 °C in a N₂ atmosphere. On the wider bandgap side, the incorporation of bromine in both deposition steps has led to a 1.78 eV Cs_xFA_{1-x}Pb(I_yBr_{1-y})₃ perovskite, which implemented in 0.125 cm² p-i-n cells has returned efficiencies of 16.5%. At the present stage, the phase stability of this 1.78 eV perovskite has been tested with 1-hour maximum power point tracking (MPPT) under 1-sun illumination, showing no losses in power output.

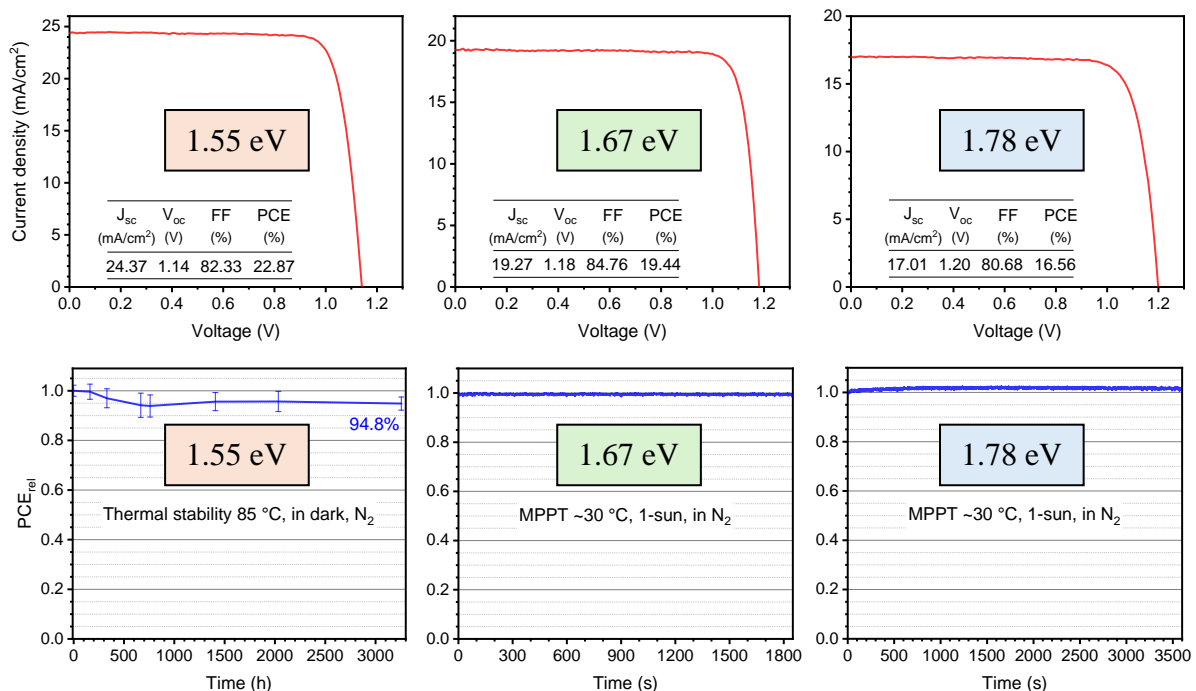


Figure 1: J-V characteristics (top), and thermal stability or MPPT tests (bottom) of solar cells using perovskites with 3 different bandgaps deposited by a 2-step hybrid deposition method.

UNVEILING THE IMPACT OF ELECTRONIC AND MATERIAL DEGRADATION FOR INVERTED PEROVSKITE SOLAR CELL VIA INHOMOGENEOUS BURIED INTERFACE

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Abstract

Achieving stable formamidinium-caesium lead perovskite solar cells under light and heat is one of the major challenges hindering the commercialization of perovskite solar cells (PSCs), while the mechanism of device degradation, especially at the interface, is unclear and concealed.^[1] Herein, by utilizing a novel polymer and organic Benzothioophene molecule (BT) blend, we construct a phase-separation hole transport layer (HTL) designed to compare with polymer PTAA and self-assembled monolayer Me-4PACz. We revealed that the efficiency difference in fresh samples arises from the crystallinity and orientation of the near HTL perovskite region, which result in defects and non-radiative recombination. However, this fails to provide guidance on the degradation pathway when aging at open-circuit condition with heat. We found that the behaviour of charge percolating and dissipating under open-circuit conditions impacts the change in the space charge region at the buried interface and the generation of mobile ions, thereby contributing to the loss of short-circuit current after aging. Devices incorporating our BT phase-separation HTL retained 85% of initial MPP efficiency for over 1,500 hours under full-spectrum simulated sunlight at 85 degrees Celsius and Open-Circuit Conditions in ambient air with a relative humidity of 50 to 60% (ISOS-L-3), five times longer than other HTL alternatives.^[2,3]

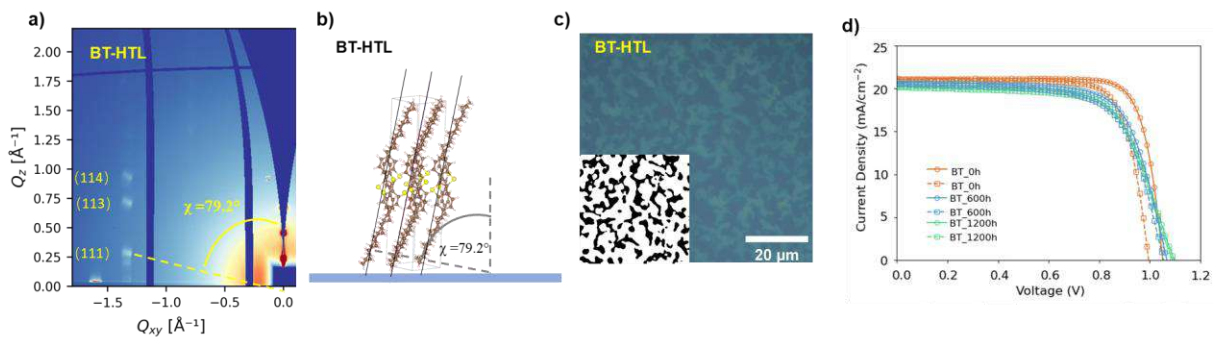


Figure: a) The GIWAX pattern for BT phase-separation HTL. b) The orientation of BT molecules in the film. c) Optical microscope images of BT phase-separation HTL. d) JV curve of BT-HTL PSC devices after different aging time under 1 Sun, 85°C, Open-circuit condition.

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ELECTRON SELECTIVE MONOLAYERS IN PEROVSKITE SOLAR CELLS - ADVANCED CHARACTERIZATION

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In recent years, self-assembled monolayers (SAMs) have revolutionized the design of perovskite solar cells (PSCs), particularly in p-i-n ("inverted") architectures, thanks to their low-temperature processing, minimal material usage, and excellent operational stability. This has made them the preferred material for hole-selective contacts on ITO. However, this preference doesn't extend to n-i-p (or "regular") architectures. Despite the widespread use of SAMs for hole-selective layers (HSL), it's remarkable that very few studies have explored electron-selective SAMs.

This study investigates a series of novel molecules for their potential as electron-selective SAMs on ITO. Charge selectivity and transfer rates were assessed using transient surface photovoltage (trSPV) across timescales ranging from 1 nanosecond to 1 second. The results demonstrate clear electron selectivity for certain molecular structures, indicating their strong electron injection capability into ITO and excellent hole-blocking properties.

This study highlights novel molecules with potential for efficient electron-selective SAMs, offering improved performance in perovskite solar cells.

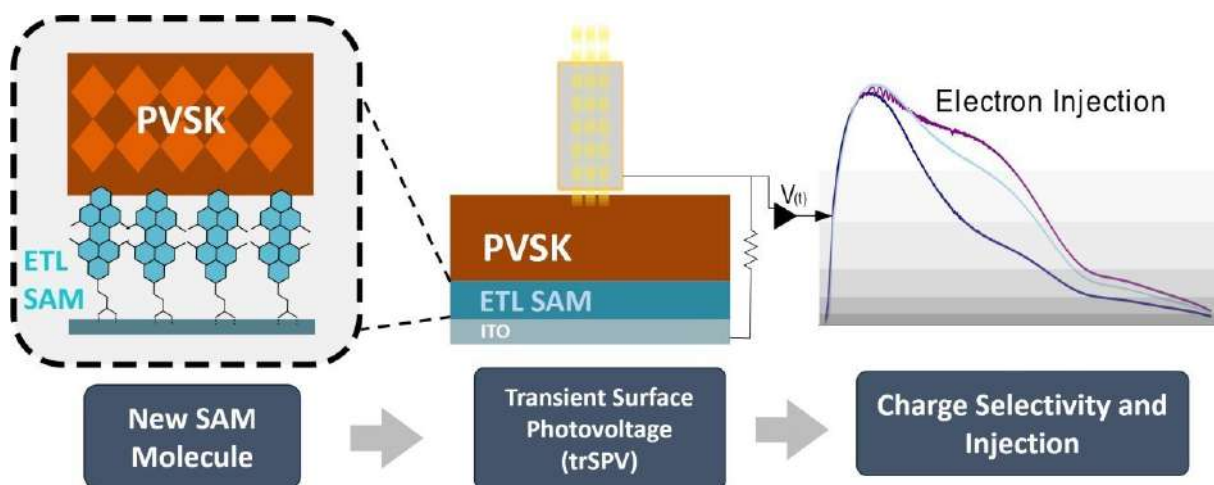


Figure 1: simplified explanatory scheme of the transient photovoltage measurement: after perovskite film deposition onto the self-assembled monolayer, the samples are subjected to pulsed laser excitation. The resulting photovoltage is a clear sign of charge selectivity.

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PLASMA-DRIVEN ENGINEERING OF METAL HALIDE PEROVSKITE INTERFACES FOR PHOTOVOLTAIC APPLICATIONS

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Metal halide perovskite (MHPs) solar cells represent a promising newcomer in the front of emerging photovoltaic technologies to address the dramatic energy crisis and climate change that we are facing. The exceptional properties of MHPs derive from their hybrid organic-inorganic nature, which allows also for low-cost and straightforward processing. Solar cells containing MHPs as absorbing layer have already achieved a power conversion efficiency of about 25,7 %, close to the efficiency of silicon-based devices. Nevertheless, a major limitation, still preventing the uptake of the technology, is related to the reduced stability of these materials when exposed to operative conditions, namely temperature, light, and moisture. Herein, an effective defect passivation of MHP surfaces is a key strategy to tackle both the stability and the enhancement of solar cell performances. Although many solution-based approaches have been tested ^[1], we propose here an innovative use of plasma, as a solvent-free, scalable, and non-invasive promising strategy to boost MHP solar cells performances ^[2]. As starting point we exposed the surface of Methylammonium Lead Iodide perovskite thin films to different plasma conditions implying the variation of power, gas, and treatment time, both for low-pressure (LPPs) and atmospheric pressure plasmas (APPs). The impact of *Ar*, *N₂*, *H₂* and *O₂* LPPs on *MAPbI₃* optochemical properties and morphology was correlated to the performance of the photovoltaic devices and rationalized by density functional theory calculations ^[3]. Herein an interesting improvement in photoluminescence was observed for the *Ar* and *H₂* treated films, while an improvement in PCE was observed only for the *Ar* treated device. This result was ascribed to the efficient removal of the superficial organic component, revealed through X-ray photoelectron spectroscopy (XPS), following suitable surface passivation by the electron transporting layer deposition. Following these results, we tested APP treatments, finding a milder morphological modification than LPP treatments but withstanding good surface passivation, as confirmed through the improved photoluminescence intensity, while the effect in terms of photovoltaic devices is still under investigations. Starting from these encouraging results, we applied plasma surface treatments to tin-based perovskites, finding a very interesting slowdown in the oxidation of the surface tin of *FaSnI₃* thin films. The collection of these results already shows the great versatility and potential of plasma-based techniques for the intelligent modification of metal halide perovskites for solar energy conversion.

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NON-CONTACT CHARACTERIZATION OF PEROVSKITES: RELATING MATERIAL PROPERTIES TO DEVICE PERFORMANCE

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The ability to reduce energy loss at semiconductor surfaces and interfaces through passivation or surface field engineering is an essential step in the manufacturing of efficient photovoltaic (PV) and optoelectronic devices. Ideally, surface modifications reduce non-radiative recombination and do not inhibit charge extraction but, oftentimes, there exists a trade-off between these effects. Understanding this behavior is complicated by the fact that non-radiative recombination and charge extraction appear as similar dynamics in time-resolved spectroscopy measurements. Therefore, a detailed understanding of perovskite material behavior requires a combination of spectroscopic measurements paired with physically accurate theoretical models. Here, we discuss a suite of measurements paired with a theoretical model that includes surface fields to uncover several key properties of the first devices to reach the >25% PCE milestone.^[1] Next, we discuss how this type of analysis can be scaled to researchers and perovskite companies that are exploring a large number of perovskite formulations, passivation techniques, and transport layers – with the goal of achieving high power output and excellent stability. Specifically, Optigon has built a metrology tool capable of performing several spectroscopic measurements simultaneously in only a few milliseconds. The tool is used to measure 100's of different perovskite samples and generate large data sets to not only test the accuracy of different theoretical models across a wide range of perovskite architectures, but also to perform machine learning to identify key features in optical measurements that relate to device performance. Just as Suns- V_{oc} measurements have been critical in the characterization and optimization of silicon PVs,^[2] we are starting to develop the key set of measurements that demonstrate high predictive power for perovskite devices.

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IMPACT OF BURIED INTERFACE TEXTURE ON ION MIGRATION IN PEROVSKITE SOLAR CELLS

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Abstract: Despite the sky-rocketed efficiency of lead-based perovskite solar cells (PSCs),¹ their poor operational stability impedes their commercialization. Among the various factors that influence device stability, ion migration has been identified as a key driver of degradation. However, inverted (p-i-n) architecture-based PSCs shows relatively higher operational stability in comparison to the regular (n-i-p) architecture-based PSCs.² In this work, we focus on the study of ion migration induced degradation in inverted architecture PSCs, which employ either a thin polymer layer or a self-assembled monolayer (SAM) for hole extraction. We demonstrate that the difference in texture imposed by the use of these hole transport layers (HTL) is an important and thus far inconspicuous factor that impacts on ion migration, and consequently on device stability. By investigating the buried interface of $\text{Cs}_{0.05}\text{MA}_{0.17}\text{FA}_{0.83}\text{Pb}(\text{I}_{0.83}\text{Br}_{0.17})_3$ (TrCa) perovskite in detail, we reveal that its texture has a strong impact on the vertical compositional stratification in the perovskite active layer. By monitoring bias-induced ion migration in devices with different HTLs, we demonstrate that the smooth polymer-based HTL results in a higher degree of ion migration than the rough SAM HTL, corresponding to a stronger degradation in the former. These results further indicate that the use of SAMs for hole extraction is a promising strategy to suppress ion migration and improve device efficiency.

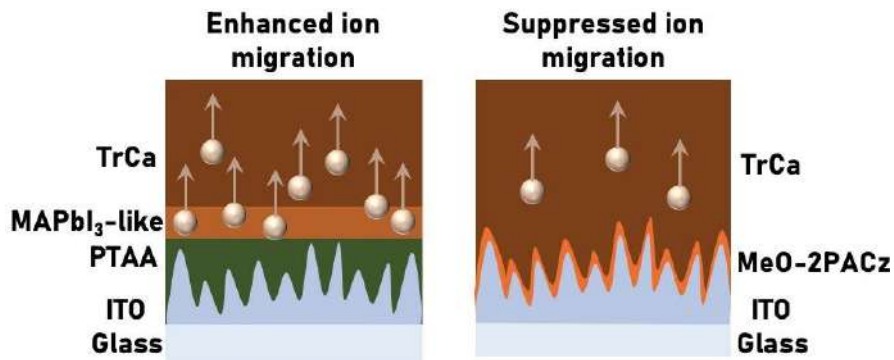


Figure: Ion migration in perovskite solar cells as a function of buried interface texture.

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THERMALLY EVAPORATED PEROVSKITES: CONCEPTUAL ADVANTAGES AND CHALLENGES TO ACCELERATE ABSORBER DEPOSITION

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The industrial production of perovskite-based single-junction and tandem solar cells has attracted considerable attention in recent years as it has the potential to revolutionize solar technology. Key concerns for the large-scale deposition of perovskite films include (i) the conformal, reproducible and high-yield deposition of the perovskite absorber layer and (ii) ensuring a throughput compatible with current industrial-scale production rates.

