

**8<sup>TH</sup> INTERNATIONAL CONFERENCE ON  
PEROVSKITE SOLAR CELLS AND  
OPTOELECTRONICS - PSCO**



**20  
25**

**Book Of Abstract**

**September, 15 – 18 2025**

**Hotel Giò Wine e Jazz Area, Congress Center**

**Perugia, Italy**

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# INVITED LECTURES

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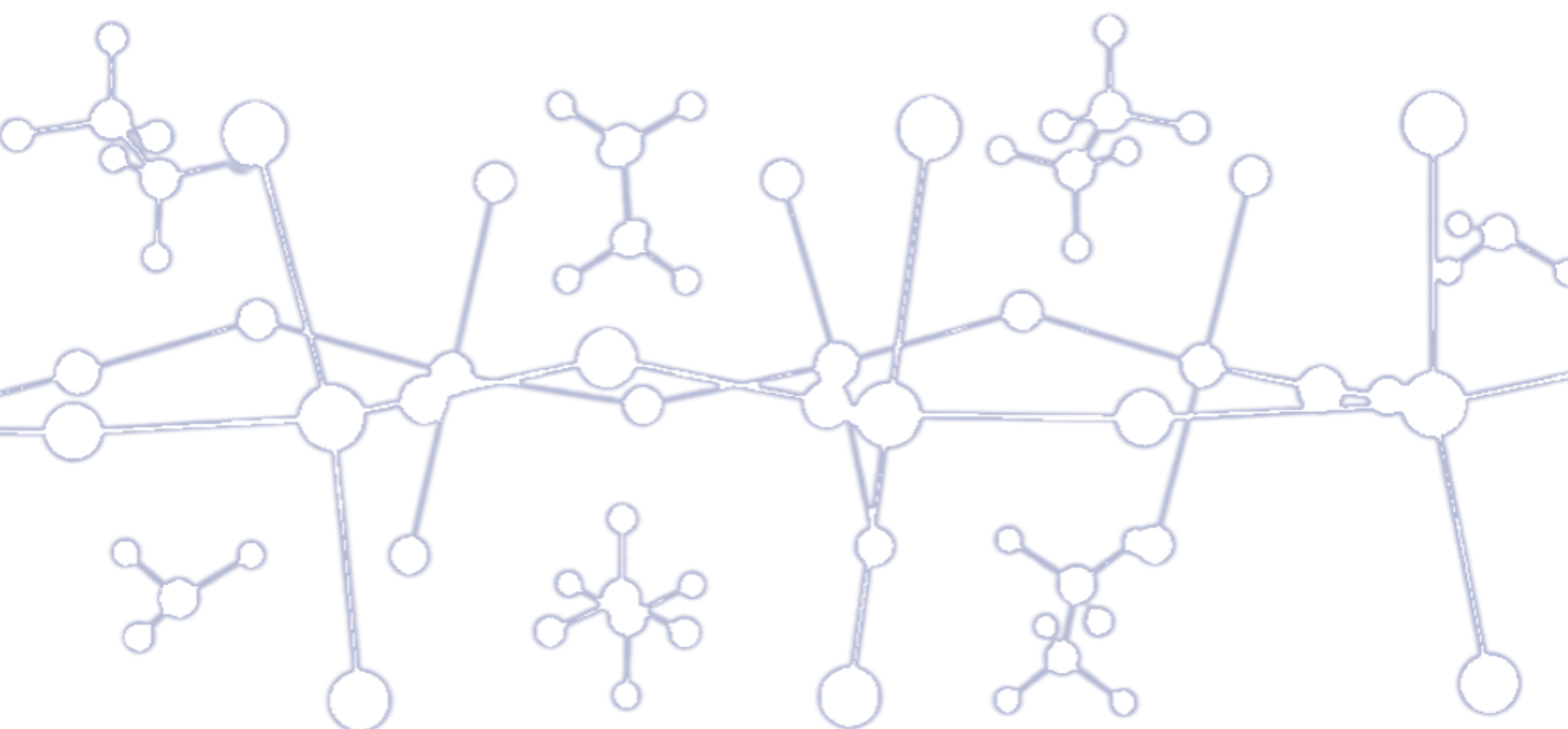
**Yuanyuan Zhou**

HKUST, HKG



Day 1 - Monday, September 15th 2025

08:30 08:50		CONFERENCE DESK
		Town Hall
Session Chair	Edoardo Mosconi, CNR – SCITEC “G.Natta” Perugia, Italy	
Session Title	Special Session - Catalysis	
09:00 09:12	Introduction to CATALYSIS Session by <b>Prof. Lorenzo Malavasi</b> , University of Pavia and INSTM, Italy	
09:12 09:24	<b>Luca Gregori</b> , University of Perugia, Italy <i>Computational modeling of perovskite for photovoltaics and photocatalysis</i>	
09:24 09:36	<b>Costanza Tedesco</b> , University of Pavia, Italy <i>Metal halide perovskites and graphitic carbon nitride heterojunctions for ammonia and hydrogen production</i>	
09:36 09:48	<b>Diego Sorbelli</b> , University of Perugia, Italy <i>Cooperative CO<sub>2</sub> activation: lessons from molecular systems for emerging catalytic materials</i>	
09:48 10:00	<b>Sofia Lerda</b> , University of Perugia, Italy <i>Computational insights into selective catalysis by dirhodium complexes</i>	
10:00 10:30	COFFEE BREAK AM	



# COMPUTATIONAL MODELING OF PEROVSKITE FOR PHOTOVOLTAICS AND PHOTOCATALYSIS

**Luca Gregori,<sup>1</sup> Edoardo Mosconi,<sup>2</sup> Filippo De Angelis<sup>1,2,3</sup>**

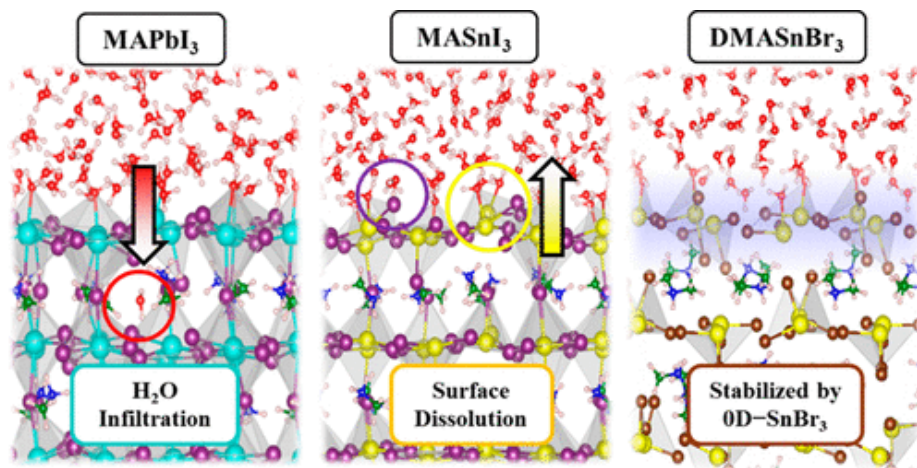
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<sup>2</sup>Computational Laboratory for Hybrid/Organic Photovoltaics (CLHYO), Istituto CNR di Scienze e Tecnologie Chimiche "Giulio Natta" (CNR-SCITEC), Via Elce di Sotto 8, 06123 Perugia, Italy.

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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.

# METAL HALIDE PEROVSKITES AND GRAPHITIC CARBON NITRIDE HETEROJUNCTIONS FOR AMMONIA AND HYDROGEN PRODUCTION

**Costanza Tedesco,<sup>1</sup> Luca Gregori,<sup>2</sup> Francesca Merlo,<sup>1</sup> Angelica Simbula,<sup>3</sup> Edoardo Mosconi,<sup>2</sup> Filippo De Angelis,<sup>2</sup> Andrea Listorti,<sup>4</sup> Lorenzo Malavasi<sup>1</sup>**

<sup>1</sup>*Department of Chemistry and INSTM, University of Pavia, Pavia, Italy*

<sup>2</sup>*Department of Chemistry, Biology and Biotechnology, University of Perugia and INSTM, Perugia, Italy*

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The request for sustainable and renewable energy sources has motivated a significant shift toward innovative methods for producing and storing clean energy through green solar fuels. Photocatalytically active heterojunctions based on metal halide perovskites (MHPs) are drawing important interest for their tuneable ability to promote several important redox reactions, in the field of green fuels production. This study investigates two composite systems: a classic double perovskite based, Cs<sub>2</sub>AgBiCl<sub>6</sub>/g-C<sub>3</sub>N<sub>4</sub>,<sup>[1]</sup> and a vacancy-ordered perovskite based, Cs<sub>2</sub>SnBr<sub>6</sub>/g-C<sub>3</sub>N<sub>4</sub>.<sup>[2]</sup> The first system has been studied and employed for both solar-driven hydrogen generation from chloride media and ammonia production from nitrogen fixation and the second one for ammonia production, due to its remarkable photofixation activity. The efficiency of the Cs<sub>2</sub>AgBiCl<sub>6</sub>/g-C<sub>3</sub>N<sub>4</sub> system depends on the relative amounts of perovskite and carbon nitride to promote the two reactions. Spectroscopic investigations and density functional theory (DFT) modelling reveal that perovskite halide vacancies are primary reactive sites for hydrogen generation and can be, together with g-C<sub>3</sub>N<sub>4</sub> nitrogen vacancies crucial also for nitrogen reduction.<sup>[1]</sup> On these bases, again through a combined experimental and computational approach, we provide a detailed framework of the mechanism supporting the efficient nitrogen reduction reaction to ammonia observed in Cs<sub>2</sub>SnBr<sub>6</sub>/g-C<sub>3</sub>N<sub>4</sub> system. The vacancy-ordered perovskite is characterized by a higher surface density of halide vacancies than the classic double perovskite and for this reason Cs<sub>2</sub>SnBr<sub>6</sub>/g-C<sub>3</sub>N<sub>4</sub> system achieves the highest ammonia evolution rate of 266 μmol g<sup>-1</sup> h<sup>-1</sup>.<sup>[2]</sup> Photoluminescence studies and differential transmission measurements stress the importance of compositional engineering in enhancing photocatalysis efficiency for both reactions. This work represents a significant advancement in photocatalytic green fuels production, especially in the field of nitrogen photofixation, proposing materials and structures that can potentially improve sustainable ammonia production, thereby contributing to energy independence and reduced carbon emissions.