In that regard, thermal evaporation enables a remarkable coating homogeneity, which can be a decisive advantage for high-yield production of perovskite-based solar cells. First, we summarize the conceptual advantages of vapor-based over solution-based fabrication methods and discuss the most crucial process parameters.^{[1],[2]} Second, we will discuss the challenges that come with accelerating absorber deposition by thermal evaporation. Achieving consistent and high film quality requires precise control of the evaporation process, while production throughput is limited by achievable deposition rates. The latter can be increased, for example, by arranging multiple deposition sources sequentially (e.g., by using a linear evaporation system), utilizing deposition sources with larger evaporation areas or by increasing the deposition rate for each individual source. This requires that the raw materials used can withstand sufficiently high temperatures before negative effects on the final film quality or degradation occur.^[3] In this context, we will provide an analysis of the most commonly employed perovskite precursor materials in terms of (i) their composition, thermal stability, evaporation behaviour and rate limitation, and (ii) the effects of evaporation rate on microstructure, film quality and device efficiency. Overall, we provide a comprehensive view of the potentials and obstacles in the production of perovskite absorbers via thermal evaporation.

In addition, we will discuss our recent results for all-vacuum processed methylammonium-free PSCs in the p-i-n architecture. We recently showed how exposed phosphonic acid functional groups impact the initial phase and final bulk crystal properties of co-evaporated perovskites and demonstrated that the surface interaction is mediated by hydrogen bonding of phosphonic acids with interfacial iodine.^[3] This results in increased formamidinium iodide (FAI) adsorption, persistent changes in perovskite structure, and stabilization of bulk α -FAPbI₃ with PCEs up to 17%. With regard to sequentially evaporated PSCs, we will present all-vacuum processed phase-pure FAPbI₃ PSCs with PCEs above 17%, among the highest value reported in the p-i-n architecture. Finally, we will present results on co-evaporated and sequentially evaporated wide bandgap PSCs at the conference.

Our work paves the way for efficient all-evaporated PSCs and their application to monolithic tandem solar cells with an up-scalable and industrially relevant deposition technique and takes a promising look at the future of this emerging solar technology.

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CHARGE TRAPPING AT THE SnO₂ / PEROVSKITE INTERFACE AND ITS IMPLEMENTATIONS FOR SOLAR CELLS

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SnO₂ is currently the most popular electron transport layer (ETL) for n-i-p perovskite solar cells. It is attractive because of its low cost, low processing temperature (< 200°C), good optical properties and wide bandgap (3.6 eV). The high performance of SnO₂ ETLs is surprising, since the energy of its conduction band minimum is expected to be well below that of lead halide perovskites, which should lead to considerable voltage losses in the solar cell.

In order to assess band alignment and charge accumulation at the SnO₂ / perovskite interface we performed time-resolved photovoltage measurements under illumination, as well as time-resolved potential steps (chronoamperometry) in the dark. Several remarkable findings were done:

- The photovoltage rise and decay have a biphasic characteristic, where about half of the photovoltage changes on a millisecond timescale and the rest on a second time scale.
- A significant amount of charge appears to be irreversibly trapped in SnO₂ / lead halide perovskite / spiro-OMeTAD devices.

Based on these observations, as well as additional photoinduced absorption and fluorescence measurements, we propose that upon application of a forward voltage bias (or illumination under open-circuit conditions) there is not only a fully reversible ionic charge displacement in the solar cell device, but also trapping of charge at the interfaces. Specifically, stepping the voltage from 0 V to 0.8 V results in ionic displacement charge of about 1.5 μC cm⁻² and a trapped charge of about 500 μC cm⁻², see Figure 1.

We propose that trapping of negative charge at the SnO₂ / lead halide perovskite aligns the conduction band level of SnO₂ with that of the perovskite. The positive counter charge at the other interface is in the form additional oxidized spiro-OMeTAD molecules.

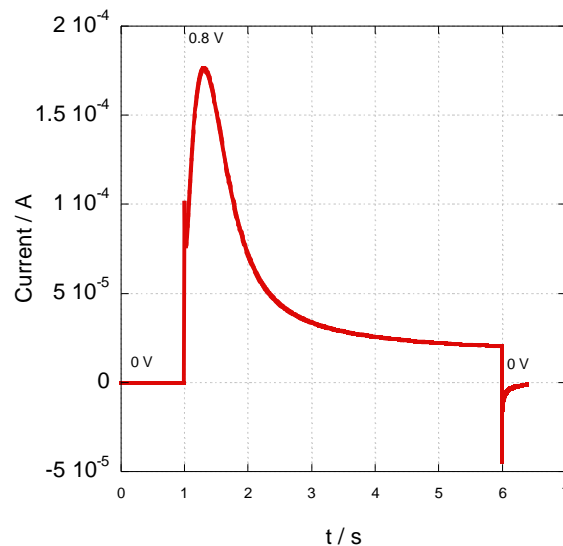


Figure 1: Potential step measurement (0 V to 0.8 V) of a SnO₂/FAPbI₃/spiro-OMeTAD solar cell in the dark.

VACUUM DEPOSITED PEROVSKITES FOR THIN FILM PHOTOVOLTAICS AND LEDs

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I will present the latest results on metal halide perovskite films prepared using different vacuum based methods, such as thermal co-sublimation and close-space sequential sublimation. The typical properties of these perovskite films will be presented including the stability. Additionally, efficient solar cells and LEDs employing these films, reaching power conversion efficiency and external quantum efficiency above 20 and 15 %, respectively will be presented.

MODIFIED HOLE TRANSPORT LAYERS FOR IMPROVED EFFICIENCY IN EVAPORATED PEROVSKITE SOLAR CELLS

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Organo-lead-halide perovskites are a promising set of materials for photovoltaic applications. However, many challenges remain before adoption into real world applications. One of these challenges is industrial scale up. Evaporation is a proven industrial technology used in thin film solar cells like cadmium telluride, is reported to reach 26% for perovskites,^[1] and has been demonstrated previously by our group for tandem applications.^[2] Here we present a method of 4 source co-deposition of perovskite using a modified hole transport layer. Using this modified hole transport layer, we demonstrate improved performance and stability over the control sample deposited within the same batch. Additionally, this new hole transport layer allows for a broader range of process conditions without additional processing steps. In this study we used in-situ and ex-situ photoluminescence to probe the perovskite growth, and probe perovskite at different stages of solar cell fabrication. This helped elucidate the perovskite formation process and how our modified layer impacts the open circuit voltage of solar cells. Solar cells have demonstrated an efficiency of over 20% for over 300 hours of maximum power point testing.

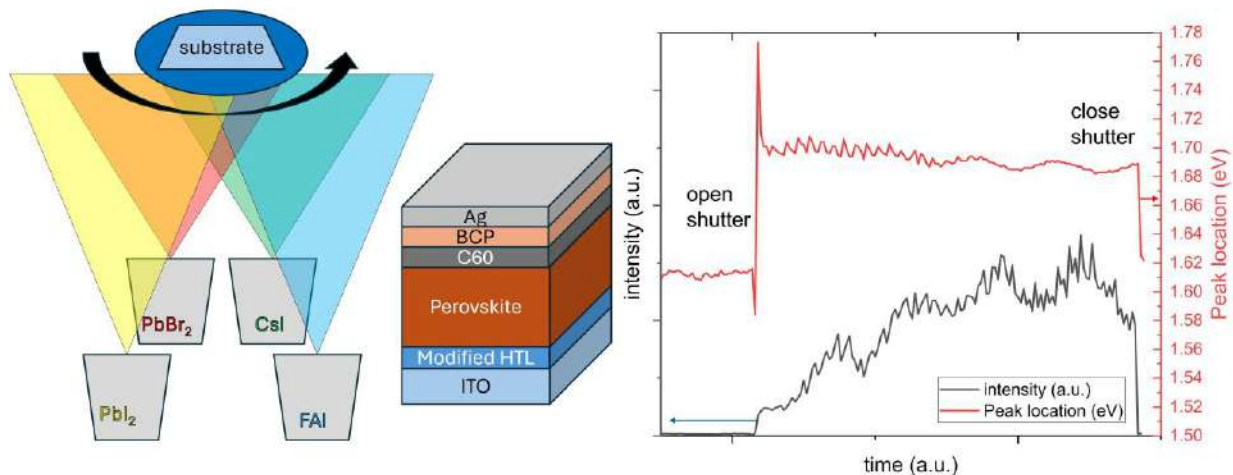


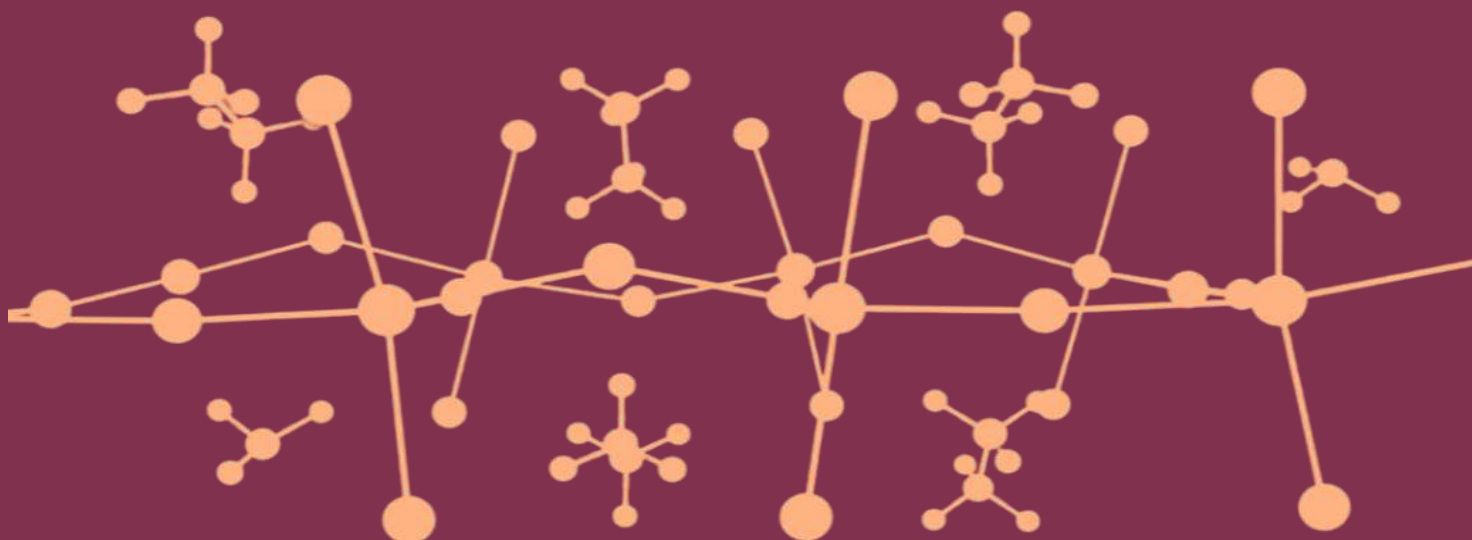
Figure 1: Diagrams of our co-evaporation process and structure of a completed solar. On the right is a graph of an in-situ PL measurement revealing the PL intensity and bandgap of the perovskite during an evaporation.

[1] J. Zhou, *et al.*, *Joule*, **2024**, 10.1016/j.joule.2024.02.019

[2] M. Roß *et al.*, *Adv. Energy Mater.* **2021**, 11, 2101460.

Day 3 - Wednesday, September 18th, 2024

08:45	09:00	Prof. Luca Gammitoni for VITALITY Project	
Session Chair:		Henry Snaith, University of Oxford, United Kingdom	
09:00	09:25	18° INVITED LECTURE - Mohammad Khaja Nazeeruddin , EPFL, Switzerland <i>Stable and efficient Perovskite Solar Cells and Modules by interface and compositional Engineering</i>	
09:25	09:50	19° INVITED LECTURE - Seigo Ito , University of Hyogo, Japan <i>Fabrication of cost-effective carbon-based multiporous-layered-electrode perovskite solar cells</i>	
09:50	10:15	20° INVITED LECTURE - Paola Vivo , Tampere University, Finland <i>Sustainable and air-stable pnictogen-based light harvesters for indoor photovoltaics</i>	
10:15	10:40	21° INVITED LECTURE - Hyunjung Shin , SKKU, South Korea <i>Highly oriented grains in alpha - formamidinium lead triiodide with non-centrosymmetric crystal structure</i>	
10:40	10:50	NEXUS PROJECT by Prof. Paul Fasl	
10:50	11:20	COFFEE BREAK	
Session Chair:		Stefan Glunz, Fraunhofer ISE, University of Freiburg, Germany	
11:20	11:45	22° INVITED LECTURE - Ute Cappel , Uppsala University, Sweden <i>Insights into perovskite properties from studies on single crystal surfaces</i>	
11:45	12:05	23° INVITED LECTURE - Atsushi Wakamiya , Kyoto University, Japan <i>Interlayer Materials for Efficient Perovskite Solar Cells</i>	
12:05	12:08	FUNANO (3 mins)	
12:08	13:33	LIGHT BUFFET LUNCH	

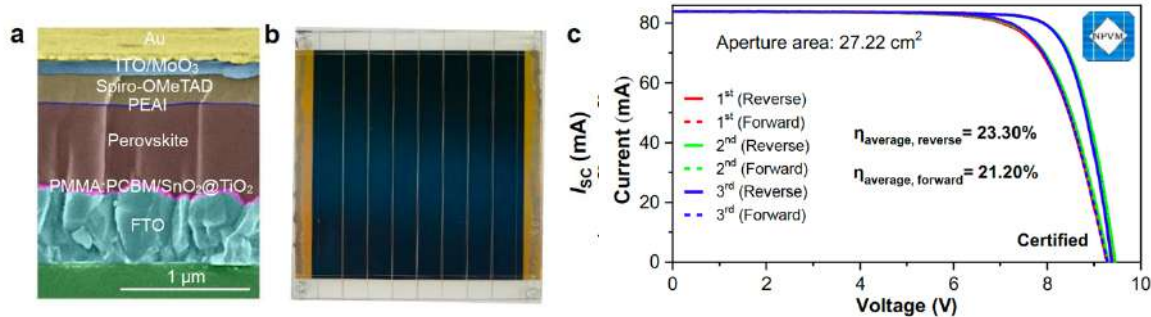


STABLE AND EFFICIENT PEROVSKITE SOLAR CELLS AND MODULES BY INTERFACE AND COMPOSITIONAL ENGINEERING

Mohammad Khaja Nazeeruddin,^{*2} Bin Ding, Yong Ding, Gao Xiaoxin, Yi Zhang, Jianxing Xia, Paul J. Dyson

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Organic/Inorganic metal halide Perovskite solar cells (PSCs) with efficiencies exceeding 26% have the potential to address energy and environmental concerns. However the lower efficiency, poor stability, and reproducibility issues of large-area PSCs compared to laboratory-scale PSCs are significant drawbacks that hinder their commercialisation. To address these challenges, we developed additives and interface engineering methods to enhance the efficiency and stability of PSCs. The resulting PSCs attained a power conversion efficiency (PCE) of 25.5% with long-term operational stability over 1000 hours. This approach enabled the fabrication of perovskite solar modules (PSMs) that achieved a certified efficiency of 23% over a 27.22 cm² aperture area, marking the highest certified PSM performance. Additionally, the PSMs displayed long-term operational stability, maintaining 94.66% of the initial efficiency after 1000 h under continuous one-sun illumination at room temperature. In this talk, we present recent progress in compositional and interface engineering approaches.



FABRICATION OF COST-EFFECTIVE CARBON-BASED MULTIPOROUS-LAYERED-ELECTRODE PEROVSKITE SOLAR CELLS

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Carbon-based multi-porous-layered-electrodes perovskite solar cells (MPLE-PSCs) have ability to be the commercialized photovoltaic panels. The porous carbon electrodes have special five functions as below,

- [1] high stability against halogen in perovskite crystal (Au and Ag can be damaged by the halogen)
- [2] high conductivity to be the back contact electrodes (the sheet resistance can be around 5 ohm/square)
- [3] strong hole-extraction ability (in place of organic hole-transporting material)
- [4] water absorption ability as activated carbon after annealing procedure at 400 °C
- [5] water blocking ability after making photovoltaic device with perovskite crystal

Using such porous carbon electrodes, MPLE-PSCs can be very stable. And, the points for the commercialization of MPLE-PSCs can be listed as,

- [1] high stability against high temperature and strong radiation against sun illumination
 - 1-1 Thermal stability at 100°C over 4500 h in dark (by Univ. of Hyogo, Japan).
 - 1-2 Damp-heat stability at 85°C-85%RH over 3,000 h in dark (by Univ. of Hyogo and Kishu Giken Kogyo, Japan).
 - 1-3 Light stability at 55°C over 10,000 h (by EPFL, Switzerland).
- [2] relatively photoenergy conversion efficiency for the utilization (11.5% as module)
- [3] cost-effective fabrication process by fully-printing method under ambient air (without glove box and dry room)
- [4] Recyclable device

In the conference, the fabrication technology and the challenging works of high thermal stability over 100°C will be presented.

SUSTAINABLE AND AIR-STABLE PNICTOGEN-BASED LIGHT HARVESTERS FOR INDOOR PHOTOVOLTAICS

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The need for energy autonomous Internet-of-Things (IoT) devices is rapidly growing, with billions of wireless sensors expected to be installed over the next decade. Indoor photovoltaics (IPVs) show promise for enabling seamless communication by harnessing the readily available indoor light in our buildings. Emerging solution-processed absorbers, such as lead halide perovskites (LHP), have recently demonstrated huge potential for efficient indoor light harvesting. However, the toxicity and bioavailability of lead are a showstopper for the potential widespread commercialization of LHP-based IPVs, given the close proximity of lead-containing devices to the end users in indoor scenarios.

Perovskite-inspired materials (PIMs), comprising Group VA pnictogen cations, such as antimony (III) (Sb^{3+}) and bismuth (III) (Bi^{3+}), have recently gained popularity as eco-friendly and air-stable absorbers.^[1] Among them, two-dimensional $\text{Cu}_2\text{AgBiI}_6$ (CABI)^[2] and $\text{A}_3\text{Sb}_2\text{X}_9$ ^[3] possess quasi-direct to direct bandgaps suitable for photovoltaic and other optoelectronic applications.^[1] Nevertheless, PIMs often crystallize in disordered structures with a large number of surface defects/vacancies and grain boundaries, which explains their modest performance as photovoltaic absorbers. Their nearly ideal bandgap for indoor light harvesting, exceptional air stability, and low toxicity motivated us to optimize their intrinsic defect tolerance by a thorough composition engineering at each of the crystallographic sites (A, B, X) of the PIM structure. This approach enabled a significant boost in the performance and operational stability of pnictogen-based devices for sustainable indoor light harvesting.

Acknowledgements: P.V. acknowledges the financial support of Jane and Aatos Erkko Foundation within the SOL-TECH project. P.V. also thanks Research Council of Finland, Decision No. 347772. This work was part of the Research Council of Finland Flagship Programme, Photonics Research, and Innovation (PREIN), Decision No. 320165.

[1] Grandhi, G.K. et al., *Adv. Funct. Mater.* **2024**, Early view, <https://doi.org/10.1002/adfm.202307441>.

[2] Samson, H.C. et al., *J. Am. Chem. Soc.* **2021**, *143*, 10, 3983.

[3] Lamminen, N. et al., *Adv. Energy Mater.* **2023**, *13*, 2203175.

HIGHLY ORIENTED GRAINS IN ALPHA – FORMAMIDIUM LEAD TRIIODIDE WITH NON-CENTROSYMMETRIC CRYSTAL STRUCTURE

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Formamidinium lead triiodide (FAPbI₃) is gaining much interest with an optimal band gap of ~ 1.5 eV. Although α -FAPbI₃ is the most thermodynamically stable photoactive phase, it can kinetically stabilize δ -FAPbI₃ in ambient. Many attempts were studied to stabilize the black α -phase, for example, pseudo-halide anion engineering, ionic liquid engineering, and incorporation of additives. Incorporating with methylammonium chloride (MACl) as an additive not only induces the stabilized α -FAPbI₃, but also affects the crystallization kinetics of α -FAPbI₃. Along with the role of methylammonium chloride (MACl) as a ‘stabilizer’ in the formation of α -FAPbI₃, we pointed out the additional role as a ‘controller’ in the crystallization kinetics.^[1] Herein, we examined the crystallization process of MACl, as higher concentration of MACl induces slower crystallization kinetics. Microscopic observations, such as electron back-scattered diffraction (EBSD), confocal photoluminescence (PL), time-resolved photoluminescence (TRPL) mapping, and conductive atomic force microscopy (C-AFM), were conducted to examine the optoelectronic properties of [001] preferentially oriented grains. Reduction in the non-radiative recombination, a longer lifetime of charge carriers and less photocurrent deviation between each grain induce higher short-circuit current density (J_{sc}) and fill factor (FF) in α -FAPbI₃ based perovskite solar cells (PSCs) with MACl 40 %. It highlights the importance of crystallization kinetics resulting in desirable microstructures for device engineering.

[1] Shin, S., Seo, S., Jeong, S., Sharbirin, A.S., Kim, J., Ahn, H., N.-G. Park, and **Shin, H.**, “Kinetic-Controlled Crystallization of α -FAPbI₃ Inducing Preferred Crystallographic Orientation Enhances Photovoltaic Performance”, *Advanced Science*, **2023**, 10, 2300798.

INSIGHTS INTO PEROVSKITE PROPERTIES FROM STUDIES ON SINGLE CRYSTAL SURFACES

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Solar cells have a great potential in replacing fossil fuels in electricity generation, if requirements of low production costs can be met. In the last years, lead halide perovskites have drastically changed the solar cell research field due to their ease of synthesis and high power conversion efficiencies, which now reach over 25%. The future success of these developments crucially depends on understanding the details charge separation, charge transport and charge recombination at the interfaces between the different layers in a solar cell as well as what parameters limit solar cell stability. X-ray based techniques such as photoelectron spectroscopy (PES) are powerful tools for obtaining electronic structure information of materials at an atomic level.

In this presentation, I will show how we have used photoelectron spectroscopy to gain insights into the fundamental surface properties of perovskites by investigating single crystals (Figure 1). Through in-vacuum cleaving it was possible to obtain clean crystalline perovskite surfaces.^[1] We have used resonance spectroscopy to map out the cation orbital contributions to the perovskite valence band in detail. Furthermore, we studied how the degradation of perovskite surfaces under heat and X-rays depends on the perovskite composition.^[2,3] Using in-situ evaporation, we investigated the interface formation with charge transport layers and metal contacts and determined the energy alignment between the layers.^[4] Finally, we investigated light induced charge movement in single crystals through time-resolved photovoltage measurements.

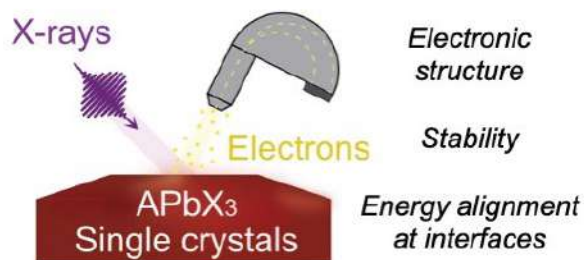


Figure 1: Schematic of investigating perovskite single crystals with photoelectron spectroscopy

[1] A. García-Fernández et al., *Small*, **2022**, 18, 2106450.

[2] B. Kammlander et al. *Chem. Comm.* **2022**, 58, 13523-13526.

[3] A. García-Fernández et al. *Phys. Chem. Chem. Phys.*, **2024**, 26, 1000

[4] A. García-Fernández et al. *Inorg. Chem.* **2023**, 62, 15412-15420.

INTERLAYER MATERIALS FOR EFFICIENT PEROVSKITE SOLAR CELLS

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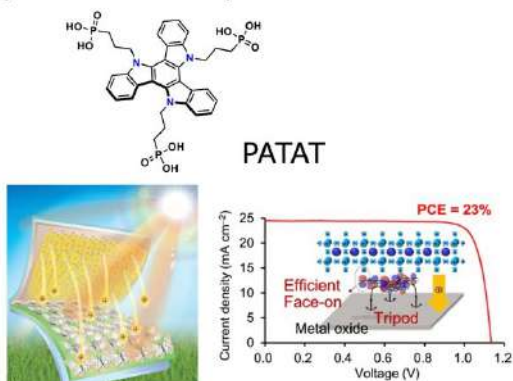
Perovskite solar cells attract attention as promising cost-effective next generation printable photovoltaics. The power conversion efficiencies (PCEs) have been substantially increased in a short period, based on the improvements of the fabrication protocols for the perovskite layer, and the development of new materials for passivation of the surface or efficient charge collection, etc. Our research approaches for perovskite solar cells are as follows.^[1-3]

1) Development of highly purified perovskite precursor materials:^[4,5] We synthesis a series of complexes of lead halides or tin halides as purified precursor for perovskite materials.

2) Development of fabrication methods for perovskite layer by solution process: Based on "dipole strategy", we designed the surface passivation organic materials.^[6-8] We develop the efficient fabrication methods of perovskite layer including top and bottom surface passivation based on the film formation mechanism.

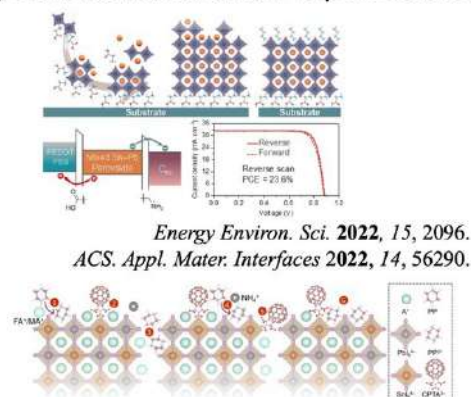
3) Development of organic semiconductors as efficient charge-collection materials from perovskite layer: We design and synthesis novel pi-conjugated materials, PATAT, in terms of control of the energy level of frontier orbitals, molecular orientation, and interface between perovskite layer.^[9]

a) PATAT: Monolayer HTM



J. Am. Chem. Soc. **2023**, *145*, 7528.

b) Surface Passivation: Dipole Strategy



Energy Environ. Sci. **2022**, *15*, 2096.

ACS Appl. Mater. Interfaces **2022**, *14*, 56290.

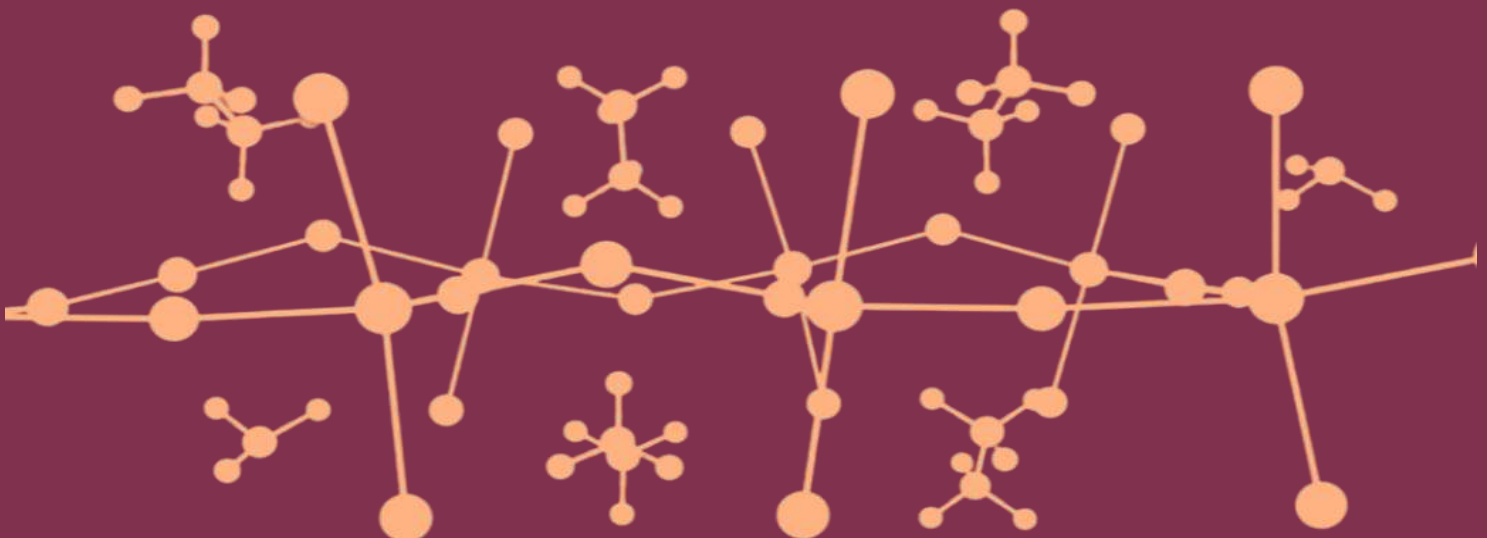
Adv. Mater. **2023**, *35*, 2208320.

Figure 1: Examples of our Interlayer Materials.

Acknowledgements: This work was partially supported by the JST-Mirai Program (JPMJMI22E2), NEDO (JPNP21016), the International Collaborative Research Program of ICR, Kyoto University, etc.

- [1] S. Hu, J. Thiesbrummel, J Pascual, M. Stolterfoht, A. Wakamiya, H. J. Snaith, *Chem. Rev.* **2024**, *in press*. (DOI: 10.1021/acs.chemrev.3c00667)
- [2] T. Nakamura, A. Wakamiya, et al. *Bull. Chem. Soc. Jpn.* **2024**, *97*, uoad025.
- [3] S. Hu, J. A. Smith, H. J. Snaith, A. Wakamiya, *Precis. Chem.* **2023**, *1*, 69.
- [4] A. Wakamiya, et al. *Chem. Lett.* **2014**, *43*, 711.
- [5] T. Nakamura, A. Wakamiya, et. al. *Nat. Commun.* **2020**, *11*, 3008.
- [6] S. Hu, A. Wakamiya, et al. *Energy Environ. Sci.* **2022**, *15*, 2096.
- [7] S. Hu, J. Pascual, A. Wakamiya, et al. *ACS Appl. Mater. Interfaces* **2022**, *14*, 56290.
- [8] S. Hu, A. Wakamiya, et al. *Adv. Mater.* **2023**, *35*, 2208320.
- [9] M. A. Truong, A. Wakamiya, et al, *J. Am. Chem. Soc.* **2023**, *145*, 7528.

	Session 1A Town Hall		Session 1B Trumpet	
Session Chair:	Paola Vivo , Tampere University, Finland		Mohammad Khaja Nazeeruddin , EPFL, Switzerland	
Session Title:	Advanced perovskite technologies		Low band gap PV	
13:33	13:45	Filippo Campana , University of Perugia, Italy <i>A comprehensive LCA study on the use of green solvents for the synthesis and processing of metal-halide perovskites</i>		Mitchell Rencheck , Electric Power Research Institute, United States <i>Managing Potential Environmental and Human Health Risks of Lead Halide Perovskite Photovoltaic Modules</i>
13:45	13:57	Camilla Bordoni , University of Bologna, Italy <i>Polymer micro-encapsulated perovskites for stable, flexible and thick radiation detectors</i>		Heon Jin , University of Oxford, United Kingdom <i>Highly efficient and stable thermal evaporated lead tin perovskites</i>
13:57	14:09	Luigi Angelo Castriotta , University of Rome Tor Vergata, Italy <i>Advancing flexible perovskite solar technology with benzamide-based molecules for greater mechanical robustness</i>		Krishanu Dey , University of Oxford, United Kingdom <i>Suppressed ion migration and compositional instabilities in mixed lead-tin halide perovskite materials and devices</i>
14:09	14:21	Min Kim , Jeonbuk National University, South Korea <i>Interfacial Crystallization of Low-Dimensional Perovskite Nanomaterials for Highly Efficient Photoelectric Devices</i>		Francesca De Rossi , CHOSE, University of Rome Tor Vergata, Italy <i>Thermosetting polyurethanes resins as primary encapsulants for flexible perovskite solar cells</i>
14:21	14:33	Wenya Song , imec, Belgium <i>Halide Perovskite Photodiode Integrated CMOS Image Sensor</i>		Isabella Poli , Istituto Italiano di Tecnologia, Italy <i>How composition affects material's properties in tin halide perovskites</i>
14:33	14:45	Anna Wąsiak-Maciejak , Saule Research Institute, Poland <i>Closing the gap: compositional and interfacial engineering for enhanced stability and performance of flexible wide bandgap devices</i>		Luca Gregori , University of Perugia, Italy <i>Reducing p-doping of tin-halide perovskites by trivalent cation doping</i>
14:45	14:57	Jin Wang , Nankai University, China <i>Conductive Passivating Contact for High Fill Factor Monolithic Perovskite/Silicon Tandem Solar Cells</i>		Giulia Folpini , CNR, Italy <i>Analysis of doping density and carrier phonon coupling in Tin-based perovskites using time resolved THz spectroscopy</i>



A COMPREHENSIVE LCA STUDY ON THE USE OF GREEN SOLVENTS FOR THE SYNTHESIS AND PROCESSING OF METAL-HALIDE PEROVSKITES

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Metal halide perovskites (MHP) in the last decades have increasingly represented a valuable active material for the development of photovoltaic devices to replace Si-based systems, which are characterised by high costs and complicated manufacturing processes. Despite the fact that several perovskites solar cells with outstanding efficiency ranging from 3.8 to 26% have been built up, most of them suffer from many drawbacks, such as the use of lead precursor and use of dangerous solvents and antisolvents for their manufacturing and processing.^[1] In fact, common diprotic solvents like *N,N*-dimethylformamide (DMF), *N*-methyl-2-pyrrolidone (NMP), or *N,N*-dimethylacetamide (DMAc) are well-known toxic and oil-derived media, deeply impacting on environmental and human health.^[2-3]

In this context, the use of alternative and greener solvents, such as those deriving from biomass valorization, constitutes a precious substitute.