[1] 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 and Sustain. Res.* **2024**, 2400040.

[2] C. Tedesco, A. Simbula, R. Pau, F. Merlo, A. Speltini, V. Armenise, A. Listorti, L. Gregori, A. A. Allothman, E. Mosconi, M. Saba, A. Profumo, L. Malavasi, *Solar RRL* **2025**, 202400778.

# COOPERATIVE CO<sub>2</sub> ACTIVATION: LESSONS FROM MOLECULAR SYSTEMS FOR EMERGING CATALYTIC MATERIALS

**Diego Sorbelli**<sup>1,2</sup>

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Understanding and controlling cooperative effects in the activation of carbon dioxide is central to the development of next-generation catalytic platforms for small molecule conversion. While cooperative reactivity is often rationalized through structural and electrostatic descriptors (e.g., the OCO bending and bond elongation in CO<sub>2</sub>, or electronegativity-driven polarization), these simplified models frequently fall short in capturing the complexity of real systems.

In this contribution, we demonstrate how a carefully designed computational protocol reveals the breakdown of these assumptions in a class of apolar and weakly polar bimetallic molecular complexes.<sup>[1-5]</sup> We uncover mechanistic pathways unexpectedly governed by electron-sharing bonds, elucidating the role of metal-metal interactions in enabling efficient CO<sub>2</sub> insertion and conversion. Furthermore, we assemble carefully selected computational approaches with the aim of assessing the nature and extent of the carbon dioxide-substrate interactions, revealing unprecedented and non-intuitive trends that challenge traditional views of reactivity based on simple descriptors. By disentangling electronic and geometric contributions to activation, our protocol provides transferable insight into the role of bond character in enabling efficient cooperative activation.

We argue that the principles extracted from these molecular systems can inform the rational design of heterogeneous or heterogenized catalysts. By rethinking the structure–reactivity relationship, our findings offer conceptual tools to inform the rational design of complex catalytic substrates, including heterogeneous systems targeting small molecule conversion.

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[1] D. Sorbelli, L. Belpassi, P. Belanzoni, *J. Am. Chem. Soc.* **2021**, *143*, 14433-14337.

[2] D. Sorbelli, L. Belpassi, P. Belanzoni, *Chem. Sci.* **2022**, *13*, 4623-4634.

[3] D. Sorbelli, L. Belpassi, P. Belanzoni, *Inorg. Chem.* **2022**, *61*, 1704-1716.

[4] D. Sorbelli, L. Belpassi, P. Belanzoni, *Chem. Sci.* **2023**, *14*, 889-896.

[5] D. Sorbelli, L. Belpassi, P. Belanzoni, *Chem. Commun.* **2024**, *60*, 1222-1238.

# COMPUTATIONAL INSIGHTS INTO SELECTIVE CATALYSIS BY DIRHODIUM COMPLEXES

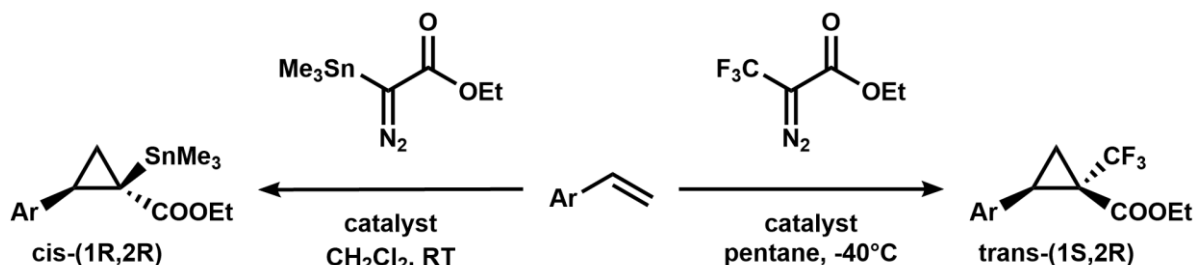
**Sofia Lerda,<sup>1</sup> Matthias Peeters,<sup>2</sup> Lorenzo Baldinelli,<sup>1</sup> Giovanni Bistoni,<sup>1</sup> and Alois Fürstner<sup>2</sup>**

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<sup>2</sup>Max-Planck-Institut für Kohlenforschung, 244 D-45470 Mülheim/Ruhr, Germany

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Dirhodium paddlewheel complexes are powerful catalysts with broad applications in asymmetric synthesis. We investigated a recently developed example that is chiral at both inequivalent metal centers despite containing only achiral ligands [1]. This heterochiral catalyst furnishes stannylated cyclopropane derivatives with excellent diastereo- and enantioselectivity. Remarkably, the same cyclopropanation reaction catalyzed by this complex gives a completely different selectivity pattern when the stannyl substituent on the diazo precursor is replaced by a fluorinated group. To investigate the origin of these contrasting outcomes, we combined conformational sampling with DFT refinement to study the two carbene intermediates and their reactivities. For the stannylated case, the calculated transition states reproduced the experimentally observed high selectivity, showing that steric effects and a N–H···O hydrogen bond cooperate to favorably yield the cis-(1R,2R) product. On the other hand, the fluorinated carbene intermediate leads preferentially to the trans-(1S,2R) cyclopropane. This switch in selectivity was found to arise from increased structural rigidity of the carbene intermediate, attributed to two key noncovalent interactions: the same hydrogen bond observed previously and an additional halogen–halogen interaction. Quantum chemical characterization revealed the latter to be primarily dominated by London dispersion, in contrast to conventional halogen bonds, which are usually driven by electrostatics [2].

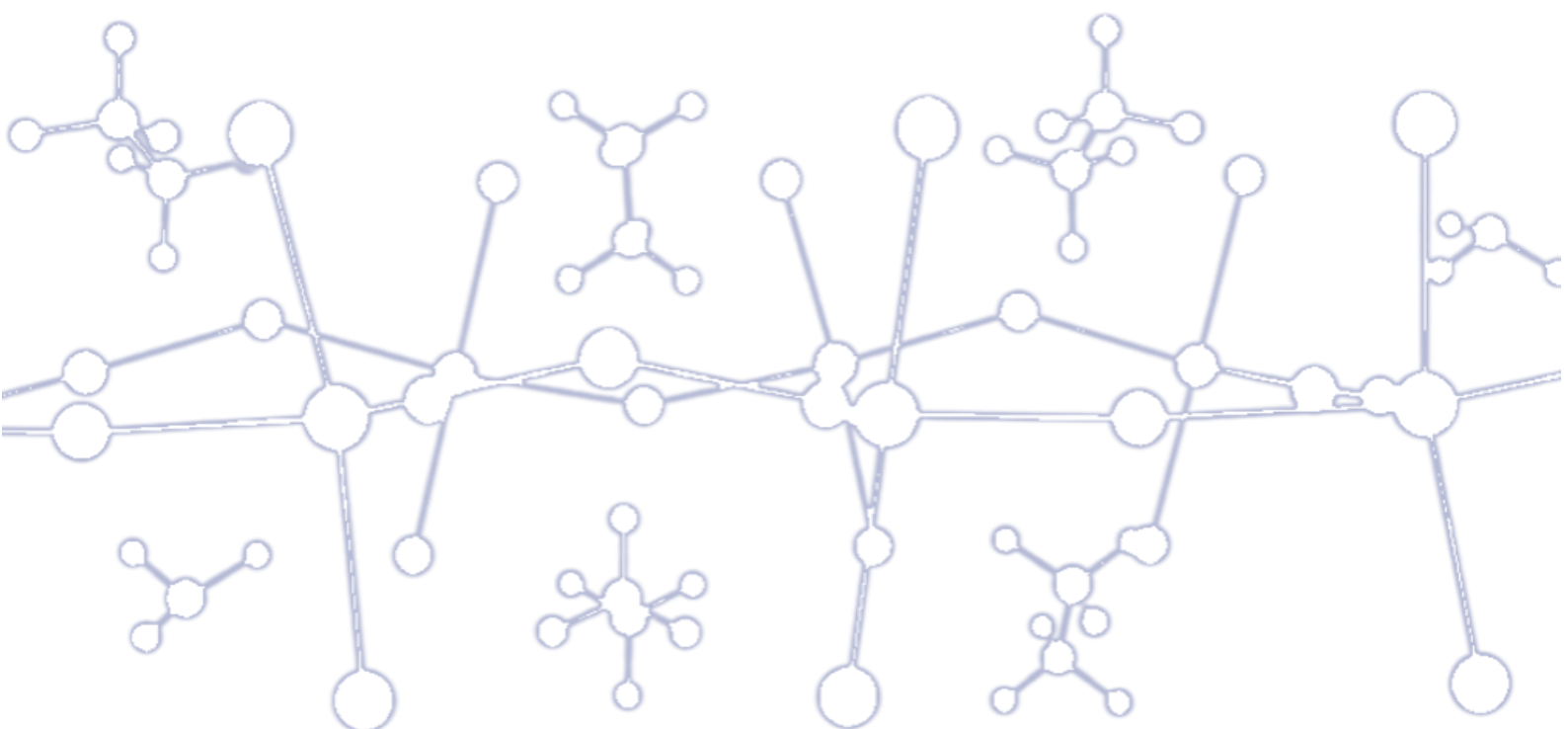


**Figure 1:** Schematic representation of the cyclopropanation reactivities promoted by the same heterochiral dirhodium catalyst. On the left, the stannylated diazo compound leads to the cis-(1R,2R) cyclopropane; on the right, the fluorinated diazo compound yields the trans-(1S,2R) product.

[1] M. Peeters, L. Baldinelli, S. Lerda, G. Bistoni, A. Fürstner, *J. Am. Chem. Soc.* **2025**, 147, 12418–12424.

[2] M. Peeters, S. Lerda, G. Bistoni, A. Fürstner, manuscript in preparation.

		<b>Town Hall</b>
<b>Session Chair</b>	<b>Paola Delli Veneri, ENEA, Italy</b>	
<b>Session Title</b>	<b>Special Session - GoPV</b>	
10:30	10:45	Introduction by <b>Paola Delli Veneri</b> , ENEA, Italy <i>GoPV Project: New generation materials for tandem solar cells</i>
10:45	11:00	<b>Gennaro V. Sannino</b> , ENEA and INSTM, Italy <i>Innovative materials for perovskite/Si tandem solar cells</i>
11:00	11:15	<b>Antonio Terrasi</b> , University of Catania, Italy <i>TCOs and selective contacts for tandem solar cells</i>
11:15	11:30	<b>Debendra Prasad Panda</b> , University of Naples "Federico II", Italy <i>Recent Progress in DMSO-Free Tin Perovskites</i>
11:30	11:45	<b>Annamaria Petrozza</b> , Istituto Italiano di Tecnologia, Italy <i>Design of Strong and Weak Intermolecular Interactions to Engineer Buried Interfaces in Inverted Wide-Bandgap Perovskite Solar Cells</i>
11:45	12:00	<b>Matteo Degani</b> , University of Pavia, Italy <i>Redefining Solar Energy with Low-Dimensional Perovskites: Breakthroughs in Active Materials and Interface Control</i>
12:00	12:15	<b>Marina Ustinova</b> , University of Rome "Tor Vergata", Italy <i>Materials for perovskite cells in single and tandem configurations</i>
12:15	12:30	<b>Filippo De Angelis</b> , University of Perugia, Italy <i>Modeling and Screening of Optimized Perovskite Material</i>
12:30	12:45	<b>Sanjay Thorat</b> , BeDimensional, Italy <i>The applications of two-dimensional materials in photovoltaic</i>
12:45	13:45	<b>REGISTRATION &amp; LIGHT BUFFET LUNCH</b>



# INNOVATIVE MATERIALS FOR PEROVSKITE/Si TANDEM SOLAR CELLS

**Gennaro V. Sannino,<sup>1,2,3</sup> L. Lancellotti,<sup>1</sup> E. Bobeico,<sup>1</sup> I. Usatii,<sup>1</sup> M. F. Caso,<sup>1</sup> M. Della Noce,<sup>1</sup> G. Nasti,<sup>1</sup> C. Serpico,<sup>1,2</sup> E. Santoro,<sup>1</sup> P. Scognamiglio,<sup>1</sup> L. V. Mercaldo<sup>1</sup> and P. Delli Veneri<sup>1</sup>**

<sup>1</sup> Italian National Agency for New Technologies, Energy and Sustainable Economic Development (ENEA), Portici(NA), Italy

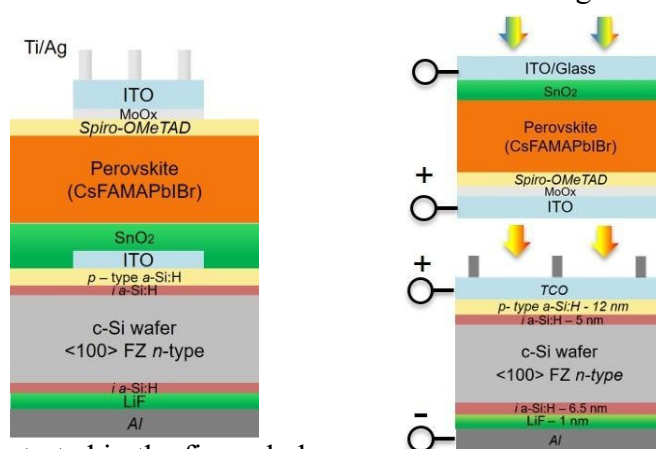
<sup>2</sup> Department of Chemical Sciences, University of Naples Federico II, Naples, Italy

<sup>3</sup> Italian National Interuniversity Consortium of Materials Science and Technology (INSTM), Florence, Italy  
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Within the GoPV project, ENEA is focusing on the development of innovative materials for high-efficiency perovskite–silicon tandem solar cells. While silicon heterojunction (SHJ) and perovskite solar cells (PSCs) individually achieve power conversion efficiencies (PCEs) above 27%, their monolithic integration enables broader spectral utilization and has already delivered record efficiencies above 34%. Despite this potential, several challenges must be addressed to enable scalable and cost-effective deployment. The main issues concern the intrinsic instability of hybrid perovskites, the parasitic absorption and processing complexity of doped amorphous silicon contacts, and the reliance on indium-based transparent conductive oxides (TCOs).

ENEA's strategy focuses on three directions: (i) replacing hybrid perovskites with the all-inorganic CsPbI<sub>3</sub>, expected to offer enhanced thermal and photostability, (ii) developing dopant-free selective contacts (MoO<sub>x</sub>, LiF, and self-assembled monolayers (SAMs)) to simplify processing and reduce optical losses, and (iii) reducing or eliminating the use of indium in TCOs. Initial results demonstrated that MoO<sub>x</sub> and LiF can provide open-circuit voltage and fill factor values comparable to conventional SHJ cells, while SAM-based approaches showed feasibility as electron-selective contacts but led to shunted devices when deposited on textured silicon. To address this issue, different SAM deposition procedures were tested to optimize coverage on textured surfaces.

In parallel, we developed low-temperature device architectures for CsPbI<sub>3</sub>-based PSCs, investigating both nip and pin configurations. PCEs up to 9% were achieved in nip devices using SnO<sub>2</sub> as electron transport layer, while up to 16% were obtained in pin devices employing 2PACz SAM as hole transport layer. Finally, proof-of-concept tandem devices were demonstrated in both four-terminal and monolithic configurations, employing the



device structures illustrated in the figure below.

# TCOs AND SELECTIVE CONTACTS FOR TANDEM SOLAR CELLS

**Antonio Terrasi<sup>1,2</sup>, Federica Florio<sup>1,2</sup>, Maria Pilar Miritello<sup>2</sup>, Salvatore La Manna<sup>2</sup>, Vanna Torrisi<sup>2</sup>, Giorgia Franzò<sup>2</sup>, Iurie Usatii<sup>3</sup>, Eugenia Bobeico<sup>3</sup>, Lucia V. Mercaldo<sup>3</sup>, Paola Delli Venere<sup>3</sup>**

<sup>1</sup>Department of Physics and Astronomy "Ettore Majorana", University of Catania, Italy

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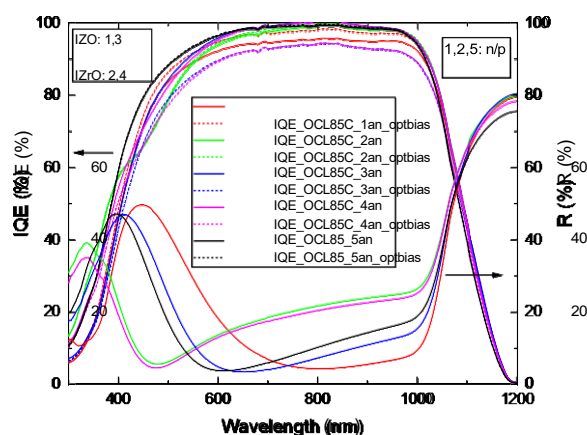
<sup>3</sup>ENEA, TERIN-SPV, Centro Ricerche Portici, Italy

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As part of the work on TCOs and selective contacts for the GOPV project, our group has identified several materials with potentially interesting electro-optical properties. For TCOs, two materials with excellent electrical conductivity and transparency, without post deposition thermal processes, were identified (see table), and their functionality is going to be tested after integration into a photovoltaic cell. IZO (Zn-doped Indium oxide) and IZrO (Zr-doped Indium oxide) films, in the range thickness 10-130 nm, have been deposited by magnetron sputtering onto silicon and glass substrates. Work functions have also been measured via photoemission at ambient pressure.

TCO	Resistivity (Ohm cm)	Mobility (cm <sup>2</sup> / V s)	Carrier density (cm <sup>-3</sup> )	Trasparency (% @ λ = 550nm)	Work Function (eV)
IZO (136 nm)	5,44 10 <sup>-4</sup>	17,4	6,61 x10 <sup>20</sup>	80	4.54
IZrO (11 nm)	6,4 x10 <sup>-4</sup>	22,7	4,82 x10 <sup>19</sup>	85	4.74

The next step was a first attempt of implementing these TCOs into semi-finished, cut from 4 inches wafers, crystalline silicon photovoltaic cells produced by the ENEA-Portici. IZO and IZrO films, both around 100 nm thick, were deposited on four structures terminated with n-type or p-type doped silicon. As comparison, the same devices were completed with ITO deposited by ENEA without breaking the fabrication process. Due to the interruption in the cell manufacturing process, with transportation from the ENEA laboratories to those at UniCT, and vice versa, the performances of the devices suffered some problems, e.g. s-shapes and lower life time for the carriers, but V<sub>OC</sub> and IQE were consistent with expectations. As an example, in figure 1 we report the IQE curves of devices deposited with our TCOs and standard ITO.