Herein, we are going to report a comprehensive LCA analysis with the aim of assessing the differences in the environmental impact when a bio-based derived solvent is adopted instead of a non-renewable and toxic one (Fig. 1).

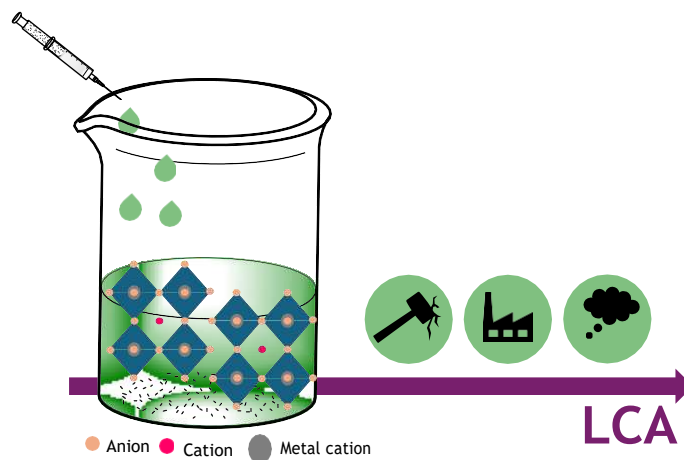


Figure 1: A Comprehensive LCA study on the use of green solvents for the synthesis and processing of metal-halide perovskites

[1] A. Srivastava, J. A. K. Satrughna, M. K. Tiwari, A. Kanwade, S. C. Yadav, K. Bala and P. M. Shirage, *Mater. Today Commun.*, **2023**, 35, 105686.

[2] F. Campana, L. Vaccaro et al.: *J. Mater. Chem. C*, **2020**, 8, 15027–15047; *ACS Sustain. Chem. Eng.*, **2020**, 8, 17154–17164; *ACS Sustain. Chem. Eng.*, **2022**, 10, 9123–9130.

[3] L. H. Chen, M. L. Meena, S. A. Lu, S. Som, C. W. Chu and C. H. Lu, *Org. Electron.*, **2024**, 129, 107037.

MANAGING POTENTIAL ENVIRONMENTAL AND HUMAN HEALTH RISKS OF LEAD HALIDE PEROVSKITE PHOTOVOLTAIC MODULES

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Perovskite solar modules (PSMs) are an emerging photovoltaic (PV) technology that can be manufactured at low costs while maintain power conversion efficiency parity with other PV technologies on the market. Currently, some PSMs utilize lead halide perovskite which contain lead ions that are more soluble in water than other available PV technologies. Depending on the concentration of lead and leaching behavior and if the module structure is compromised, there is potential for unique environmental and human health risks. Assessment of the potential lead leaching risk could be performed in conjunction with PSM development to mitigate risk during deployment, among other options. Therefore, prior to commercialization, it is important to understand, identify, and begin to address the associated environmental and human health risks.

This study puts the potential lead leaching risks associated with PSMs into perspective by assessing potential lead leaching risks for PSMs, through the lens of U.S. regulation and policy, and supports creation of a framework that can be applied across different PSM designs and assemblies. The U.S. regulations that pertain to environmental and human health risks associated with

lead leaching are identified and discussed. The identified regulations are leveraged to inform metrics for experimental testing of lead leaching, and characterization approaches are proposed to assess the potential risk of lead leaching during operational scenarios (fire, weather events, end of life management, etc.). Fig. 1 provides an example of potential methodology to assess the potential of lead leaching from a PSM fire scenario. Furthermore, strategies used for existing PV technologies are analyzed to understand ways that manufacturers have overcome environmental and human health risks, along with technological solutions specific to PSMs to mitigate leaching. The goal of this work is to create a framework to elucidate, propose, and assess potential methods and pathways for overcoming potential environmental and human health risks associated with potential lead leaching risks of PSMs.

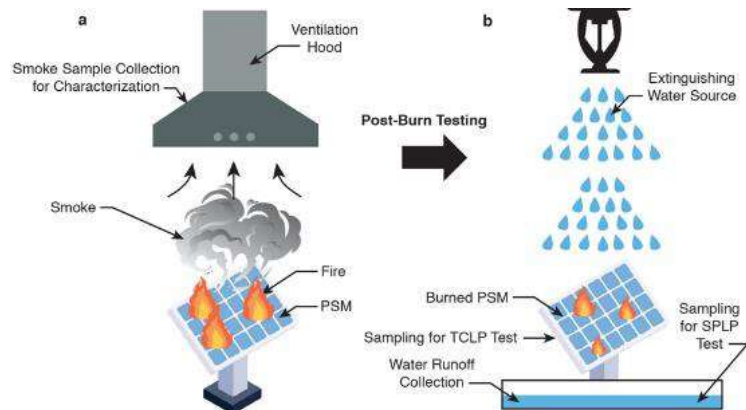


Fig 1. A schematic of (a) the potential burn testing experimental set-up and (b) subsequent methodology for assessing hazardous waste and contamination in rainwater runoff from simulated rainfall.

POLYMER MICRO-ENCAPSULATED PEROVSKITES FOR STABLE, FLEXIBLE AND THICK RADIATION DETECTORS

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The demand for low-cost, flexible, and lightweight X-ray detectors has grown extensively recently. Metal halide perovskites can meet all the demands of innovative X-ray detectors and have rapidly outperformed the sensitivity of standard radiation detectors^[1].

Here we present perovskite films fabricated by simple, low-cost, air-process, dry mechanochemical synthesis of CsPbBr₃ in a poly(butyl methacrylate) (PBMA) matrix^[2]. The precursors are pressed into free-standing thick disks up to several hundreds of micrometres, which can be laminated onto a substrate with patterned electrodes. The resulting photoconductors are investigated as detectors of ionizing radiation. By tuning the polymer content, it is possible to achieve an extremely stable direct radiation detection with good sensitivity. The devices are stable in air and they are radiation hard, making them suitable for ionizing radiation detection in real-life applications. The perovskite-polymer composites are further investigated in vertical devices. The vertical electrode geometry allows to attain more than double the sensitivity than that of a planar photoconductor, with the same thickness (100 µm) and at the comparable applied electric field. The sensitivity can be further improved increasing the active layer thickness up to 500 µm. When laminated onto PET plastic substrate, the devices show outstanding flexibility properties reaching a bending radius of 1 mm with unaltered radiation response for 100 µm thick device. Moreover, vertical geometry is suitable to implement a pixelated matrix for imaging.

To conclude, the synthesis of polymer micro-encapsulated perovskite pellets through simple, dry processes is promising for the development of flexible, stable, and highly sensitive radiation detectors with imaging capabilities.

[1] Dudipala K.R. et al, *Adv. Mater.* 2023, 2304523

[2] B. Huisman et al, *Adv. Funct. Mater.* 2023, 2308844

HIGHLY EFFICIENT AND STABLE THERMAL EVAPORATED LEAD-TIN PEROVSKITES

Heon Jin¹, Henry Snaith¹

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Multi-junction tandem solar cells, utilizing complementary bandgaps, offer the potential to surpass the detailed balance limit for single-junction perovskite solar cells (PSCs). Through the tunability of perovskite bandgaps and recent advancements in mixed lead-tin (Pb:Sn) narrow bandgap PSCs, it is now possible to create highly efficient multi-junction solar cells solely using perovskites, achieving certified PCEs of up to 26.4% in all-perovskite tandem solar cells.

However, there are two main challenges when using Pb:Sn perovskites. Firstly, methylammonium (MA) has been traditionally used in the most efficient Pb:Sn PSCs, but its thermal and chemical stability concerns prompt the search for MA-free alternatives with solution process. Second, conventional solution processing methods remain prevalent in lab-scale Pb:Sn PSCs fabrication. There were many attempts to thermal evaporate Pb:Sn as this method presents significant advantages, including high-quality thin film fabrication, precise thickness control, elimination of toxic solvents, large-scale compatibility, and reproducibility. Vacuum evaporation can also be applied to the fabrication of all-perovskite tandem solar cells without damaging underlying layers. Although vacuum deposition has proven successful in achieving high-efficiency and large-area PSCs for Pb-based perovskites, its application to Pb:Sn perovskites is less unexplored. Ball *et al.* and Igual-Munoz *et al.* are among the few to report Pb:Sn PSCs using vacuum evaporation.^[1-3]

In this work, we demonstrate that through careful control of the environment and some fine-tuning, it is possible to deposit Pb:Sn perovskite films of high quality through thermal evaporation. We compare devices made using this method to those made from similar state-of-the-art solution processed methods. Our work demonstrates that it is possible to approach the performance of solution processed devices within a workable processing window using vacuum evaporation. Our champion devices reach PCEs of 17%, surpassing previously set records of 14% for thermally coevaporated Pb:Sn devices. This was done without requiring additional passivation or bulk additive, which are used in the previous solution based reports.

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ADVANCING FLEXIBLE PEROVSKITE SOLAR TECHNOLOGY WITH BENZAMIDE-BASED MOLECULES FOR GREATER MECHANICAL ROBUSTNESS

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Flexible perovskite solar cells have garnered significant interest for their potential in lightweight, high-efficiency applications. However, issues like poor interfacial adhesion and significant deformation of flexible substrates at the perovskite-substrate interface have hindered their performance. By integrating entinostat into the hole transport material poly(bis(4-phenyl)(2,4,6-trimethylphenyl)amine), we have enhanced adhesion and decreased voids at this interface. These improvements have increased the power conversion efficiency of the flexible perovskite solar cells to 23.4% and raised the certified aperture efficiency of minimodules to 19.0%. Further developments in surface coverage and stability are being pursued with two new molecules, tucidinostat and domatinostat. Initial findings indicate that these additions may significantly enhance film crystallinity and uniformity, potentially redefining performance standards for the durability and efficiency of flexible perovskite solar cells. Our continued research seeks to refine the molecular engineering of perovskites to optimize photovoltaic efficiency for commercial application.

SUPPRESSED ION MIGRATION AND COMPOSITIONAL INSTABILITIES IN MIXED LEAD-TIN HALIDE PEROVSKITE MATERIALS AND DEVICES

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Despite the meteoric rise in the development of a variety of perovskite electronic and optoelectronic devices, the phenomenon of ion migration remains a common and longstanding Achilles' heel limiting their performance and operational stability. In this talk, I will share our research on understanding the ionic transport in methylammonium (MA)-free mixed Pb-Sn perovskites using field effect transistors (FETs) and solar cells as two different platforms.

Firstly, we demonstrate that mixed Pb-Sn based FETs do not suffer from ion migration effects as significantly as their pure-Pb counterparts, thereby reliably exhibiting hysteresis-free p-type transport with high mobility reaching 5.4 cm²/Vs, which is one of the highest reliably-reported long-range mobilities for 3D hybrid perovskite thin films [1]. The reduced ion migration is visualized through photoluminescence microscopy under bias and is manifested as an activated temperature dependence of the field-effect mobility with a low activation energy (~ 48 meV) consistent with the presence of the shallow defects present in these materials. In fact, to the best of our knowledge, such activated temperature dependence of FET mobility is also reported for the first time in the field of 3D halide perovskites. Next, we perform scan-rate dependent current-voltage (and hysteresis) measurements and temperature dependent impedance spectroscopy measurements on optimized MA-free Pb and Pb-Sn perovskite solar cells, which demonstrate the suppressed motion of ions in Pb-Sn devices as compared to their Pb-only analogues, thereby generalizing our earlier observations from FETs [2]. We also obtain mechanistic insights into these experimental observations by conducting first-principles calculations, which reveal the key role played by Sn vacancies in increasing the migration barrier for iodides due to severe local structural distortion in the lattice. Finally, we also show our preliminary results on the improved photostability of mixed-halide perovskite compositions with Pb-Sn alloying under a host of processing, atmospheric and excitation conditions, which will have significant implications for the development of future perovskite optoelectronic devices with extended stability [3].

All in all, our results emphasize the relatively unexplored bright prospects of tin substitution in Pb halide perovskite materials for (opto)electronic applications.

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INTERFACIAL CRYSTALLIZATION OF LOW-DIMENSIONAL PEROVSKITE NANOMATERIALS FOR HIGHLY EFFICIENT PHOTOELECTRIC DEVICES

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This study focuses on the interfacial crystallization of perovskite nanomaterials, a key process in the development of highly efficient photoelectric devices. By manipulating the crystallization behavior of low dimensional nanocrystals incorporated with functional small molecules at the air surface of perovskite layers, we have achieved significant enhancements in the photovoltaic performance and material stability of the resulting nanomaterials. The research presents a detailed understanding of the thermodynamically stable crystallization dynamics based on DFT calculations and its impact on the microstructural and photovoltaic efficiency of the perovskite nanomaterials. Our innovative approach leads to a marked improvement in the performance of photoelectric devices, addressing critical challenges in the field of renewable energy. This work not only offers new insights into the fundamental aspects of mixed dimensional perovskite crystallization but also paves the way for the next generation of high-efficiency optoelectronic devices.

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THERMOSETTING POLYURETHANES RESINS AS PRIMARY ENCAPSULANTS FOR FLEXIBLE PEROVSKITE SOLAR CELLS

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Flexible perovskite solar cells (f-PSCs) hold the promise to be game-changers for a wide range of applications (e.g. IoT, portable and wearable electronics, space), where flexibility, conformability, lightweight and high power-to-weight ratio are instrumental and sought-after.

Beside their remarkable efficiency, as high as 25% ^[1], f-PSCs present additional appealing features: f-PSC fabrication is based on abundant materials and low-cost manufacture via solution processes ^[2]; series-interconnected monolithic modules have been demonstrated on large area substrates, reaching up to 15.5% PCE on 100 cm² ^[3]. Yet, as for their counterparts on rigid glass, f-PSC long-term stability is still an open issue, depending on several factors, both intrinsic and extrinsic ^[4]. An effective encapsulation, able to ensure f-PSCs long-term stability providing protection from extrinsic agents, such as moisture, water, and oxygen, without compromising the overall flexibility of the device, is of extreme interest.

Thermosetting polyurethanes (PUs) arise as promising candidates: they are inert toward the perovskite layer, and their curing reaction can easily be performed at room temperature, directly on the f-PSC. Moreover, minimal modifications on the precursors' skeleton can tune flexibility, barrier properties, and transparency.

We present the successful implementation of a low-cost thermosetting PU resin as the encapsulant for 1 cm² f-PSCs ^[5]. Two encapsulation strategies are proposed: the PU is applied only on the back of the device (i.e., in contact with the metal electrode) or on both the back and the front, onto the PET substrate. Besides preserving the device flexibility, the double encapsulation strategy allows for very long stability under a highly damp atmosphere (RH > 75%), reaching T80 of over 550 hours (i.e., 23 days), clearly outperforming the unencapsulated control devices, whose T80 is 6 hours only.

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HALIDE PEROVSKITE PHOTODIODE INTEGRATED CMOS IMAGE SENSOR

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Many of the advantageous perovskite properties applied in solar cells are also relevant for photodiodes and imagers. High absorption coefficients and high carrier mobilities can, e.g., reduce pixel cross talk, making perovskites also a promising material class to increase responsivity and reduce response time. In this work, we developed a perovskite photodiode (PePD) stack through energy landscape optimization and defect passivation. Such PePDs present a leakage current below 5×10^{-7} A/cm² and an external quantum efficiency (EQE) close to 80%, leading to an at least 100 dB linear dynamic range between -2 V and -1 V. The PePD stack was then monolithically integrated on top of fully processed silicon read-out integrated circuits (Si-ROICs, 512×768 pixels) with 5- μ m pixel pitch (Figure 1a), one of the first-of-a-kind to the best of the authors' knowledge. High resolution color-images (Figure 1b,d) were taken using this PePD integrated CMOS image sensor, demonstrating an elevated technology readiness level of perovskite-based optoelectronics in image sensing. We close our presentation with an outlook on possible implementations of the perovskite performance advantages for future imaging applications.

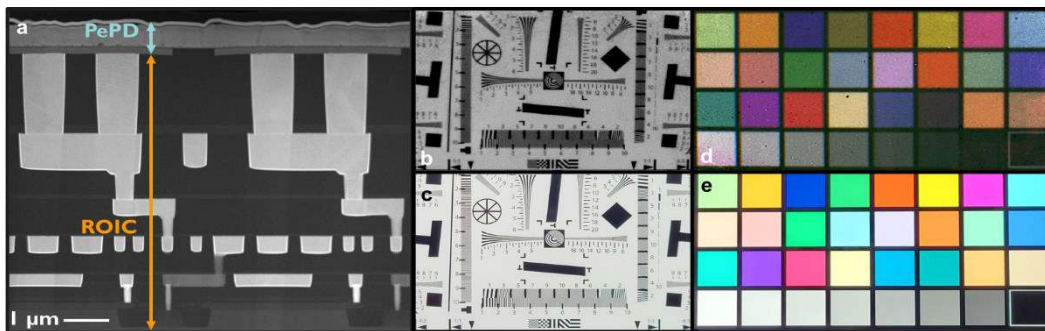


Figure 1: (a) A cross-sectional scanning transmission electron microscopy (STEM) image of the image sensor including the Si-ROIC and the PePD. An intensity image of resolution chart from (b) the PePD image sensor and (d) a smart phone. A color image of a color checker from (c) the PePD image sensor and (e) a smart phone.