**Figure 1:** Internal Quantum Efficiency for photovoltaic solar cells with IZO, IZrO deposited at UniCT (1,2,3,4) and ITO deposited at ENEA (5)

# RECENT PROGRESS IN DMSO-FREE TIN PEROVSKITES

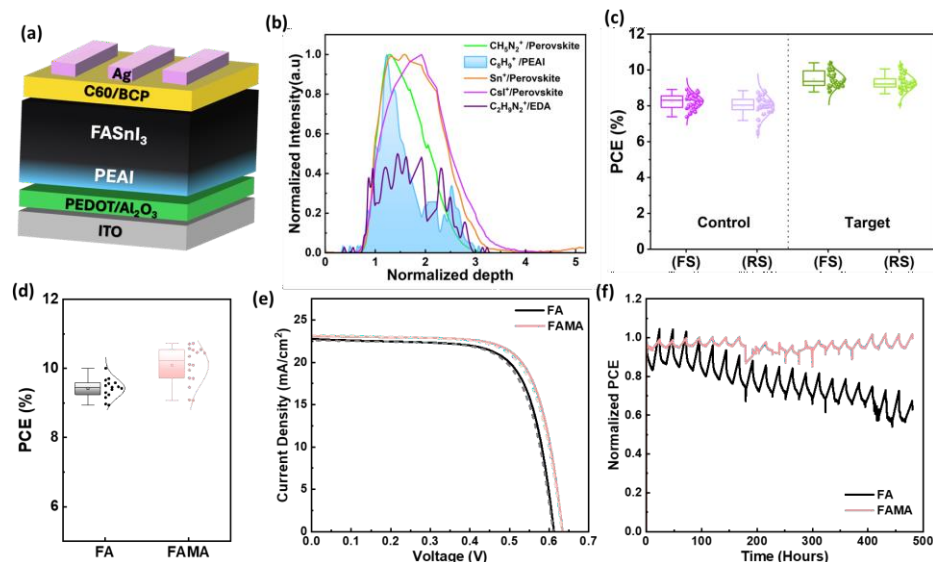
**Debendra Prasad Panda,<sup>1</sup> Muhammad Okash Ur Rehman,<sup>1</sup> Rabeb Issaoui,<sup>1</sup> Madineh Rastgoo,<sup>1</sup> Lorenzo Miele,<sup>1</sup> and Antonio Abate<sup>1,2</sup>**

<sup>1</sup>Department of Chemical, Materials and Industrial Production Engineering, University of Naples Federico II, Naples 80125, Italy

<sup>2</sup>Helmholtz-Zentrum Berlin für Materialien und Energie (HZB), Hahn-Meitner-Platz 1, 14109 Berlin, Germany

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Dimethyl sulfoxide (DMSO) is a widely used solvent for processing perovskite solar cells (PSCs). Although it regulates the crystallisation dynamics, it also induces several detrimental effects, such as catalysing the deprotonation of A-site cations, promoting interfacial void formation, and facilitating iodine extraction from the perovskite film, eventually leading to device degradation. Besides, it oxidises Sn<sup>2+</sup> to Sn<sup>4+</sup>, which results in self p-doping, limiting the performance of tin-PSCs.<sup>[1,2]</sup> Therefore, DMSO-free processing route is crucial for efficient tin-PSCs. Previously, we have demonstrated an alternative solvent system, a mixture of DEF (N,N-Diethylformamide) and DMPU (N,N-Dimethylpropyleneurea) for tin-PSC fabrication, which can completely suppress the Sn<sup>2+</sup> oxidation. Recently, by using a pyridinium additive, we improved the crystallisation dynamics and achieved a PCE of 9.5%. Later, the introduction of a n-dopant, DMBI has shown excellent improvement compared to the reference devices, demonstrating a PCE of 9.7%. Further, by employing a unique interface diffusion strategy, where bulky PEA<sup>+</sup> cations from the bottom interface of perovskite diffuse into the bulk during film formation, we have achieved a PCE of 10.4% (Figure 1a-c). Recently, we have achieved PCE of 10.7% by substituting formamidinium with methylammonium cation, which suppresses the lone pair expression and enhances the efficiency and stability of tin-PSCs (Figure 1d-f).



**Figure 1.** (a) Schematic of device architecture. (b) ToF-SIMS measurement showing PEA<sup>+</sup> located in the perovskite region of the stack. (c) Statistics of PCE of Control and PEA<sup>+</sup> diffused tin-PSCs. (d) Statistics of PCE of FA and FAMA-based devices. (e) Champion J-V and (f) PCE tracked under maximum power point.

[1] Di Girolamo, *et al.* *ACS Energy Lett.* **2021**, *6*, 959–968.

[2] Panda, D. P., *et al.* *ACS Energy Lett.* **2025**, *10*, 3789–3798.

# DESIGN OF STRONG AND WEAK INTERMOLECULAR INTERACTIONS TO ENGINEER BURIED INTERFACES IN INVERTED WIDE-BANDGAP PEROVSKITE SOLAR CELLS

**Annamaria Petrozza**

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The interfaces between the charge extraction layers and the perovskite layer are critical in defining the performance and stability of wide-bandgap (WBG) perovskite solar cells (PSCs). They govern multiple critical factors affecting the operation of photovoltaic devices such as the energetics of the contact, and the crystallization process of the thin film, thus its structural and electronic quality. Self-assembled monolayers (SAMs) have emerged as promising candidates as hole-selective materials for inverted PSCs, thanks to the flexibility provided by the large library of their functional groups. Herein, we outline a molecular hybridization strategy through the incorporation of the histamine molecule into the [4-(3,6-dimethyl-9H-carbazol-9yl)butyl]phosphonic acid (Me-4PACz), which is one of the most common hole extracting layers. Playing with intermolecular strong and weak interactions, we can contextually act on multiple processes. The proton transfer from the phosphonic acid group of the Me-4PACz to the ethylamine functional group of histamine enables the design of the interface dipole to facilitate hole extraction and minimize recombination losses. Then, the protonated amines balance the nucleation of halide components and stabilize the halide ions in the perovskite, avoiding their migration. Thus, three-dimensional nanovoids and tensile stress at the bottom surface were reduced, stabilizing the buried interface. Finally, the  $\pi$ - $\pi$  interactions between the imidazole moiety and Me-4PACz improve the molecular assembling of the SAM, reducing disorder at the interfacial contact. The general impact of these results has been tested on PSCs based on lead mix-halide perovskites with two different bandgaps. The inverted WBG PSCs with 1.77 eV bandgap present a power conversion efficiency (PCE) of 20.34%, and maintain 95.5% of the initial PCE after 1000 hours of continuous illumination. The highly challenging WBG PSCs with 1.83 eV bandgap deliver a PCE of 18.99% with a  $V_{oc}$  as high as 1.364 V-ranking among the highest reported PCEs and  $V_{oc}$  values for such large bandgap.

# REDEFINING SOLAR ENERGY WITH LOW-DIMENSIONAL PEROVSKITES: BREAKTHROUGHS IN ACTIVE MATERIALS AND INTERFACE CONTROL

**Matteo Degani<sup>1</sup>, Riccardo Pallotta<sup>1</sup>, Francesco Toniolo<sup>1</sup>, Masoud Karimipour<sup>2</sup>, Chang-Qi Ma<sup>3</sup>, Alessandro Mirabelli<sup>4</sup>, Tianyu Xu<sup>3</sup>, Samuel D. Stranks<sup>4</sup>, Monica Lira Cantù<sup>2</sup>, and Giulia Grancini<sup>1</sup>**

<sup>1</sup>University of Pavia, Italy

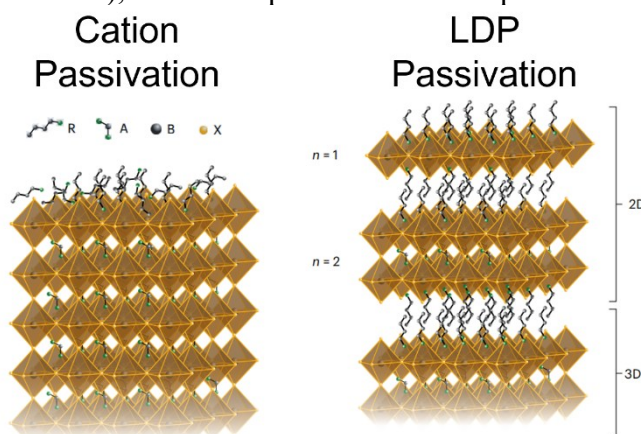
<sup>2</sup>Institute of Nanoscience and Nanotechnology (ICN2), Spain

<sup>3</sup>Suzhou Institute of Nano-Tech and Nano-Bionics, China

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The use of large organic molecules, either as active materials or as passivating agents for perovskite surfaces, has emerged as a highly effective strategy. Indeed, by controlling the crystal growth of perovskites, it is possible to obtain efficient active layers with a large bandgap [1]. On the other hand, the incorporation of organic salts effectively suppresses interfacial defects, mitigates non-radiative recombination, and consequently enhances both the efficiency and long-term stability of perovskite solar cells (PSCs). Depending on their chemical nature and deposition conditions, these cations can self-assemble into ultrathin molecular layers or induce the formation of low-dimensional perovskite phases, each imparting distinct structural and electronic effects on device operation [2]. The effectiveness of such passivation strategies also depends on the device architecture (regular or inverted), and two representative examples will be presented [3–4].



**Figure 1:** Schematic representation of passivation using large organic molecules

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- [4] F. Toniolo, L. Pancini, A. Oranskaia, N. Mrkyvkova, P. Siffalovic, R. Pallotta, M. Degani, F. Doria, U. Schwingenschlögl, G. Grancini, submitted

# OPTIMIZATION OF NARROW- AND WIDE-BANDGAP SUBCELLS FOR EFFICIENT 4-TERMINAL ALL-PEROVSKITE TANDEM SOLAR CELLS

**Marina Ustinova<sup>1,2</sup>, Erica Magliano<sup>2,1</sup>, Federico Trezzini<sup>1</sup>, Renhao Zheng<sup>1</sup>, Francesco Toschi<sup>2</sup>, Aldo Di Carlo<sup>1,2</sup>**

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Perovskite solar cells are considered highly promising for next-generation photovoltaics due to their tunable bandgap and low-cost fabrication. All-perovskite tandem architectures can overcome the efficiency limitations of single-junction devices, but their practical realization is hindered by instability of Pb-Sn narrow-bandgap absorbers and interfacial losses in wide-bandgap cells. Addressing these challenges requires optimization of perovskite composition and charge transport layers.