Acknowledgements: Part of this work received financial support from the Fund for Scientific Research Flanders (FWO) under Project number S004322N (GigaPixel).

HOW COMPOSITION AFFECTS MATERIAL'S PROPERTIES IN TIN HALIDE PEROVSKITES

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Tin halide perovskites (chemical formula ASnX_3 , with A=methylammonium MA^+ , formamidinium FA^+ or cesium Cs^+ and X= iodide I) have gained much attention in various fields of research. Among these, the main explored application is thin film photovoltaics, thanks to the achievable ideal bandgap, ranging between 1.3 and 1.4 eV. However, despite the promise, their power conversion efficiency has not reached levels comparable to lead-based solar cells (>25%). Both the soft nature of tin-halide lattice and the facile oxidation of tin(II) to tin(IV) induce relatively low defect formation energies, implying a significant probability of defects formation and causing low power conversion efficiencies in devices.^[1] Tin halide perovskites are indeed characterized by a severe intrinsic p-doping which might be detrimental for photovoltaic applications, but highly favourable for diverse electronic devices, such as field-effect transistors and thermoelectrics.

While the optoelectronic properties of tin halide perovskites have been extensively studied, e.g. by looking at the photoluminescence efficiency and monitoring the dynamics of photogenerated carriers,^[2-4] charge transport properties have received less attention. In this study we explore the effect of A-site cations and X-halide anions on structure, morphology, electronic and photophysical properties of tin halide perovskites. Simply tuning the chemical composition, we are able to change the chemistry of defects and electronic properties of the material.^[5,6] These fundamental properties are highly relevant to optimize the semiconductor to achieve not only photovoltaic devices with high power conversion efficiencies but also to foster its development as an electronic material.

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CLOSING THE GAP: COMPOSITIONAL AND INTERFACIAL ENGINEERING FOR ENHANCED STABILITY AND PERFORMANCE OF FLEXIBLE WIDE BANDGAP DEVICES

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The capacity to manufacture perovskite solar cells (PSCs) on lightweight and flexible substrates through cost-effective solution-based processes, is a significant advantage, positioning perovskite as a superior alternative to conventional silicon photovoltaics^[1]. Moreover, widely tunable bandgap enables surpassing the Shockley-Queisser efficiency limit of a single-junction device by stacking together perovskites of different bandgaps^[2]. The combination of these properties opens up possibilities for fabricating large-area, flexible, all-perovskite tandems. Despite the enormous progress made in the efficiency enhancement of wide-bandgap perovskite solar cells, stability remains a substantial constraint^[2].

In this work, we developed a strategy of perovskite composition engineering, coupled with perovskite/hole transporting layer interface engineering, leading to significant enhancements in the light stability of flexible wide bandgap devices. Attributed to composition engineering, a notable decrease in ion migration has been attained, resulting in substantially reduced halide segregation and lowered defect formation under light exposure. Additionally, a novel self-assembling hole-transporting molecule with multiple anchoring groups will be presented. This planar molecule, based on carbazole moiety, provides a uniform coating and enhanced hole extraction, thereby further improving device performance and reliability. Unencapsulated wide-bandgap devices (1.76 eV), fabricated using the implemented methodology, retained 100% of initial performance after 2000 hours of continuous light exposure at 40°C in inert atmosphere. Importantly, significantly improved long-term stabilities at elevated temperatures were observed. We reached 90% and 85% of the initial performance after 1000 hours of light soaking at 70°C and 1000 hours in the Damp Heat test (85°C, 85% relative humidity), respectively. The champion flexible devices, with an active area of 1cm², yielded a power conversion efficiency exceeding 15% for the single-junction wide bandgap device, and 22.4% for the all-perovskite tandem.

This work provides an important insight into the development of large-area, flexible wide bandgap devices, as it highlights an area in the device where non-optimum operation occurs, providing important implications for the stability and performance, paving the way for the commercialization efforts of all-perovskite tandem technology.

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REDUCING P-DOPING OF TIN-HALIDE PEROVSKITES BY TRIVALENT CATION DOPING

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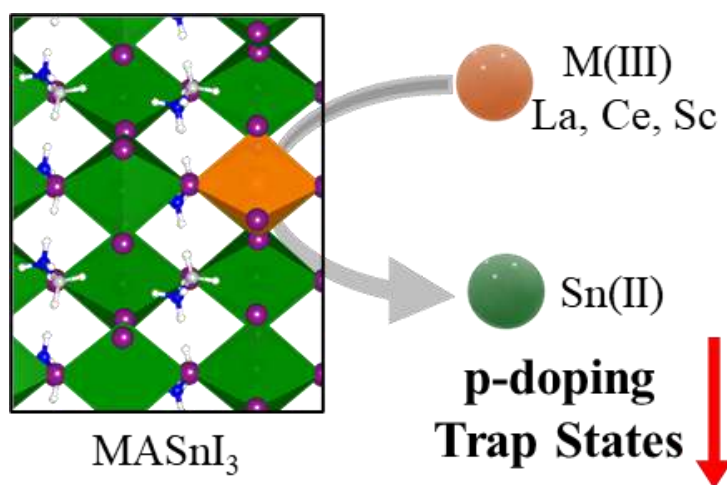
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We investigate trivalent doping of tin-halide perovskites as a means to decrease p-doping and controlling defect activity. Through density functional theory calculations and experimental characterization, we demonstrate that doping with scandium, lanthanum and cerium successfully accomplishes Fermi level upshift, reducing background carrier concentration and defect densities, thereby improving material performance. Solar cells fabrication and testing highlights the efficacy of doping, with scandium delivering increase photocurrent and open circuit voltage compared to control devices, despite being non optimized. This research underscores the potential of cation doping in enhancing the functionality of p-doped tin perovskites for advanced optoelectronic applications.



CONDUCTIVE PASSIVATING CONTACT FOR HIGH FILL FACTOR MONOLITHIC PEROVSKITE/SILICON TANDEM SOLAR CELLS

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Undesirable defects on the surface of wide bandgap perovskite films and inherent interface problems limit the further development of perovskite/silicon tandem solar cells (PK/Si TSCs). Herein, zwitterionic molecules of bis(2-hydroxyethyl)dimethylammonium chloride (BDAC) is introduced on the perovskite surface (Fig. 1a), which promotes the growth along with (111) facets with better moisture resistance (Fig. 1b), passivates positive and negative local defects, inhibits the formation of Pb⁰ (Fig. 1c, d), and transforms the perovskite surface into a more n-type conductive contact layer that facilitated charge separation (Fig. 1e-i). These combined enhancements enable a PCE of 21.4% with an enhanced V_{OC} of 80 mV and an FF of 82.84% for the inverted single-junction device prepared by the two-step method (Fig. 1j), and the PCE of PK/Si TSC increased from 26.71% to 28.67% with excellent operational stability (Fig. 1l). Moreover, the scaling-up device with an active area of 11.879 cm² delivers a PCE of 24.46%, and a mini-module consisting of 9 large-area PK/Si TSCs is designed and fabricated with a power conversion power of more than 2W (Fig. 1m, n).

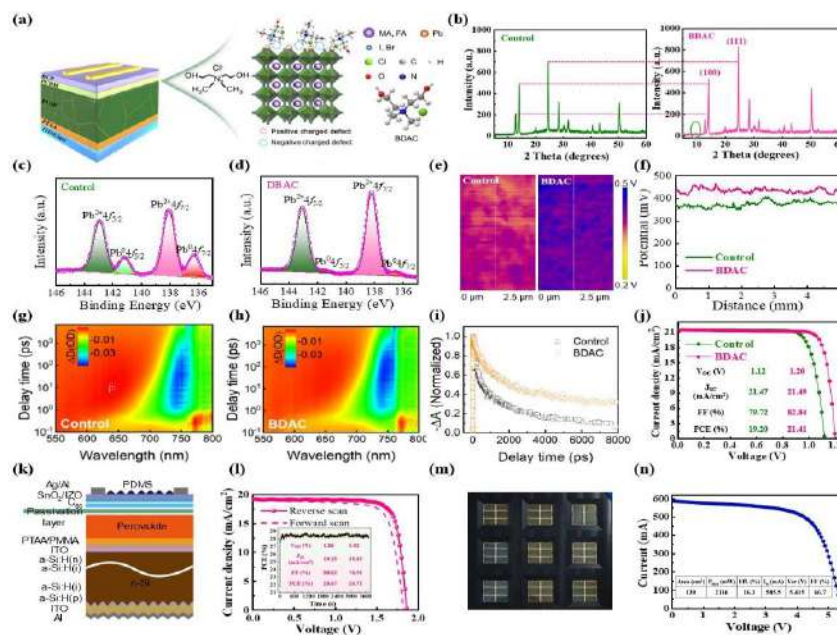


Figure 1 (a) Schematic diagram of device structure and interaction mechanism between BDAC and perovskite. (b) XRD patterns of control and BDAC-treated perovskite. (c) Pb 4f core-level spectra for (c) control and (d) BDAC-treated perovskite films. Kelvin Probe Force Microscope of (e) control and (f) BDAC-treated films. Transient absorption spectrum images of (g) control and (h) BDAC-treated films. (i) Exciton decay dynamics of Control and BDAC films. (j) J–V curves of the champion control and target single junction devices. (k) Device architecture of the monolithic PK/Si TSCs. (l) J–V curves of the champion PK/Si TSC with an aperture area of 0.5003 cm², the inset shows the performance parameters and steady-state power outputs. (m) Photograph of mini-module of PK/Si TSCs. (n) J–V curves of mini-module of PK/Si TSCs, the inset shows the performance parameters.

Analysis of doping density and carrier phonon coupling in Tin-based perovskites using time resolved THz spectroscopy

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Tin-based halide perovskites (THPs) have emerged as promising candidates for both photovoltaics and near - IR light emitting applications thanks to their high carrier mobilities low band gap, ideal for pairing with silicon in tandem solar cells^[1,2]. A key characteristic of THPs is the remarkable stability of acceptor defects such as Sn vacancies and I interstitials, resulting in a large population of self – doping holes that can negatively impact device performance if not adequately managed. As such, it is of critical importance to devise strategies to both quantify and control the dopant hole densities in THPs by compensating the oxidation state of Sn during material fabrication using additives such as SnF₂.

In this context, terahertz (THz) spectroscopy represents a powerful tool to characterize the carrier populations and dynamics in THPs. THz radiation is sensitive to mobile charge carriers^[3], as well as their coupling with lattice phonons^[4]: this can shed light on charge transport properties in THPs, as low frequency phonons in the THz range have been shown to limit their thermal and electrical conductivity. However, as the doping density affects both transparency to THz radiation and carrier phonon coupling, THz absorption spectroscopies can be used as a sensitive, contactless probe to characterize the self – doping density even in samples where it has been brought down to levels comparable to background carrier densities suitable for device applications (e.g. 10¹⁵ cm⁻³), and that could be challenging to characterize by traditional Hall effect measurements. Furthermore, time resolved THz spectroscopy after optical excitation of the material allows to follow the dynamics of photogenerated carriers with ps temporal resolution.

In this work, we study FACsSnI₃ thin films with both high and low doping concentrations with time resolved THz spectroscopy, and develop a robust technique to study doping hole density by fitting the THz conductivity with a Drude – Smith model. By supporting our results with DFT calculations, we also investigate the effect of doping concentration and defect states on optical phonon frequencies and their coupling to charge carriers.

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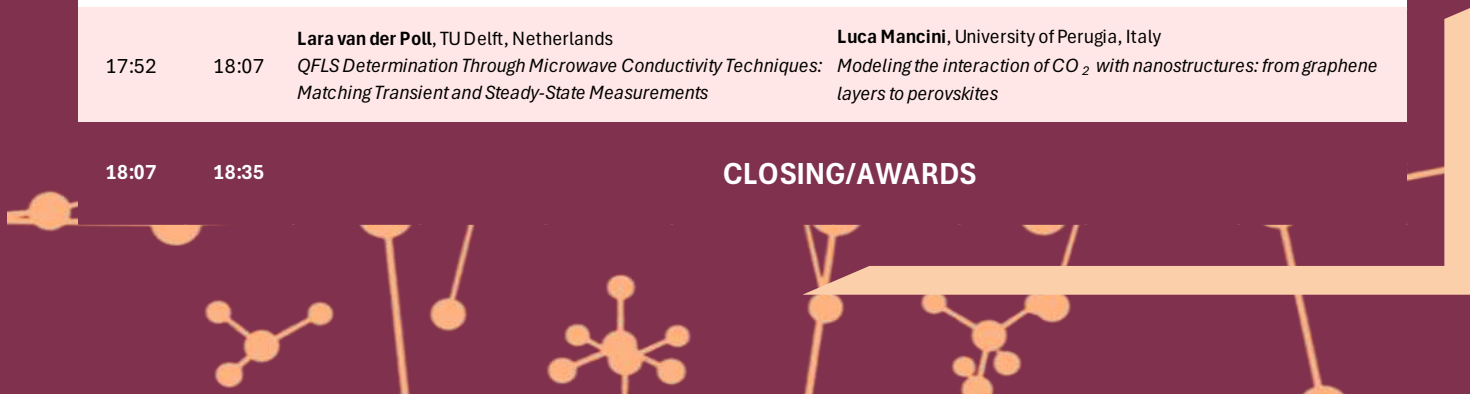
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14:57		15:05		COMFORT BREAK			
		Session 2A Town Hall		Session 2B Trumpet			
Session Chair:		Edoardo Mosconi, CNR-SCITEC Perugia, Italy		Maria Antonietta Loi, University of Groningen, Netherlands			
Session Title:		Computational insight into perovskites		AI for perovskite thin-film			
15:05	15:17	Daniele Meggiolaro , CNR-SCITEC Perugia, Italy <i>On the route towards efficient tin-halide perovskite solar cells: a theoretical perspective</i>		Esther Hung , University of Oxford, United Kingdom <i>A novel halobismuthate perovskite derivative with excellent piezoelectricity</i>			
15:17	15:29	Mostafa Othman , EPFL, Switzerland <i>Suppression of Stacking Faults for Stable Formamidinium-Rich Perovskite Absorbers</i>		Ulrich Paetzold , Karlsruhe Institute of Technology, Germany <i>Augmenting in situ monitoring of perovskite thin-film formation using deep learning</i>			
15:29	15:41	Xin Wu , City University of Hong Kong, Hong Kong <i>Theoretically guided material design, interface engineering and device optimization for efficient and stable perovskite/organic tandem solar cells</i>		Justus Just , MAX IV Laboratory, Lund University, Sweden <i>Integrating Robotic High-Throughput Processing with Synchrotron Based InSitu Multimodal Analysis—Homogenous Crystallization of Mixed Br-I Perovskites</i>			
15:41	15:53	Tommaso Moretti , University of Perugia, Italy <i>Harnessing halogen bonding in tuning optoelectronics properties of low-dimensional perovskites</i>		Valentina Larini , University of Pavia, Italy <i>Recycling and reuse of critical components of perovskite solar cells: from device efficiency to life cycle assessment</i>			
15:53	16:05	Claudio Quarti , Materials Research Institute, University of Mons, Belgium <i>Atomistic simulations of mixed halide perovskites: is compositional disorder detrimental?</i>		Salvatore Valastro , CNR-IMM, Italy <i>Improved radicchio seedlings growth under CsPbI3 perovskite rooftop in a laboratory- scale greenhouse for agrivoltaics application</i>			
16:05	16:17	Federico Brivio , University of Perugia, Italy <i>NMR crystallography of 2D hybrid perovskites</i>		Tom Aernouts , imec, Belgium <i>Long-term perovskite module outdoor performance in different outdoor regions</i>			
16:17		16:52		COFFEE BREAK			
		Session 3A Town Hall		Session 3B Trumpet			
Session Chair:		Filippo De Angelis, University of Perugia, Italy		Daniele Meggiolaro, CNR-SCITEC, Italy			
Session Title:		Exploring PVK dynamics and innovation		Perovskite photonics and device engineering			
16:52	17:07	Vanira Trifiletti , University of Milano - Bicocca, Italy <i>Doping in quasi-zero dimensional halide perovskite</i>		Thomas William Gries , Helmholtz-Zentrum Berlin, Germany <i>Lumos Maxima: Unveiling the Mysteries of Photoluminescence Quenching</i>			
17:07	17:22	Lauren Tidmarsh , University of Surrey, United Kingdom <i>Influence of heavy ions on perovskite photovoltaics operating in space</i>		Giacomo Giorgi , University of Perugia, Italy <i>Optoelectronic features of 2d and quasi-2d halide perovskites</i>			
17:22	17:37	E Laine Wong , Istituto Italiano di Tecnologia, Italy <i>Understanding the role of PbI2 and Pb in the photoemission studies of polycrystalline perovskite thin films</i>		Sergey Tsarev , Ethz, Switzerland <i>Monolithic multiband triple junction perovskite photodetectors for color filter-free imaging</i>			
17:37	17:52	Gebhard Matt , ETH Zurich, Kovalenko Lab, Switzerland <i>Time-Domain Signal Balancing LiDAR with Centimeter Resolution Based on Metal-Halide Perovskite</i>		Davide Regaldo , Istituto Italiano di Tecnologia, Italy <i>A Lateral Heterojunction Device as a Tool to Study Perovskite-Based Solar cells</i>			
17:52	18:07	Lara van der Poll , TU Delft, Netherlands <i>QFLS Determination Through Microwave Conductivity Techniques: Matching Transient and Steady-State Measurements</i>		Luca Mancini , University of Perugia, Italy <i>Modeling the interaction of CO₂ with nanostructures: from graphene layers to perovskites</i>			

18:07 18:35

CLOSING/AWARDS



ON THE ROUTE TOWARDS EFFICIENT TIN-HALIDE PEROVSKITE SOLAR CELLS: A THEORETICAL PERSPECTIVE

D. Meggiolaro¹

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Metal halide perovskites (MHP) are outstanding materials for photovoltaics due to their excellent optoelectronic properties, such as direct band gaps, large absorption cross sections and long lifetimes and diffusion paths of the photo-generated charge carriers.^[1] So far lead-based perovskites dominated the field by providing efficiencies of 26% in solar cell devices. In parallel, an increasing interest is arising in the development of tin-based perovskites (THP) to replace toxic lead and possibly rivaling the efficiencies of lead-based perovskites. The efficiency of THPs, however, is seriously limited by the native p-doping and the easy oxidation of tin(II) to tin(IV), compromising both the efficiency and the long-term stability of the material.^[2] Understanding the fundamental photo-physics and the defect chemistry of this class of materials is essential for guiding experiments through an advancement in the field.