In this work, we designed a wide-bandgap top cell and a mixed Pb-Sn perovskite (with 1.26 eV bandgap) bottom cell for the fabrication of 4-terminal all-perovskite tandem solar cells. Through improved passivation of the wide-bandgap perovskite layer, as well as its interfaces with the charge transport layers—specifically self-assembled monolayers such as MeO-2PACz and Me-4PACz as HTLs and PCBM/AZO as ETLs—we enhanced the  $V_{OC}$  and fill factor (FF), achieving a power conversion efficiency (PCE) of 15%. To address the problem of instability of the low-band gap perovskite subcell containing PEDOT:PSS, alternative HTL materials were applied. Furthermore, we present a comparative study of the influence of various additives on the performance of Pb-Sn perovskite solar cells. The best combination of additives significantly enhanced  $V_{OC}$  and FF of the  $APb_{0.5}Sn_{0.5}I_3$  solar cells (A=Cs, MA, and FA) up to 0.9V and 78%, respectively. The stabilized PCE of 18.9 % was achieved in the encapsulated p-i-n single junction solar cells. For further improvement of the intrinsic photostability of the Pb-Sn perovskite absorber layer, the fabrication process for the alternative narrow-band-gap absorber  $FAPb_{0.5}Sn_{0.5}I_3$  was optimized. Preliminary results have demonstrated a PCE of 14%, highlighting the potential of  $FAPb_{0.5}Sn_{0.5}I_3$  for further development to achieve more stable and efficient bottom subcell, suitable for tandem applications. The combination of the obtained subcells in the 4-terminal all-perovskite tandem cells provided the PCE of 22.5 %.

*We acknowledge the GOPV project RdS2019-21 CSEAA\_00011 - TIPO A - Ministry of Environment and Energy Security (MASE) – CUP E83C23000840001*



# MODELING AND SCREENING OF OPTIMIZED PEROVSKITE MATERIAL

**Filippo De Angelis,<sup>1,2,3</sup>**

<sup>1</sup>*University of Perugia, Italy*

<sup>2</sup>*INSTM, Italy*

<sup>3</sup>*SKKU Institute of Energy Sci. & Tech. (SIEST), SKKU, Korea*

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Perovskite solar cells are making their way to the market despite intrinsic instability issues remain. Also, replacing lead by less toxic elements remains a major challenge, with tin likely being the only suitable alternative. While lead-based perovskites are affected by instability related to iodide oxidation, tin based materials are plagued by stability of Sn(IV) phases, which are related to the lower oxidation potential of tin compared to lead. A related phenomenon is the stability of tin vacancies, which introduce significant p-doping in tin-halide perovskites, while their lead-based counterpart are essentially intrinsic semiconductors. Defect activity clearly controls doping and could also contribute to the instability towards Sn(IV) phases. Controlling doping and defect activity thus represents a pathway towards obtaining stable perovskites with optimal optoelectronic properties. The different defect activity of tin- and lead-based materials is at the origin of their respective thermal and phot-induced degradation phenomena, including halide demixing and loss of I<sub>2</sub> in lead-halide perovskites.

Here we present results of advanced modelling studies on the defect mediated degradation pathways of prototypical lead- and tin-based materials. We show that iodine chemistry dominates lead-based perovskites while Sn-vacancies are central in promoting both material p-doping and formation of Sn(IV) phases. Interestingly, while p-doping dominates in the bulk, Sn oxidation is only favoured at surfaces or grain boundaries. Thus achieving uniform thin films coupled with proper surface passivation strategies represent a pathway towards achieving more stable THP-based devices. We further unveil the key factors determining the stability of mixed-halide THPs against photoinduced halide segregation phenomena. Molecular and ionic strategies to mitigate p-doping in THPs are also presented.

# LOW-TEMPERATURE STRAIN-FREE SEMI-SOLID/LIQUID ENCAPSULATION FOR PEROVSKITE SOLAR CELLS AND MODULES

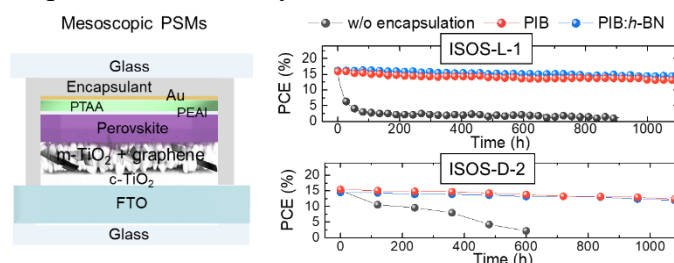
**Sanjay Thorat,<sup>1</sup> Cosimo Anichini,<sup>1</sup> Jessica Barichello,<sup>2</sup> Paolo Mariani,<sup>2</sup> Miguel Molina García,<sup>1</sup> Marilena I. Zappia,<sup>1</sup> Elena Magliano,<sup>2</sup> Luca Gabatel,<sup>1</sup> Antonio E. Del Rio Castillo,<sup>1</sup> Sara Pescetelli,<sup>2</sup> Luigi Vesce,<sup>2</sup> Fabio Matteocci,<sup>2</sup> Sebastiano Bellani,<sup>1</sup> Aldo Di Carlo,<sup>2</sup> and Francesco Bonaccorso<sup>1</sup>**

<sup>1</sup>BeDimensional S.p.A., Via Lungotorrente Secca 30R, 16163 Genova, Italy

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Perovskite solar cells (PSCs) are emerging as a high-efficiency photovoltaic technology, but their instability is posing challenges to their commercialization. Recent stability assessments have been conducted on perovskite solar farms,<sup>[1]</sup> but reliable accelerated aging tests on large-area cells still remain insufficient. To achieve a Levelized Cost of Energy (LCoE) comparable to commercial silicon photovoltaics, perovskite solar modules (PSMs) are expected to provide stable output for at least 20 years in outdoor conditions, while withstanding thermomechanical stresses caused by temperature fluctuations. In this study, we present an innovative industrially compatible encapsulation process by laminating low-temperature strain-free semi-solid/liquid encapsulant adhesives onto PSC/PSMs. In addition, the incorporation of two-dimensional (2D) hexagonal boron nitride (*h*-BN) flakes, produced by liquid-phase exfoliation,<sup>[2]</sup> into the polymeric matrix enhances the barrier and thermal management characteristics of the encapsulant. The proposed encapsulated PSCs and PSMs withstood multifaceted accelerated aging tests, including ISOS-D1 preconditioning (240 h), ISOS-D2 (85°C, >1000 h), ISOS-L1 (light soaking, >1000 h), as well as a customized thermal shock test (200 cycles) and modified humidity freeze test (10 cycles), retaining more than 80% of their initial power conversion efficiency.<sup>[3]</sup> Our results represent a significant progress towards the realization of long-term stable PSMs by using industrially compatible laminable advanced composite encapsulants enabled by 2D materials.



**Figure 1:** a) Schematic of the cell layout in which the non-compact layers of the device are fully covered by the encapsulant. b) Evolution of power conversion efficiency in time of the PSC not encapsulated, encapsulated with PIB and PIB:h-BN under ISOS-L-1 and ISOS-D-2 conditions.

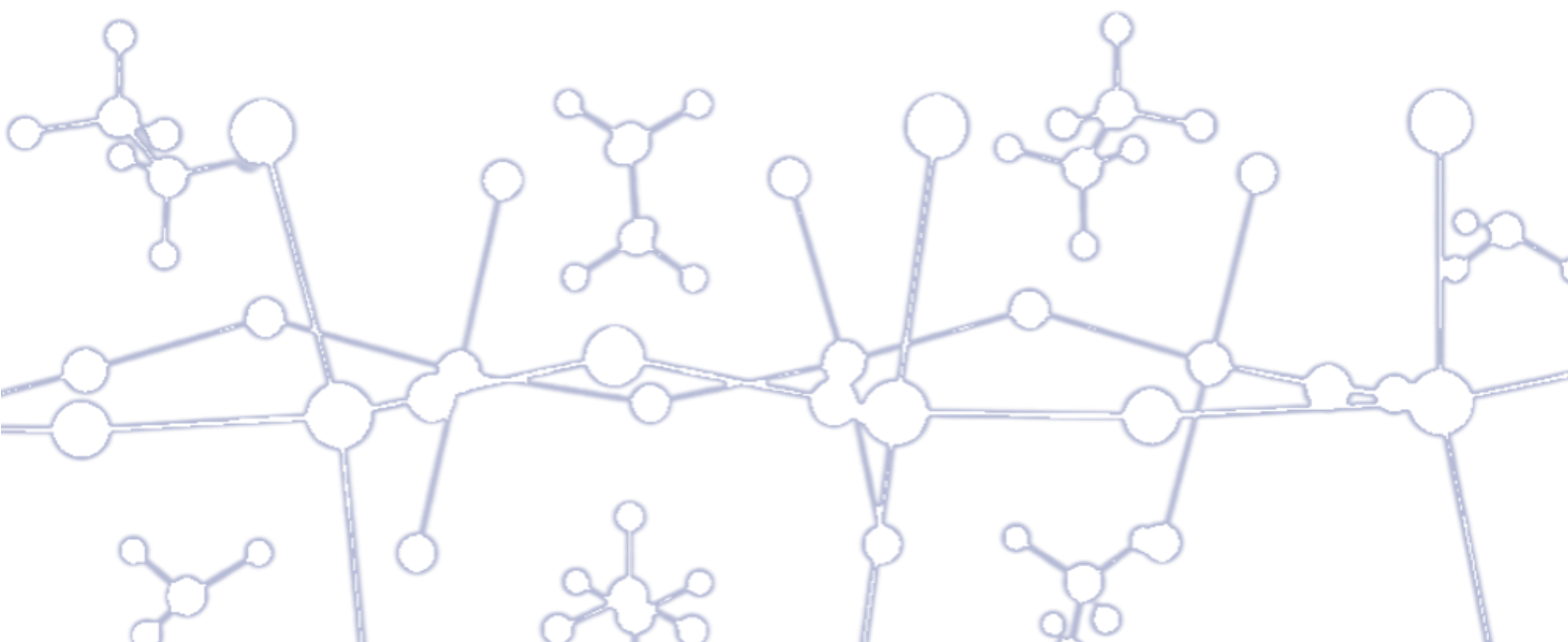
**Acknowledgements:** This project received funding from the European Union's DIAMOND Horizon Europe research and innovation action under grant agreement No. 101084124. This project received funding from the Italian Ministero della Transizione Ecologica (MITE), GoPV project.