In this presentation we provide a theoretical account of the charge carrier photo-physics and the defect chemistry of THPs. In the first part the main aspects of the defect chemistry of THPs will be discussed to show the origin of the heavy p-doping of these materials, but also the existence of non-radiative recombination channels.^[3] The role of defects in promoting intrinsic degradation paths will also be discussed. Hence, the discussion will focus on the analysis of the electron-phonon coupling and the hole polaron in this class of materials.

In the second part of the presentation effective strategies to mitigate the negative effects of p-doping will be analyzed. Discussion will be focussed on understanding the role of additives, such as SnF₂,^[4] and the chemical composition of the perovskite on the internal defects equilibria. The alloying of the halide site as well as the doping with trivalent metals will be analyzed by a computational perspective as potential strategies to reduce the p-doping of THPs.^[5]

Acknowledgements: D.M. acknowledges the European Union's Horizon Europe research and innovation program under grant agreement no. 101082176 – VALHALLA.

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A NOVEL HALOBISMUTHATE PEROVSKITE DERIVATIVE WITH EXCELLENT PIEZOELECTRICITY

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Ferroelectricity is the phenomena of spontaneous electric polarization $P \neq 0$ which is reversible under an external electric field. All ferroelectric materials also exhibit piezoelectricity; strain-induced electric polarization or conversely, electric-field-induced strain. . Molecular ferro- and piezo-electric materials have recently attracted interest over traditional piezo-ceramics due to simpler processing methods, their lightweight nature and mechanical flexibility. Here we develop a novel, lead-free organic-inorganic halobismuthate, TIBI. We study the structural origins of its ferroelectric nature using VT scXRD and ssNMR and demonstrate ferroelectricity and record-breaking piezoelectricity for a halobismuthate.

SUPPRESSION OF STACKING FAULTS FOR STABLE FORMAMADINIUM-RICH PEROVSKITE ABSORBERS

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The poor intrinsic perovskite absorber stability is arguably a central limitation challenging the prospect of commercialization for photovoltaic (PV) applications^[1–3]. Understanding the nanoscopic structural features that trigger instabilities in perovskite materials is essential to mitigate device degradation. Using nanostructure characterization techniques, we observe the local degradation to be initiated by material loss manifested in stacking faults pathways, forming inherently in the (011)-faceted perovskite domains in different popular formamidinium-lead triiodide-rich perovskite compositions. We introduce —an asymmetric sulphur (S)—containing additive (the obtained material is named hereafter as target) into the Cs_{0.17}FA_{0.83}PbI₃ perovskite precursor which manipulates the perovskite crystal growth and results in majorly oriented in-and out-of-plane (001) perovskite domains. Combining in-depth experimental analysis and density functional theory calculations, we find that the additive lowers the perovskite formation energy at room temperature, leading to a direct crystallization of the perovskite phase without the need for an antisolvent quenching step. This facilitates the fabrication of high-quality large area 5 cm by 5 cm blade-coated perovskite films and devices. Encapsulated target devices, with an active area of 0.2 cm², retained > 93 % of their initial power conversion efficiency (PCE) for > 2100 hours at room temperature, and additionally, 1 cm² active area target devices maintained T_{80} (the duration for the PCE to decay to 80 % of the initial value) for > 500 hours at 65 °C, all under continuous 1-sun illumination at the maximum power point tracking in ambient conditions. Our demonstration of scalable and stable perovskite solar cells represents a promising step towards achieving a reliable perovskite PV technology.

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2. Jiang, Q. *et al.* Towards linking lab and field lifetimes of perovskite solar cells. *Nature* **623**, 313–318 (2023).
3. Macpherson, S. *et al.* Local nanoscale phase impurities are degradation sites in halide perovskites. *Nature* **607**, 294–300 (2022).

AUGMENTING IN SITU MONITORING OF PEROVSKITE THIN-FILM FORMATION USING DEEP LEARNING

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To enable large-scale production of commercial perovskite solar cells (PSCs), fabrication processes must be transferred from small-area laboratory devices to large areas while ensuring consistent thin film quality across device areas and batches. Due to the complex formation of perovskite thin films from precursor solution, sophisticated *in situ* metrology is required for monitoring, optimizing, understanding, and controlling the entangled phases of drying, nucleation, and crystal growth. Applying *in situ* photoluminescence imaging allows recording the perovskite thin-film formation while providing spatial and spectral resolution.^[1] Exploring this *in situ* data reveals important information from the formation process, but the limits of human analysis are exceeded due to the data's complexity. However, deep learning (DL) methods are promising tools to investigate such complex, multi-dimensional data. DL-augmented characterization leverages the power of machine learning to monitor, predict, understand, and ultimately control the formation of perovskite thin films by exploiting the capability of these techniques to reveal correlations between *in situ* monitoring data and solar cell performance metrics.

Accordingly, we apply DL to predict the final power conversion efficiency (PCE) before the thin films are finalized into functional PSCs providing early insight into the perovskite thin film quality.^[2] Next to predicting device level performance, the DL-augmented *in situ* method detects perovskite material inconsistencies by differentiating between small variations in precursor molarity and molar ratio. To make the correlations between *in situ* data and the corresponding PCEs humanly understandable, we employ explainable artificial intelligence (XAI).^[3] XAI explains which data features are important to predict PSC performance and provides a data-driven explanation of why they are important. Additionally, we translate these insights into actionable recommendations for optimizing perovskite thin-film fabrication. Remarkably, these insights are generated by analyzing the given dataset without performing additional laborious experiments.

Finally, by combining *in situ* forecasting of various quenching scenarios with PCE prediction, *in situ* recommendations are generated using DL to inform whether vacuum quenching should be terminated or whether it is beneficial to continue to quench. These DL-based recommendations enable the implementation of active control of the perovskite material formation process.

Overall, our research demonstrates that DL and XAI are crucial for enhancing perovskite research allowing more detailed analyses of information-rich experimental characterization data, revealing valuable insights that would be difficult to identify without DL-augmented metrology.

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THEORETICALLY GUIDED MATERIAL DESIGN, INTERFACE ENGINEERING AND DEVICE OPTIMIZATION FOR EFFICIENT AND STABLE PEROVSKITE/ORGANIC TANDEM SOLAR CELLS

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The advent of solution-processed metal halide perovskite and organic semiconductors, and their subsequent integration into solar cells, holds the potential to revolutionize photovoltaic technology. While perovskite solar cells (PVSCs) and single-junction organic solar cells (OSCs) have achieved impressive power conversion efficiencies of over 26% and 19% respectively, their maximum efficiency is inherently limited to around 30% according to the Shockley-Queisser model., the fabrication of perovskite/organic tandem solar cells (POTSCs) with multiple light absorbers of significantly varied bandgaps is a promising alternative to overcome this limitation, potentially boosting solar cell efficiency to over 40%. However, their efficiencies are currently limited to around ~25% due to challenges related to theoretical study, material innovation, and device optimization of the sub cells and interconnecting layers (ICLs), highlighting the need for further development.

To address this issue, we have developed a theory-guided approach to materials design, interface engineering and device fabrication, realizing remarkable photovoltaic performance. We have developed a theory-guided method to design a mixed-cation surface passivation system, CE, to simultaneously all types of defects in wide-bandgap (WBG) perovskites, effectively suppressing the non-radiative recombination and realizing a record open-circuit voltage (V_{oc} , 1.35 V) and a high fill factor (FF) of 83.29% of 1.84-eV PVSCs. These improvements lead to a remarkable PCE of 24.47% when applied to fabricated POTSCs.^[1] Furthermore, we developed a quaternary organic bulk-heterojunction (BHJ) blend composed of two donor materials, PM6 and D18, and two acceptor materials, Y6 and L8-BO, to enhance the charge extraction capabilities of electrons and holes in organic sub cell, contributing to increased FFs of over 78%. In addition, a self-assembly monolayer, 2PACz, was incorporated into the ICL to reduce the energy barrier and manage the charge collection from organic BHJ to the recombination layer. Combining this with carefully tuning of the thickness of ICLs under the guidance of optical modelling to suppress parasitic absorption, POTSCs with a record PCE of 25.52% (certified 24.65%) with outstanding stability and an unprecedented FF of 83.47% was realized. Our findings prove the potential of POTSCs to rival the energy-lifetime yield of other solution-processed perovskite-based TSCs via comprehensive theoretical study, novel material innovation, and careful device optimization.

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INTEGRATING ROBOTIC HIGH-THROUGHPUT PROCESSING WITH SYNCHROTRON BASED IN-SITU MULTIMODAL ANALYSIS —HOMOGENOUS CRYSTALLIZATION OF MIXED BR-I PEROVSKITES

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Optoelectronic material properties and especially conversion efficiencies of next-generation semiconductors are a result of the complex interplay between precursors, intermediates, spectators and products during synthesis processes. Therefore, the discovery of optimized synthesis processes has become an important part in material discovery approaches. A knowledge based discovery and tuning of synthesis processes requires a fundamental understanding of its systematics, pathways and kinetics. Due to the complexity of synthesis interactions, a multitude of experiments with a wide variation of parameters, investigated from complementary perspectives, is required.

To this extend we developed a platform (in-FORM), which integrates robotic high-throughput solution processing with synchrotron based in-situ multimodal process analysis. It is based on a small-footprint, robotic, roll-to-roll slot-die coating system, which is fully integrated into a hard X-ray beamline for real-time in-situ process analysis at the MAX IV synchrotron. We measure simultaneously and at the same spot from the same incident X-ray beam a combination of X-ray spectroscopy (X-ray absorption and fluorescence), X-ray diffraction (XRD) and X-ray excited optical luminescence (XEOL).

This allows for a complementary investigation of the local structure, crystalline phase, chemical composition, oxidation states, and optoelectronic properties, unraveling formation and evolution processes during and after slot-die ink deposition.

Aiming to optimize the synthesis of mixed bromide-iodide metal-halide perovskites for a wide range of resulting absorber band-gaps while achieving high opto-electronic material quality, we utilized our in-situ platform. We investigated the full formation process, from precursor solutions to final films, under a wide range of synthesis parameters using a combinatorial approach. Our results show how the choice of solvents and co-solvents determines Br/I intermixing and segregation during the synthesis process. Measurements with high-temporal resolution (10ms) during rapid gas quenching reveal how rapid quenching processes can be utilized to achieve homogenous Br/I distributions. By enabling a fundamental understanding of the complex interplay between solvents and intermediates, we pave the way towards the development of greener solvent processes and environmental friendly up-scaling.

HARNESSING HALOGEN BONDING IN TUNING OPTOELECTRONICS PROPERTIES OF LOW-DIMENSIONAL PEROVSKITES

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Two-dimensional (2D) perovskites have attracted significant attention due to their potential applications in optoelectronics and photovoltaics. However, the stability of these materials is a major concern, as they are susceptible to degradation in the presence of moisture and air.

We investigate how halogen bonding between cations and inorganic layers affects the stability and the performance of 2D hybrid perovskites (2DHP). Density functional theory calculations have been carried out to study the energetics and the electronic structure of these materials.

The main target is the identification of an organic cation showing the HOMO and LUMO energy levels aligned to the valence band (VB) and conduction band (CB) edge of the inorganic states and, at the same time, showing a geometry and steric hindrance suitable to be adapted in the 2DHP inorganic network. An additional target will be the effect of the halogen bond interaction on the structure of the final 2DHP. The introduction of aromatic rings, conjugated multiple bonds or electron donor/acceptor substituents can allow a fine tuning of the frontier orbital energy levels in the cations, promoting their proper alignment with the VB or CB edges.

The data obtained will contribute to a better understanding of the influence of cations on the perovskites structure, optimizing the stability and the charge transport of the material.

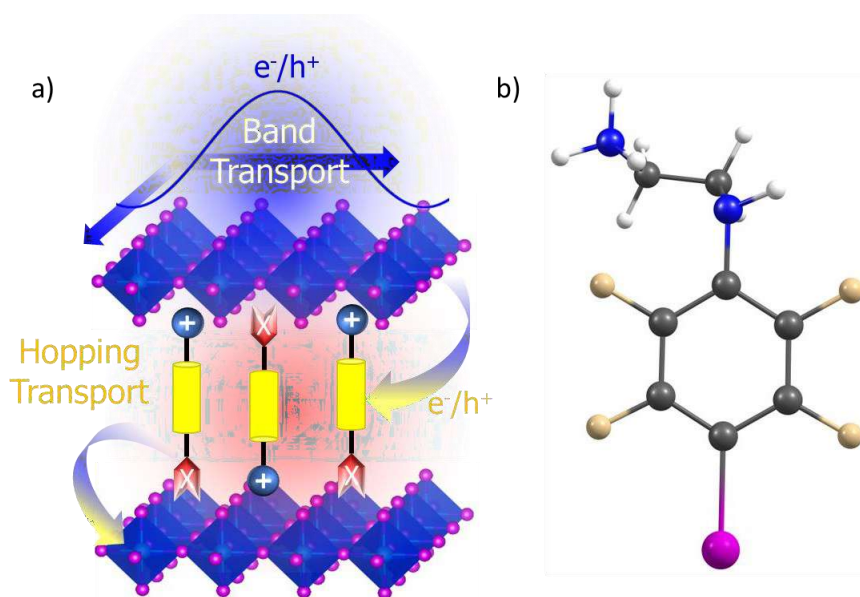


Figure: a) Crystal structure of a generic 2D Perovskite with X-donor cations separating the inorganic layer
b) One of the one of the engineered cations

RECYCLING AND REUSE OF CRITICAL COMPONENTS OF PEROVSKITE SOLAR CELLS: FROM DEVICE EFFICIENCY TO LIFE CYCLE ASSESSMENT

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If Earth's economical systems continue to rely on linearity, by 2060 we will need at least two planets to meet the current materials demand.^[1] This renders the circular design of new technologies a crucial strategy to achieve sustainable production and consumption, as required by the 12th Sustainable Development Goal of the Agenda 2030.^[2]

Within the photovoltaic (PV) field, perovskite solar cells (PSCs) have become promising alternatives to more energy-demanding, mainstream technologies. Although PSCs are not commercial products yet, their market size is forecasted to steadily grow in the next years.^[3] Moreover, since up to 80% of products' environmental impacts are determined at the design phase, foreseeing an end-of-life strategy for PSCs is likewise fundamental.^[4]

In this work we demonstrated the recovery of several critical components of PSCs, such as the environmentally impacting tin oxide (SnO₂)-coated indium tin oxide (ITO) substrates, the toxic lead iodide (PbI₂) and the expensive N²,N²,N²,N²,N⁷,N⁷,N⁷,N⁷-octakis(4-methoxyphenyl)-9,9'-spirobi[9H-fluorene]-2,2',7,7'-tetramine (Spiro-OMeTAD), by employing green and safe solvents (deionized water, ethanol and ethyl acetate). To test the efficacy of our method, we fabricated PSCs employing all recovered materials. Recovered devices maintained 98.4% of the PCE displayed by fresh devices. Moreover, we tested the wider applicability of our recovery protocol by performing multiple recovery iterations. In order to further insert the protocol into a circular perspective, we purified the solvents used for materials recovery by distillation, achieving the removal of 97.4%, 99.8% and 100% of contaminants from deionized water, ethanol and ethyl acetate, respectively. Finally, we performed a life-cycle assessment (LCA) analysis, comparing Si PV and PSCs landfill end-of-life strategy with our PSCs recovery end-of-life strategy. We found that recovered devices outperform landfilled PSCs and Si PV in all considered midpoint impact categories. Moreover, by performing multiple recovery iterations, global warming potential, abiotic depletion potential and cumulative energy demand indicators are progressively reduced, ultimately demonstrating the benefits of our recovery method.

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ATOMISTIC SIMULATIONS OF MIXED HALIDE PEROVSKITES: IS COMPOSITIONAL DISORDER DETRIMENTAL?

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By combining impressive electronic properties together with wide compositional “tailorability”, solution-processed halide perovskites are emerging as ideal candidates for opto-electronics.^[1] The possibility of tuning their chemical compositions via halide mixing, in particular, paves the way for band gap modulation within the full visible spectrum,^[2] which is a key requirement for the development of color-tunable LEDs,^[3] and wide band gap components in silicon-based PV cells.^[4] On the other hand, such compositional inhomogeneity represents an intrinsic source of disorder in these semiconductors, hence leading to the fundamental question “*whether such disorder may negatively influence the intrinsic electronic properties of halide perovskites, and to which extent?*” This question was early investigated via optical spectroscopy, namely using Urbach tail and photoluminescence linewidth analyses.^[5] Still, complex phenomena as light-triggered ion diffusion and formation of halide segregated domains hinders the rationalization of the experimental findings, hence calling for complementary theoretical simulations.

We hence performed parameter-free, periodic Density Functional Theory (DFT) simulations of mixed halide perovskite atomistic models. Cutting edge hybrid DFT calculations including spin-orbit-coupling point out that halide substitution does not lead to formation of intragap trap states, both in the dilute limit and in the case of homogeneously distributed iodine/bromine ions. Only in the case of halide segregation, the valence band maximum localizes in the iodine-rich domain, the bromine-rich domain acting as a barrier to hole diffusion.^[6] We also included thermal-driven vibrational motion, resorting to DFT-based molecular dynamics simulations.^[7] This allows to grasp the influence on the electronic properties due to “static” compositional disorder from iodine/bromine mixing and “dynamic” structural disorder associated with phonons, at once. Band gap broadening resulting from real-time ion dynamics falls in reasonable agreement with linewidth from photoluminescence,^[8] finite-temperature simulations showing very small inhomogeneous contribution to broadening, both for pure halide and homogeneously dispersed iodine/bromine compositions. The increased broadening in segregated phases due to enhanced electron-phonon scattering, potentially associated with charge carrier recombination, also parallels experimental finding and we relate it to increased inhomogeneous, static contribution. This peculiar behaviour is associate with lattice mismatch at the iodine-rich/bromine-rich interface. All in all, our theoretical analyses point out that halide mixing does not negatively influences the electronic properties of perovskite semiconductors, except in the case of halide segregation, where more complicated mechanisms appear.

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IMPROVED RADICCHIO SEEDLINGS GROWTH UNDER CsPbI₃ PEROVSKITE ROOFTOP IN A LABORATORY-SCALE GREENHOUSE FOR AGRIVOLTAICS APPLICATION

Valastro Salvatore,¹ Spampinato Carlo,^{1,2} Calogero Gaetano,¹ Smecca Emanuele,¹ Mannino Giovanni,¹ Arena Valentina,¹ de Jong Bastiaan,³ Cinà Lucio,³ Balestrini Raffaella,⁴ Sillo Fabiano,⁵ La Magna Antonino,¹ Alberti Alessandra¹

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Agrivoltaics offers a sustainable solution for land's use by integrating photovoltaic (PV) systems with crop cultivation. Traditional opaque PV modules can hinder plant growth due to shading effects. Semi-transparent (ST) PV technologies, including organic, dye-sensitized, and perovskite solar cells (PSCs), entail high light transmission with efficient electricity generation, making them promising for open-field farms and greenhouses.

In this context, PSCs could represent the best choice for agrivoltaics applications owing to high efficiency and low-cost fabrication processes. Recent papers show different stable and efficient ST-PSC architectures suitable for agrivoltaics^[1], but they lack information regarding how the integration of PSCs impacts plant growth and its genomics. For this reason, this study investigates through a multidisciplinary approach the viability and the agronomic implications of growing radicchio seedlings in a laboratory-scale greenhouse with a ST-perovskite-coated rooftop with respect to a bare glass reference system (Fig.1). Perovskite rooftop is made of a ST 130 nm-thick CsPbI₃:EuI₂^[2] layer. The experiment is performed indoor by illuminating radicchio seedlings through perovskite and glass rooftop for 15 days with a 12 LEDs tower acting as a solar simulator. Despite a lower daily light integral under the perovskite rooftop, seedlings exhibit accelerated growth with larger leaves, indicating potential benefits from the unique spectral filtering behavior of the perovskite layer. RNA-sequencing analysis over three replicas reveals differential gene expression patterns in seedlings grown under perovskite and glass rooftops, suggesting adaptive responses to environmental variations. Furthermore, photovoltaic device simulations demonstrate a positive balance between annual energy production and consumption by integrating perovskite PV rooftop in several kind of greenhouses.

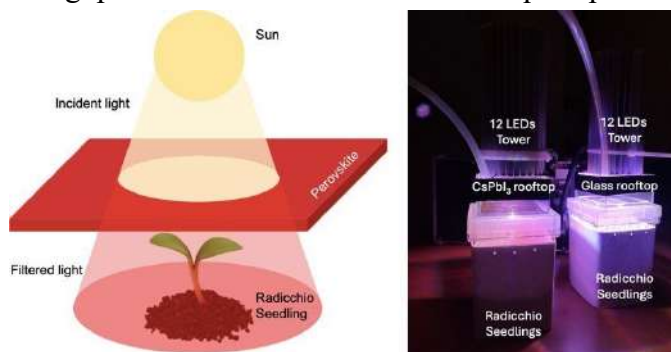


Figure 1: Schematic and setup of the experiment

Acknowledgements: The authors acknowledge the project SAMOTHRACE “Sicilian micro and nanotechnology research and innovation centre” funded by PNRR-MUR (ECS_00000022, CUP B63C22000620005) and the CNR-funded project VertiGrow (CUP B15F21004410005). This activity was partially supported by the national project, BEYOND NANO Upgrade (CUP G66J17000350007).

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NMR CRYSTALLOGRAPHY OF HYBRID PEROVSKITES

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Nuclear magnetic resonance (NMR) crystallography became a valid tool for integrating and supporting conventional X-ray diffraction (XRD)^[1-2]. Specifically, NMR has the advantage of picking up local non-periodic features, and it is well sensible to light-weight atomic species that are otherwise difficult to detect or distinguish with XRD without resorting to neutrons-based techniques.

The parallel development of the GIPAW^[3] (Gauge Including Projector Augmented Waves) methodology within the DFT framework opened the way to simulations with periodic boundaries of the NMR response that do not require the definition of complex cluster models. In this work, we perform a set of NMR spectra of structures taken from *ab-initio* molecular dynamic trajectories to investigate different configurations of 2D hybrid halide perovskites and their time evolution. We show how the B-site metal NMR response can differentiate between various types of perovskite surfaces, making it an ideal way to probe the structural properties of novel synthesized materials. The same method allows for studying the dynamics of the softer organic component and returning a more realistic description of the materials compared to one-shot frozen DFT simulations.

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LONG-TERM PEROVSKITE MODULE OUTDOOR PERFORMANCE IN DIFFERENT OUTDOOR REGIONS

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Our research focuses on improving the performance and stability of the perovskite modules while we scale the module to industrial size. In this work, we share our approach in scaling our perovskite module to 800 cm² while optimising the layer stack for outdoor stability. This work unveils our findings on the long-term (up to +3 years) outdoor behaviour of perovskite modules of varying sizes at different climate conditions. The modules studied share nearly identical layer stacks and perovskite composition. Thanks to a scalable and reproducible, operationally stable perovskite formulation, and a photo and thermally stable layer stack, a foundation for equitable outdoor performance comparisons among samples in long-term outdoor operation studies is possible. The analysis of data permits the establishment of a correlation of the module performance with irradiance levels, temperatures, seasons, and climates. Our approach integrates a feedback loop based on the in-lab characterization and outdoor results to enhance understanding, enabling adjustments for prolonged lifetimes. Preliminary findings indicate, regardless of irradiance levels or climate conditions, a consistent burn-in period within the initial 3 months, resulting in a performance decline of approximately 30%, followed by stabilization. As the dataset will expand by an additional 6 months, extending through September, we anticipate gaining a more nuanced understanding of module behaviour potentially leading to the development of enhanced module versions. Finally, perovskite performance time series will be implemented for the samples tested for over a year at the different testing sites using different forecasting methods (statistical and machine learning) thus demonstrating the expected lifetime of the different modules at the different locations.

This work has been financed by the European Union through the TESTARE project (Grant ID: 101079488) and by the European Regional Development Fund and the Republic of Cyprus through the DegradationLab project (Grant ID: INFRASTRUCTURES/1216/0043).

DOPING IN QUASI-ZERO DIMENSIONAL HALIDE PEROVSKITE

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Many technological advances have been made possible by nanoscale phenomena: unique optical and electronic phenomena occur on length scales smaller than 10 nanometres. Halide perovskites can self-assemble into low-dimensional bulk materials, thus combining easy synthesis processes, low production costs and the possibility of exploiting the charge confinement phenomena. In low-dimensional perovskites, metal halides are partially isolated from each other by the cations: the isolation level generates the two-, one-, or quasi-zero dimensional confinement. In particular, quasi-zero dimensional perovskites have been explored for several applications (e.g., photovoltaics, thermoelectric, lasing, photodetectors, memristors, capacitors, and LEDs).^[1]

In particular, here the thermal voltage response of bismuth-based perovskite derivatives is discussed and a path to increase the electrical conductivity by applying chalcogenide doping has proven effective. The films were produced by drop-casting or spin coating, and sulphur was introduced in the precursor solution using bismuth tri-ethylxanthate. The physical-chemical analysis confirms the substitution. X-ray diffraction, Raman spectroscopy and grazing-incidence wide-angle X-ray scattering were employed to confirm the structure. X-ray photoelectron spectroscopy, CHNS, scanning electron microscopy and energy-dispersive X-ray spectroscopy were employed to study the composition and morphology of the produced thin films. UV-visible and photoluminescence, inverse photoemission and ultraviolet photoelectron spectroscopies have been used to investigate the energy band gap. We proved that the sulphur introduction caused resistivity reduction by two orders of magnitude, and reported on thermal voltages exceeding 40 mV K⁻¹ near 300 K in doped and undoped bismuth-based perovskite-derivates.^[2]

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LUMOS MAXIMA: UNVEILING THE MYSTERIES OF PHOTOLUMINESCENCE QUENCHING

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Photoluminescence (PL) phenomena play a crucial role in elucidating material properties and optimizing semiconductor materials and optoelectronic devices. Among the multitude of available characterization techniques, PL dominates as both widely adopted and highly favored, owing to its ubiquity and effectiveness in contactless probing of structural, electrical, and optical properties. Despite the widespread use of PL, the phenomenon of PL quenching – the observed decrease in PL intensity – remains poorly understood. While researchers often interpret changes in PL amplitude as indications of either improved or deteriorated charge extraction in perovskite half-cells (PHCs), there is a scarcity of systematic studies on this phenomenon, leaving the interpretation of PL data ambiguous. In this study, we address the understanding of PL by employing an approach sensitive to spatial charge separation to investigate the effects of charge extraction on PL quenching or boost. We validate the presence of significant PL quenching following enhancements in charge extraction in the most commonly utilized metal oxides in state-of-the-art perovskite solar cells (s. **Fig. 1**), supported by 2D drift-diffusion simulations. Our findings further demonstrate that the mechanism of charge extraction is fundamentally different in PHCs based on metal oxides compared to PHCs based on self-assembled monolayers (SAMs). This mechanistic difference has drastic consequences for the observed PL spectra. From our findings, we establish a comprehensive protocol for the reliable measurement and analysis of PL spectra. By providing a deeper understanding of the charge carrier extraction mechanisms in PHCs, our work paves the way for the accelerated optimization of semiconductor devices, thereby advancing the fields of optoelectronics, quantum photonics, physics, material science, and chemistry.

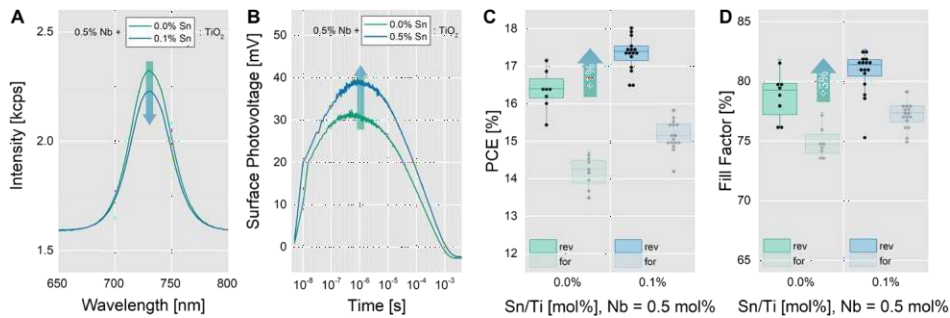


Fig. 1. In a modified $\text{TiO}_2/\text{CsPbI}_3$ PHC, PL quenching (A) is accompanied by improved electron extraction, as quantified in transient surface photovoltage measurements (B). For finished solar cells, power conversion efficiency is improved by 1% (C) due to a fill factor improvement of 3% (D).

INFLUENCE OF HEAVY IONS ON PEROVSKITE PHOTOVOLTAICS OPERATING IN SPACE

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The use of perovskite photovoltaics in space is an area of growing interest. This is driven by its numerous attractive properties such as high efficiencies and high power/per weight, as well as the potential for multijunction architectures that can be produced at a much lower cost than current III-V technologies. To date, numerous studies have been published on the stability of perovskite photovoltaics under proton irradiation with promising outcomes, However, heavy ions are also present in all areas in space, which are known to cause issues for electronic devices^[1], from low Earth orbit to travelling into deep space. Electronic devices and systems can be affected through degradation in performance or have a complete failure^[2]. However, to date, no study outlines the impact of heavy ion irradiation on the stability of perovskite photovoltaics.

In this work, the effect of heavy ion irradiation on the stability of perovskite solar cells has been investigated with a particular emphasis on the impact of heavy ions that are commonly encountered in space. We will discuss the energy deposition mechanisms and the influence of this heavy-ion bombardment on the optoelectronic properties of the perovskite. In particular, we will discuss the degradation modes (e.g. removal of cations and anions, generation of strain) and strategies that can be used to stabilise this

Finally, we will outline design strategies to counter the degradation pathways to ensure the promise of perovskite photovoltaics for operation in a space environment.

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STRUCTURAL & OPTOELECTRONIC FEATURES OF Pb-FREE 3D, QUASI-2D, AND 2D HALIDE PEROVSKITES

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2D and quasi-2D halide perovskites (HPs) represent an emerging class of dimensionally reduced perovskites characterized by an intrinsic enhanced resistance towards heat and moisture. Noticeably, whereas the initial solar devices exploiting such low-dimensional class of compounds were accompanied by photoconversion efficiencies (PCEs) quantitatively smaller than the 3D counterpart,^[1] today PCEs for such systems achieve values of up to ~ 25%.^[2] The success of 2D and quasi-2D HPs also stems from the fact that their potential technological applicability is broad by virtue of the structure's tunability, which in turn is function of the number of inorganic layers and the combination of halogens and organic cations. Accordingly, they may find applicability in several optoelectronic fields, *i.e.*, among the others, lighting and photodetection. Motivated by this extraordinary versatility, in recent years we have paid particular attention to the theoretical, unbiased, characterization of the electronic and optical properties of this class of halide perovskites.

In the present contribution, we overview some of our results obtained by combining Density Functional and Many-Body Perturbation Theories, describing and discussing the optical properties of several flavors — Pb-based, Pb-less, and Pb-free — of 2D and quasi-2D HPs.^[3-5] Finally, back to the 3D realm, we show preliminary results of interfacial systems formed by mixed Sn/Ge HPs surfaces and passivating oxide buffer layers, discussing the impact of the latter ones in the structural and electronic features of the overall system.

Acknowledgements: Authors acknowledge the NEDO project “Development of materials for Pb free perovskite tandem solar cells”. G.G. also acknowledges the European Union - NextGenerationEU under the Italian Ministry of University and Research (MUR) National Innovation Ecosystem Grant ECS00000041 – VITALITY and the PRIN 2022 project (CUP J53D23003480006).