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13:45 14:00		OPENING PSCO 2025	
		<b>Town Hall</b>	
<b>Session Chair</b>		<b>Filippo De Angelis, University of Perugia, Italy</b>	
<b>Session Title</b>		<b>Session 1 – Invited Lectures</b>	
14:00	14:25	1° INVITED LECTURE - <b>Nam Gyu Park</b> , SKKU, South Korea <i>Perovskite solar cells from nip to pin</i>	
14:25	14:50	2° INVITED LECTURE - <b>Rui Wang</b> , Westlake University, China <i>Recent progress on perovskite-based photovoltaics</i>	
14:50	15:15	3° INVITED LECTURE – <b>Pablo Boix</b> , ITQ (UPV-CSIC), Spain <i>Turning crystallization into a characterization tool for perovskite-based devices</i>	
15:15	15:40	4° INVITED LECTURE – <b>Seigo Ito</b> , University of Hyogo, Japan <i>Ion migration in carbon-based multi-porous-layered-electrode perovskite solar cells (MPLE-PSCS)</i>	
15:40	15:45	1° SPONSOR SPEACH - DJK Europe GmbH	
15:45 16:15		<b>COFFEE BREAK PM</b>	
		<b>Town Hall</b>	
<b>Session Chair</b>		<b>Filippo De Angelis, University of Perugia, Italy</b>	
<b>Session Title</b>		<b>Session 2 – Invited Lectures</b>	
16:15	16:40	5° INVITED LECTURE - <b>Saiful Islam</b> , Oxford University, United Kingdom <i>Like people, perovskites are not perfect: atomistic insights into molecular passivation &amp; defect migration</i>	
16:40	17:05	6° INVITED LECTURE - <b>Joseph M. Luther</b> , National Renewable Energy Lab, United States <i>Chirality in hybrid metal halide semiconductors and quantum dots</i>	
17:05	17:30	7° INVITED LECTURE – <b>Sascha Feldmann</b> , Ecole Polytechnique Fédérale de Lausanne, Switzerland <i>Tracking charge, spin and light polarization in space &amp; time in halide perovskites</i>	
17:30	17:33	2° SPONSOR SPEACH - NIREOS	



# PEROVSKITE SOLAR CELLS FROM NIP TO PIN

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Meeting the escalating electricity demands of our advancing society, particularly at the terawatt scale, requires achieving high power conversion efficiency and low cost per peak watt in solar cell technology simultaneously. Before the advent of perovskite solar cells (PSCs), only a limited range of materials and technologies could satisfy both criteria. This presentation will detail the evolution towards practical solid-state perovskite solar cells and outline future research directions in this field. Beginning with an overview of initial technologies, the discussion progresses to the emergence of solid-state perovskite solar cells. The initial implementations of methylammonium lead iodide (MAPbI<sub>3</sub>) perovskite as sensitizers in liquid-electrolyte-contained structures yielded disappointing results, with efficiencies as low as 3-4% in 2009 and susceptibility to MAPbI<sub>3</sub> dissolution. A breakthrough occurred in 2012 with a pioneering study demonstrating a 9.7% efficient PSC that remained stable for 500 hours, achieved by employing a solid hole transporting material. This key advancement rendered PSCs a viable and durable technology. Power conversion efficiency of 27% has been recently achieved from the inverted (PIN) structure with formamidinium lead iodide (FAPbI<sub>3</sub>), making it a strong competitor to existing solar technologies. With their immense potential for sustainable energy, PSCs represent a game-changing solution and will be ready for commercialization once stability challenges are successfully addressed.

# RECENT PROGRESS ON PEROVSKITE-BASED PHOTOVOLTAICS

**Rui Wang**,<sup>1</sup>

<sup>1</sup> *Department of Materials Science and Engineering at Westlake University, Zhejiang Province, PR China*  
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Perovskite materials, most notably organo-lead iodide species, have recently demonstrated great potential in future high-performance photovoltaics. Our group has made contributions to addressing the complex scientific challenges in perovskite solar cells, leveraging a multidisciplinary background that spans materials science, information science, and energy science. Leveraging cross-disciplinary expertise, new hole transport materials and amidinium-based modifier molecules were designed and synthesized to achieve precise modulation of perovskite properties. Innovative characterization methodologies were employed to elucidate new mechanisms for the enhancement of device stability and regulate the surface electronic state of perovskite materials. Through the development of thick-film preparation techniques and electrical passivation strategies, high-efficiency perovskite/CIGS tandem solar cells were successfully realized. In this talk, I will present our recent progress in improving the stability, efficiency, and reproducibility of perovskite-based photovoltaics and discuss the potential for commercialization

# TURNING CRYSTALLIZATION INTO A CHARACTERIZATION TOOL FOR PEROVSKITE-BASED DEVICES

**Pablo P. Boix**

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Metal halide perovskites combine exceptional optoelectronic properties with structural and chemical versatility, making them compelling alternatives to conventional semiconductors. Yet, their instability and performance limitations demand deeper insights into the fundamental links between crystallization, material evolution, and device operation. While crystallization control is often viewed primarily as a synthetic challenge, it can also serve as a powerful characterization platform.

We demonstrate humidity-driven in situ nanocrystal composite formation, enabling real-time monitoring of 0D–3D perovskite evolution with photoemission efficiencies above 90% and enhanced stability suitable for photocatalysis<sup>[1-2]</sup>. Confined monocrystal growth integrated into high-performance memristors provides a direct window into electroformation processes and resistive switching mechanisms<sup>[3]</sup>. Complementarily, advanced impedance spectroscopy captures phase dispersion effects associated with ionic modulation, while current–voltage curve reconstruction reveals recombination resistances and guides optimization pathways in tin-based solar cells<sup>[4-5]</sup>.

Altogether, this multidimensional framework illustrates how crystallization can act as both a driver of improved device performance and a versatile probe of material properties across length scales. By turning crystallization into a characterization tool, we uncover key degradation pathways, identify stability–efficiency trade-offs, and provide actionable insights for the design of robust, application-oriented perovskite devices.

**Acknowledgements:** *This work is part of the project PID2023-151880OB-C31 funded by MICIU/AEI/10.13039/501100011033 and by ERDF/EU. The work was partially funded by Generalitat Valenciana for the funding via Pla Gent-T (grant ESGENT 010/2024). These results are part of the grant CNS2023-144270 funded by MICIU/AEI/10.13039/501100011033 and by European Union NextGenerationEU/PRTR*

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[5] O. Solís et al., *ACS Energy Lett.*, **2024**

# ION MIGRATION IN CARBON-BASED MULTI-POROUS-LAYERED-ELECTRODE PEROVSKITE SOLAR CELLS (MPLE-PSCS)

**Seigo Ito**<sup>1</sup>

<sup>1</sup>*Graduate School of Engineering, University of Hyogo, Japan.*  
[itou@eng.u-hyogo.ac.jp](mailto:itou@eng.u-hyogo.ac.jp)

Organic-inorganic metal halide perovskite solar cells (PSCs) were developed by Prof. T. Miyasaka's group in 2009, and the PCE has rapidly increased over 26.6%, now. In order to fabricate cost-effective and high-stable PSCs for the commercialization, our group has focused on the fabrication of multi-porous-layered-electrode PSCs (MPLE-PSCs), which have exceptional stability (experimental acceleration test over 3,000 h in damp-heat tests (85 °C and 85% RH.) in accordance with IEC 61215:2021).

In this study, we compared the operational performance of MPLE-PSCs using 5-AVA-MAPbI<sub>3</sub> and CsFAPbI<sub>3</sub> under varying scan rates and capacitance conditions. The 5-AVA-MAPbI<sub>3</sub>-based devices exhibited notable ion migration and charge accumulation, particularly at high scan rates, which may negatively affect the operational performance. In contrast, CsFAPbI<sub>3</sub>-based devices showed stable  $J-V$  characteristics, reduced hysteresis, and consistent photocurrent generation under continuous illumination[1]. However, while the long-term stability of 5-AVA-MAPbI<sub>3</sub> is well-established in the literature, long-term data for CsFAPbI<sub>3</sub> remain limited, emphasizing the need for further investigation. These findings highlight the importance of selecting appropriate perovskite materials and optimizing device architectures to enhance stability and accelerate the commercialization of MPLE-PSCs.

In the conference, we will discuss the origin of capacitance and ion migration of MPLE-PSCs in details.

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[1] R. Tsuji, S. Ito, *et al.*, *ACS Energy Lett.* **2025**, *10*, 1275–1283.

# LIKE PEOPLE, PEROVSKITES ARE NOT PERFECT: ATOMISTIC INSIGHTS INTO MOLECULAR PASSIVATION & DEFECT MIGRATION

**Saiful Islam**<sup>1</sup>

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Further breakthroughs in perovskite solar cells and optoelectronics require advances in new compositions and underpinning materials science. Indeed, a deeper understanding of these halide perovskite materials requires atomic- and nano-scale characterization of their transport, electronic, defect and stability behaviour. This presentation will describe recent combined atomistic modelling and experimental studies on metal halide perovskites<sup>[1-4]</sup> in two fundamental areas related to improving operational stability in optoelectronic devices: (i) insights into passivating perovskites with molecular compounds including surface interactions of amino-silane additives; (ii) investigating the effects of different sized A-cations, B-site cation dopants and mixed Pb-Sn compositions on iodide-ion migration in halide perovskites.

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  - [4] A.N. Arber et al., *Chem. Mater.*, **2025**, 37, 4416.