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UNDERSTANDING THE ROLE OF PbI_2 AND Pb IN THE PHOTOEMISSION STUDIES OF POLYCRYSTALLINE PEROVSKITE THIN FILMS

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Since its emergence, perovskite solar cells have continuously surpassed expectation with its soaring power conversion efficiency despite being solution processed – a fabrication method that is known to produce abundance of defects. Though often quoted ‘defect-tolerant’, understanding and control of the types and distributions of the many defects in polycrystalline perovskite films are crucial for the achievement of stable and highly efficient photovoltaic devices. Since 2015, ultraviolet photoemission electron spectroscopy and microscopy have been used to directly probe the presence, spatial distribution, and trapping dynamics of hole traps in lead-based perovskite films. [1-2] The presence of these hole traps are typically characterized by the presence of occupied mid-gap states in the band gap of perovskites that stretches from the valence band edge up to the fermi level. Thus far, these mid-gap states have been attributed to a combination of defects i.e. PbI_2 defects, grain boundary defects, and polytype defects. [3-4]

Here, we investigate the origin of these mid-gap photoemission using spectroscopic low energy and photoemission electron microscope. By changing the stoichiometry of $\text{Cs}_{0.15}\text{FA}_{0.85}\text{PbI}_{1.5}\text{Br}_{1.5}$ perovskite thin films, we observed that the photoemission intensity of these mid-gap states seem to be correlated to the amount of excess PbI_2 in the samples. In contrast, these mid-gap photoemission spectra are strangely absent in Sn-based perovskites with similar compositions. Using microprobe low energy electron diffraction (Figure 1), we show that the presence of PbI_2 diffraction on the sample surface has a negative correlation with the presence of these mid-gap photoemission. In addition, we further correlate the rise of these mid-gap photoemission upon laser irradiation with the disappearance of the PbI_2 diffraction. Based on these observations, we thus attribute the origin of these mid-gap photoemission spectra to be the spectra of metallic Pb , a decomposition product of PbI_2 . The absence of these mid-gap photoemission in the Sn-based perovskites is thus due to the propensity of Sn^{2+} to oxidize and form various Sn^{4+} compounds such as SnI_4 and SnO_2 rather than decomposition to metallic Sn .

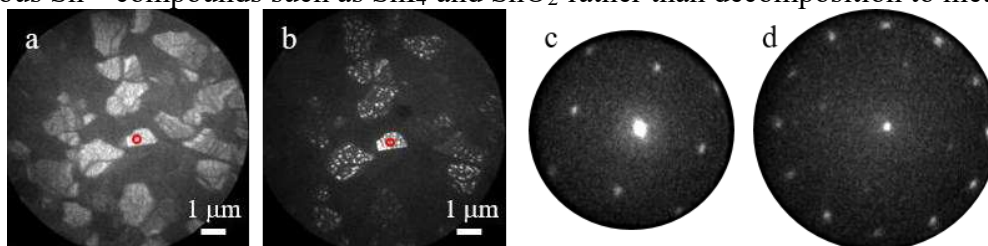


Figure 1: (a-b) Low energy electron microscopy images showing the perovskite grains with similar crystal orientation (a) and the distribution of PbI_2 on the grain surfaces. (c-d) Low energy electron diffraction of perovskite (c) and PbI_2 (d) measured at the grain highlighted in (a & b).

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MONOLITHIC MULTIBAND TRIPLE JUNCTION PEROVSKITE PHOTODETECTORS FOR COLOR FILTER-FREE IMAGING

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Modern color image sensors struggle to enhance sensitivity and color fidelity because of inherent limitations in light utilization efficiency^[1]. A significant factor contributing to these limitations is the use of passive optical filters, which absorb a substantial amount of incoming light, thereby reducing the quantum efficiency of the sensors. We introduce an innovative architecture for color detector arrays that employ multilayer monolithically stacked lead halide perovskite thin-film photodetectors. We utilize perovskite bandgap tunability^[2] to selectively absorb the visible light spectrum's red, green, and blue regions, eliminating the need for color filters. This design significantly outperforms conventional color-filter arrays and stacked silicon (Foveon) photosensors, exhibiting superior quantum efficiency and color accuracy while avoiding demosaicing artifacts. This study paves the way for the next generation of image sensors by utilizing conceptually novel architectures with improved light utilization.

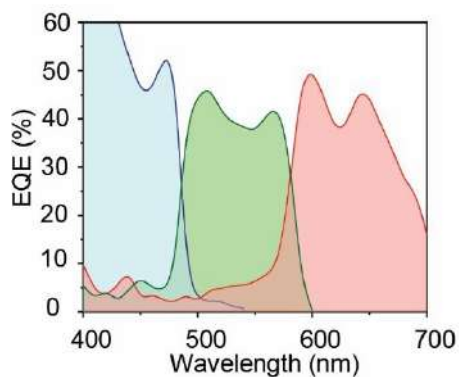


Figure 1: External quantum efficiency of a triple junction perovskite photodetector, experimentally obtained.

Acknowledgments: The work was financially supported by ETH Zürich through the ETH+ Project SynMatLab: Laboratory for Multiscale Materials Synthesis.

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TIME-DOMAIN SIGNAL BALANCING LiDAR WITH CENTIMETER RESOLUTION BASED ON METAL-HALIDE PEROVSKITE

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We report on a novel photodetector design operating on the principle of non-equilibrium charge carrier concentrations. For the first time, it realises a ‘balanced operational mode’ in which the fast response is neither free charge carrier lifetime nor transit-time limited. Instead, it directly measures the time between light pulses and demonstrates a time resolution of 170ps, corresponding to a light propagation distance of 5cm. The high operational speed originates from an efficient diffusive photocurrent enabled by the high absorption coefficient and the good charge transport properties of the metal halide perovskite CsPbBr₃. The CsPbBr₃ absorber is tens of microns thick and is fabricated by a custom-developed confined melt processing between transparent electrodes. A comprehensive electro-optical characterisation completes this work. The free carrier lifetimes and mobilities are studied at microscopic and macroscopic length scales using transient photoluminescence, time-resolved photocurrent, time-of-flight and optical pump and microwave/THz probe spectroscopy.

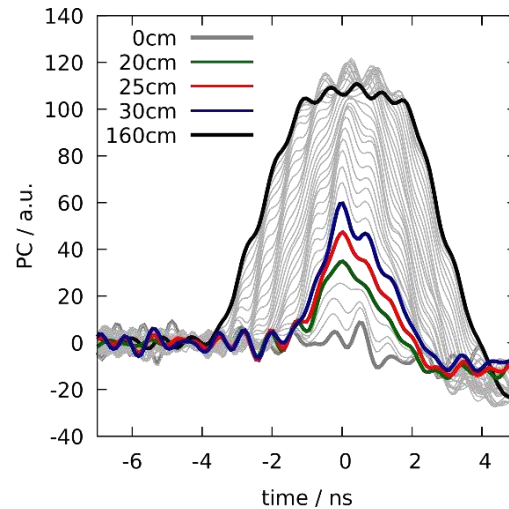
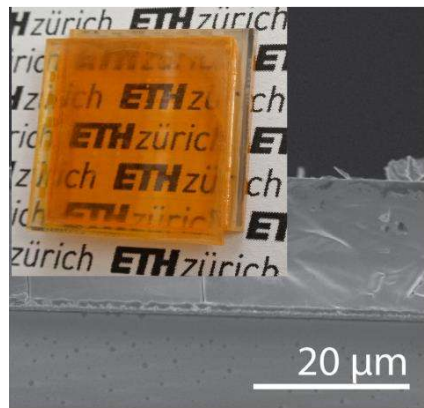


Figure 1: Left: SEM cross-section of the crystalline CsPbBr₃ film on a glass substrate. The inset shows a photograph of the semi-transparent photodetector. Right: transient photocurrent in the ns timescale measured with an optical time-delay in 5cm steps (~170ps) between 0 to 160cm.

A LATERAL HETEROJUNCTION DEVICE AS A TOOL TO STUDY PEROVSKITE-BASED SOLAR CELLS

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Halide perovskite solar cells demonstrated a dramatic increase in efficiency in the last decade mainly thanks to improvements in the bulk material quality, as well as the choice of suitable selective carrier transport layers (SCTLs). More recently, improvements have come from interface optimization strategies, such as defect passivation. Nevertheless, the interactions between the perovskite (PSK) and SCTLs are still unclear and will become more and more important to improve both efficiency and stability of PSK solar cells.

In our study, we quantified the optoelectronic interactions at the SCTL-PSK interfaces employing a lateral heterojunction device (LHJ) (Figure 1A). The device is composed of a glass substrate, on which two different SCTLs (TiO_x and NiO_x) are deposited in a lateral electrode configuration with a well-defined 100 μm – long channel between them. The two SCTLs sit on two separate ITO electrodes that serve as contacts. We measured a ≈600 meV work function (WF) difference between the SCTLs, which constitutes the built-in voltage (V_{bi}) of our device.

To complete the structure, a Pb-based perovskite layer is deposited on top, thus filling the channel and creating a p-i-n device which develops in the horizontal direction, i.e. in the sample plane. We tracked the surface electrostatic potential variation along the PSK channel employing high-spatial-resolution (≈11 μm) X-ray photoemission spectroscopy (XPS) both in dark short circuit, and under applied bias, by recording the I_{3d5/2} core level binding energy (BE_I) of the PSK.

We discovered that the substrate built-in voltage was still present on top of the PSK surface: a linear potential drop (V_{drop}) of about 600 meV was recorded across the channel by XPS in dark, short circuit conditions, implying a nearly undoped PSK. Indeed, by fitting the data with a 2D drift-diffusion (DD) model, we found N_{dop}=10¹¹ cm⁻³ to be the maximum PSK doping density able to sustain such a long-range linear drop (Figure 1B).

Furthermore, we could control (and even invert) the potential drop by applying a voltage bias (V_{app}) to the electrodes, which adds up to V_{bi} (V_{drop}= V_{bi}- V_{app}) (Figure 1C).

Our results indicate that the tested PSK is nearly intrinsic and its Fermi level is controlled by the substrate over which it is deposited, and can be modulated by an external bias voltage.

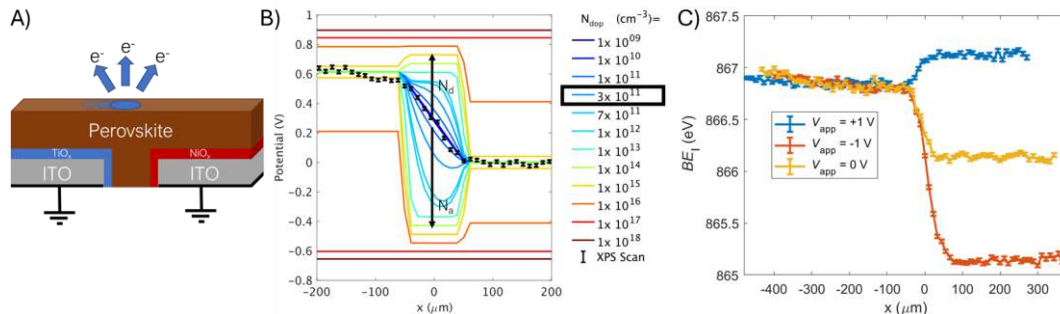


Figure 1: Schematic of the LHJ device under XPS measurement (A), XPS scan in dark short circuit compared with the outcome of DD simulations for varying N_{dop} , either in the form of acceptors (N_a), or donors (N_d) (B), highlighted is the maximum allowed N_{dop} to fit the experiment. In (C), XPS scans under applied bias V_{app} are reported.

QFLS DETERMINATION THROUGH MICROWAVE CONDUCTIVITY TECHNIQUES: MATCHING TRANSIENT AND STEADY-STATE MEASUREMENTS

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The performance of metal halide perovskite solar cells is currently limited by a low Fill Factor (FF) and open circuit voltage (V_{OC}). Besides hampered collection at the contacts and other high-resistance components, non-radiative carrier recombination in the perovskite bulk and at the interfaces between the perovskite and transport layers is a major contributor to these losses. Valuable insights herein can be provided by accurately determining the quasi-Fermi level splitting (QFLS). This work proposes a new method to determine the intensity-dependent QFLS using steady-state microwave conductivity measurements with chopped monochromatic LED illumination. Additionally, it shows that the QFLS can be accurately simulated by use of the kinetic parameters obtained from fitting time-resolved microwave conductivity (TRMC) traces with a simple model (**Figure 1a**). This method was employed on triple-cation perovskites comprising $\text{Cs}_{0.05}\text{MA}_{0.10}\text{FA}_{0.85}\text{Pb}(\text{I}_{0.97}\text{Br}_{0.03})_3$ (CsMAFA) as well as bilayers with C60.^[1] TRMC traces were recorded with multiple photon intensities and fitted, as shown in **Figure 1b**. Moreover, the measured and simulated QFLS are included in **Figure 1c**. These figures show an exceptionally convincing overlap of the measured and simulated values. Furthermore, when we compare the QFLS of the bilayers at 1 sun in **Figure 1d**, we see that the deposition order influences the resulting QFLS. Applying the perovskite on top of C60 results in an increased QFLS, indicating a passivating effect, while applying C60 on top of the perovskite film results in a reduced QFLS, indicating voltage losses across that interface. All in all, the presented method for QFLS determination can aid in the evaluation of the quality of the perovskite/transport layer interface.

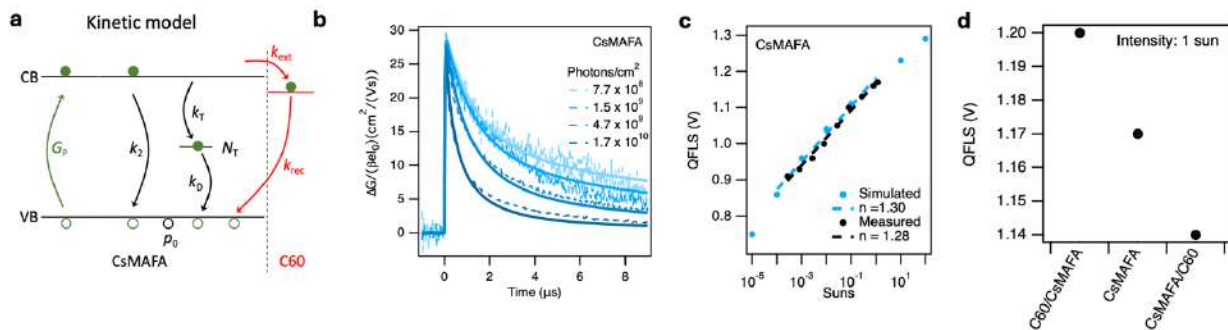


Figure 1: (a) The kinetic model employed for the fitting of the TRMC measurements, adapted from ref.^[1] (b) TRMC traces measured with multiple photon intensities (dotted lines) with fits (full lines). (c) QFLS as a function of light intensity for CsMAFA. The plots contain the measured QFLS as well as the simulated QFLS from the TRMC fits. (d) Measured QFLS at 1 sun intensity for the bare CsMAFA film and the C60/CsMAFA, CsMAFA/C60 bilayers.

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[1] Long-lived Charge Extraction in CsMAFA-based Perovskites in n-i-p and p-i-n Structures. Jiashang Zhao, Lara M. van der Poll, Sander L. Looman, Jin Yan, Jos Thieme, Bahiya Ibrahim, and Tom J. Savenije. *Manuscript under review.*

MODELING THE INTERACTION OF CO₂ WITH NANOSTRUCTURES: FROM GRAPHENE LAYERS TO PEROVSKITES

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The characterization of the chemical and physical properties of nanostructures makes it possible to design a new class of nanomaterials with various applications, ranging from energy storage to photovoltaics and carbon neutrality technologies. The investigation of novel technologies aimed at regulating and reducing the quantity of carbon dioxide released into the atmosphere is becoming a present-day priority. New porous materials are generally considered a promising medium for the effective adsorption of CO₂ upon their surfaces or within their pores. Graphene and its derivatives, being one of the thinnest materials whose properties may be altered by functionalization, represent a promising class of nanomaterials^[1,2]. In this context, molecular dynamics (MD) simulations are powerful instruments for predicting the structure and reactivity of various systems, guiding experimental synthesis and research towards approaches that minimize costs and negative effects. In this contribution, using a new force field based on the Improved Lennard-Jones formulation of the potential^[3], extensive theoretical MD simulations have been carried out to study the interaction of CO₂ with carbon-based nanostructures, in order to predict and characterize the selectivity and absorption properties. Once the nature of the interaction and the effective potential have been correctly identified and analysed, the same approach can be used to characterize the interaction of CO₂ with different materials, including perovskites. The analysis can, therefore, represent a starting point to guide more accurate theoretical and/or experimental investigations with a wide range of possible applications, including the effect on the stabilization of the perovskite itself^[4,5] and the possible role as photocatalytic site for the CO₂ conversion^[6].

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