# CHIRALITY IN HYBRID METAL HALIDE SEMICONDUCTORS AND QUANTUM DOTS

**Joseph M. Luther,<sup>1,5</sup> Md. Azimul Haque,<sup>1</sup> Young-Hoon Kim,<sup>1</sup> Shripathi Ramakrishnan,<sup>1,2</sup> Ruyi Song,<sup>3</sup> Andrew Greider,<sup>4</sup> Junxiang Zhang,<sup>5</sup> Qiuming Yu,<sup>2</sup> Seth R. Marder,<sup>1,5</sup> Volker Blum,<sup>3</sup> Yuan Ping,<sup>4</sup> Matthew C. Beard,<sup>1,5</sup>**

<sup>1</sup>*National Renewable Energy Laboratory, Golden, CO, USA*

<sup>2</sup>*Cornell University, Ithaca, NY, USA*

<sup>3</sup>*Duke University, Durham, NC, USA*

<sup>4</sup>*University of Wisconsin, Madison, WI, USA*

<sup>5</sup>*University of Colorado, Boulder, CO, USA*

[joey.luther@nrel.gov](mailto:joey.luther@nrel.gov)

In hybrid metal halide semiconductors based on the family of halide perovskites, interesting effects can arise from inclusion of chiral molecules. Chiroptical properties result and are typically induced from structural symmetry breaking by incorporating a chiral “A-site” organic cation within the structure. Restricting this to A-sites limits the compositional space. Another route involves highly efficient “remote chirality transfer” where chirality can be imposed on an otherwise achiral hybrid metal halide semiconductor by a proximal chiral molecule that is not interspersed as part of the structure yet leads to large circular dichroism dissymmetry factors (gCD) of up to 10<sup>-2</sup>. Density functional theory calculations reveal that the transfer of stereochemical information from the chiral proximal molecule to the inorganic framework is mediated by selective interaction with divalent metal cations. Anchoring of the chiral molecule induces a centro-asymmetric distortion, which is discernible four to five inorganic layers into the metal halide lattice. These properties enable a new class of devices with additional functionality regarding photons with controlled polarizations, and spin based magneto devices.

# TRACKING CHARGE, SPIN AND LIGHT POLARIZATION IN SPACE & TIME IN HALIDE PEROVSKITES

**Sascha Feldmann**<sup>1</sup>

<sup>1</sup>*Ecole Polytechnique Fédérale de Lausanne, Switzerland*  
[sascha.feldmann@epfl.ch](mailto:sascha.feldmann@epfl.ch)

Solution-processable semiconductors like halide perovskites and certain molecules are promising for next-generation spin-optoelectronic applications.<sup>[1]</sup> Yet, we don't fully understand what governs spin and light polarization in these materials, and even less how these are affected by chirality.<sup>[2]</sup>

In this talk, I will give an overview of our recent efforts to understand the spin-optoelectronic performance of these materials through time-, space- and polarization-resolved spectroscopy and microscopy.

For investigating halide perovskite films, we pushed broadband circular dichroism to diffraction-limited spatial and 15 fs time resolution for creating a spin cinematography technique to witness the ultrafast formation of spin domains due to local symmetry breaking and spin-momentum locking.<sup>[3]</sup>

I will then briefly explain the fundamentals and artefacts involved in measuring circularly polarized luminescence reliably and introduce an open-access methodology and code to do so.<sup>[4]</sup> Finally, I will show our most recent development of a transient sensitive broadband full-Stokes spectroscopy with unprecedented time and polarization resolution to track the emergence of chiral light emission.<sup>[5]</sup>

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[1] *Nature Reviews Materials* **8**, 365 (2023).

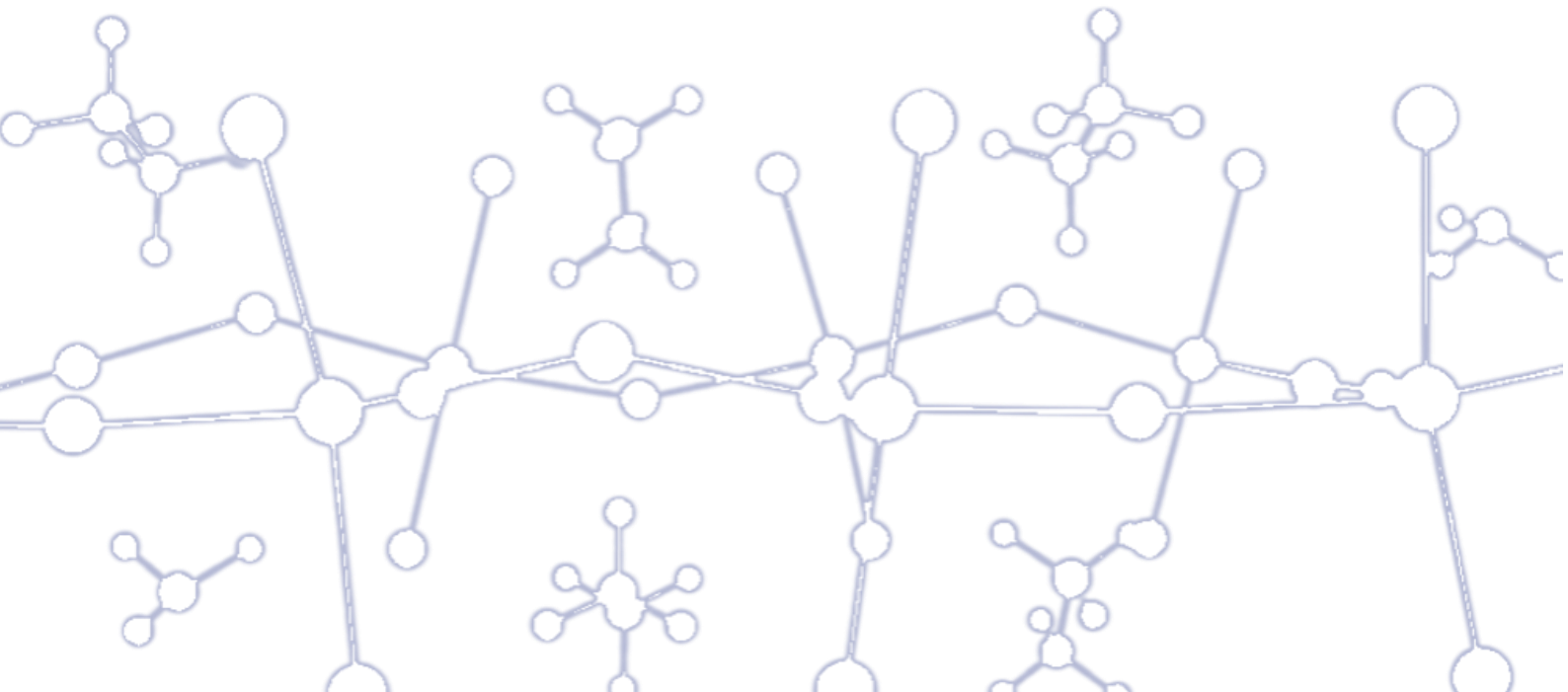
[2] *Nature Reviews Chemistry* **9**, 208 (2025).

[3] *Nature Materials* **22**, 977 (2023).

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[5] *Nature*, <https://doi.org/10.1038/s41586-025-09197-3> (2025).

	Town Hall		Trumpet	
Session Chair	Maria Vasilopoulou, University of Athens, Greece		Selina Olthof, University of Wuppertal, Germany	
Session Title	Session 2A – Characterization 1		Session 2B – Stability 2	
17:33 17:45	<b>Matthias Diethelm</b> , Fluxim AG, Switzerland <i>Probing ionic conductivity and electric field screening in perovskite solar cells: a novel exploration through ion drift currents</i>		<b>Matteo Degani</b> , University of Pavia, Italy <i>Circular recovery of critical components in perovskite solar cells via green solvent processing for high-efficiency and low-impact devices</i>	
17:45 17:57	<b>Cecilia Daniela Costa</b> , Istituto Italiano di Tecnologia, Italy <i>Water-based recycling strategies for lead recovery from end-of-life perovskite solar cells</i>		<b>Muhammad Bilal</b> , Queen Mary University of London, United Kingdom <i>Insights into degradation pathways of triple-cation perovskite thin films under outdoor and indoor conditions: a comparative analysis</i>	
17:57 18:09	<b>Jiaxing Du</b> , Oxford University, United Kingdom <i>Inter-layer diffusion of excitations in 2D perovskites revealed by photoluminescence reabsorption</i>		<b>Gurpreet Kaur</b> , Oxford University, United Kingdom <i>Crystallization via aerosol processing mitigates intrinsic quantum confinement effects and boosts optoelectronic performance of FAPbI3 films</i>	
18:09 18:21	<b>Karen Radetzky</b> , Uppsala University, Sweden <i>In situ interface formation and characterization for inverted architecture perovskite solar cells</i>		<b>Markus Griesbach</b> , University of Bayreuth, Germany <i>Exploring photoinduced phase segregation in mixed halide perovskite powders</i>	
18:21 18:25	<b>COMFORT BREAK</b>			



# PROBING IONIC CONDUCTIVITY AND ELECTRIC FIELD SCREENING IN PEROVSKITE SOLAR CELLS: A NOVEL EXPLORATION THROUGH ION DRIFT CURRENTS

**Matthias Diethelm,<sup>1,a</sup> Tino Lukas,<sup>1</sup> Joel Smith,<sup>1</sup> Akash Dasgupta,<sup>1</sup> Pietro Caprioglio,<sup>1</sup> Moritz Futscher,<sup>2</sup> Roland Hany,<sup>3</sup> Henry J. Snaith<sup>1</sup>**

<sup>1</sup>Department of Physics, University of Oxford, Clarendon Laboratory, Oxford OX13PU, UK

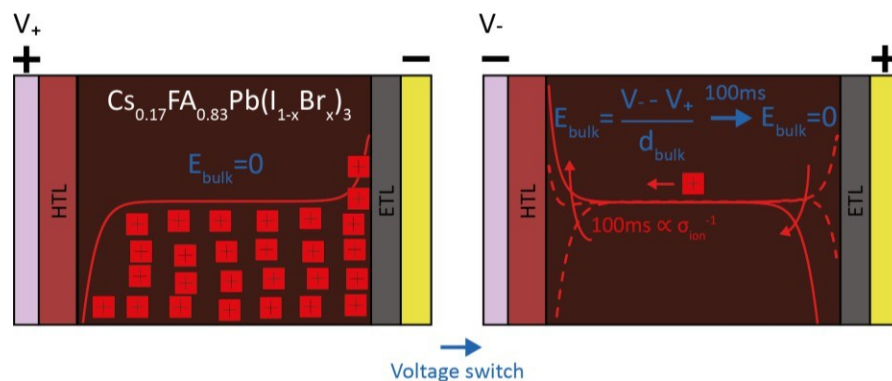
<sup>2</sup>Empa, Swiss Federal Laboratories for Materials Science and Technology, Laboratory for Thin Films and Photovoltaics, CH-8600 Dübendorf, Switzerland

<sup>3</sup>Empa, Swiss Federal Laboratories for Materials Science and Technology, Laboratory for Functional Polymers, CH-8600 Dübendorf, Switzerland

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It is widely accepted that mobile ions are responsible for the slow electronic responses observed in metal halide perovskite-based optoelectronic devices, and strongly influence long-term operational stability. Electrical characterisation methods mostly observe complex indirect effects of ions on bulk/interface recombination, struggle to quantify the ion density and mobility, and are typically not able to fully quantify the influence of the ions upon the bulk and interfacial electric fields. We analyse the bias-assisted charge extraction (BACE) method for the case of a screened bulk electric field, and introduce a new characterisation method based on BACE, termed ion drift BACE. We reveal that the initial current density and current decay dynamics depend on the ion conductivity, which is the product of ion density and mobility. This means that for an unknown high ion density, typical in perovskite solar absorber layers, the mobility cannot be directly obtained from BACE measurements. We derive an analytical model to illustrate the relation between current density, conductivity and bulk field screening, supported by drift-diffusion simulations. By measuring the ion density independently with impedance spectroscopy, we show how the ion mobility can be derived from the BACE ion conductivity. We highlight important differences between the low- and high-ion density cases, which reveal whether the bulk electric field is fully screened or not. Our work clarifies the complex ion-related processes occurring within perovskite solar cells and gives new insight into the operational principles of halide perovskite devices as mixed ionic-electronic conductors. <sup>[1]</sup>



**Figure 1: Graphical abstract**

[1] M. Diethelm, T. Lukas, J. Smith, A. Dasgupta, P. Caprioglio, M. Futscher, R. Hany and H. J. Snaith, *Energy Environ. Sci.* **2025**, 18, 1385–1397.

# CIRCULAR RECOVERY OF CRITICAL COMPONENTS IN PEROVSKITE SOLAR CELLS VIA GREEN SOLVENT PROCESSING FOR HIGH-EFFICIENCY AND LOW-IMPACT DEVICES

**Matteo Degani,<sup>1</sup> Valentina Larini,<sup>1</sup> Riccardo Pallotta,<sup>1</sup> Fabiola Faini,<sup>1</sup> Lorenzo Pancini,<sup>1</sup> Filippo Doria,<sup>1</sup> Changzeng Ding,<sup>2</sup> Chang-Qi Ma,<sup>2</sup> Giulia Grancini<sup>1</sup>**

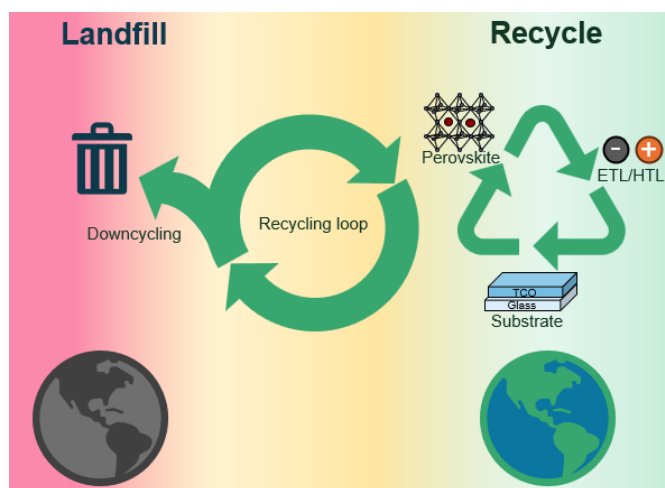
<sup>1</sup>University of Pavia, Italy

<sup>2</sup>Suzhou Institute of Nano-Tech and Nano-Bionics, China

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Environmental imperatives and international regulations are increasingly demanding sustainable solutions for the end-of-life management of perovskite solar cells (PSCs). In this context, we demonstrate a robust and circular recycling approach employing green solvents to recover and reuse the most critical and environmentally impactful components of PSCs.<sup>[1]</sup> In particular, transparent conductive oxide (TCO)-coated glasses—accounting for 56% of the total cost and 96% of the carbon footprint of PSC modules—are efficiently refurbished from n-i-p architectures using dimethyl sulfoxide to selectively dissolve the upper device layers. Employing the recovered substrates, new-generation PSCs are produced reaching a champion power conversion efficiency (PCE) of 22.6%, matching that of devices based on fresh components.<sup>[2]</sup>

The iterative reuse of these components underscores the technical feasibility of the proposed protocol. Furthermore, a comparative life cycle assessment (LCA) between this recovery strategy and conventional landfill treatment for both PSCs and silicon photovoltaics demonstrates the clear environmental advantages of the recycling route, including lower energy consumption and a reduced ecological footprint. This study highlights a scalable and environmentally responsible pathway toward the circular manufacturing of perovskite solar technologies.



**Figure 1:** Schematic representation of virtuous versus non virtuous PSC-derived waste disposal

[1] Larini, V., Ding, C., Wang, B., Pallotta, R., Faini, F., Pancini, L., Zhao, Z., Cavalli, S., Degani, M., De Bastiani, M., Doria, F., Ma, C.-Q., You, F. and Grancini, G., *EES Solar* **2025**, 1(3), 378–390.

[2] Larini, V., Ding, C., Faini, F., Pica, G., Bruni, G., Pancini, L., Cavalli, S., Manzi, M., Degani, M., Pallotta, R., De Bastiani, M., Ma, C. Q. & Grancini, G., *Advanced Functional Materials* **2023**, 2306040, 1–8.

# WATER-BASED RECYCLING STRATEGIES FOR LEAD RECOVERY FROM END-OF-LIFE PEROVSKITE SOLAR CELLS

**Cecilia Daniela Costa**,<sup>1</sup> **Dongho Kang**,<sup>2</sup> **Fillipo Drago**,<sup>3</sup> **Annamaria Petrozza**,<sup>2</sup> **Isabella Poli**<sup>1</sup>

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The most efficient halide perovskite solar cells (PSC) rely on the use of Pb, which remains essential for achieving high photovoltaic performance. Furthermore, metal alternatives have lower availability than Pb.<sup>[1]</sup> However, one of the main barriers to the large-scale commercialization of PCS modules is the toxicity associated with lead, particularly if devices are discarded in landfills at the end of their life cycle.<sup>[2]</sup> Recycling therefore emerges as a solution to mitigate environmental risks while recovering valuable materials. Moreover, from an economic standpoint, the recovery of strategic materials such as conductive glass, HTL materials, and metal contacts can make the process more cost-effective.

Common recycling approaches involve polar aprotic solvents such as dimethylformamide (DMF),  $\gamma$ -butyrolactone (GBL), or dimethyl sulfoxide (DMSO) to dissolve the perovskite layer.<sup>[3-4]</sup> However, their toxicity raises serious health and environmental concerns. Water-based recycling processes are more environmentally friendly, yet they often result in incomplete recovery, typically yielding PbI<sub>2</sub> while leaving behind high concentrations of Pb in the aqueous waste.<sup>[5]</sup> Moreover, most recycling protocols are tested in as-fabricated devices, while end-of-life devices may undergo structural and chemical changes due to ageing.

Our work focuses on the recovery of strategic materials from end-of-life devices, aiming to close the loop through reintegration into the production cycle. We avoid the use of toxic solvents and ensure that no Pb is released into the environment. We develop water-based Pb recovery strategies using metal-organic frameworks (MOF) as green adsorbents. To minimize the environmental impact of the adsorbent, we selected materials with high natural availability and low toxicity. Additionally, we compare ball milling, a low-energy, solvent-free synthesis method, with the conventional solvothermal approach to produce these MOFs, moving toward scalable and sustainable recycling solutions.

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[1] A. B. Gian, *European Commission, Study on the EU's list of Critical Raw Materials – Final Report* **2020**.

[2] G. Flora, *Interdiscip. Toxicol.* **2012**, *5*(2), 47–58.

[3] B. J. Kim, *Nature Communications* **2016**, *7*, 11735.

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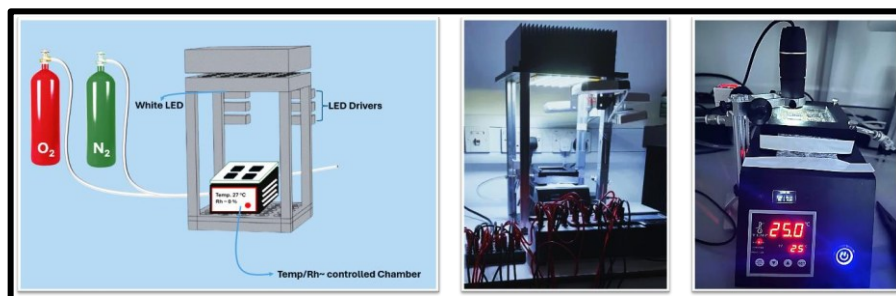
[5] F. Schmidt, *Journal of Hazardous Materials* **2023**, *447*, 130829.

# INSIGHTS INTO DEGRADATION PATHWAYS OF TRIPLE-CATION PEROVSKITE THIN FILMS UNDER OUTDOOR AND INDOOR CONDITIONS: A COMPARATIVE ANALYSIS

**Muhammad Bilal,<sup>1</sup> Madsar Hameed,<sup>1</sup> Jing Li,<sup>1</sup> Joe Briscoe,<sup>1</sup> Zhe Li<sup>1\*</sup>**

<sup>1</sup>*School of Engineering and Materials Science, Queen Mary University of London, UK*  
[m.bilal@qmul.ac.uk](mailto:m.bilal@qmul.ac.uk), [zhe.li@qmul.ac.uk](mailto:zhe.li@qmul.ac.uk)

The remarkable tunability of perovskite materials perfectly aligns with the requirements of indoor photovoltaic applications, presenting a promising alternative to conventional batteries for powering the Internet of Things (IoT).<sup>[1]</sup> The power conversion efficiency (PCE) of mixed perovskite solar cells under indoor conditions has exceeded 40%, but there is a lack of rational data on the stability and degradation pathways of perovskites under indoor low-light conditions.<sup>[2]</sup> To address this challenge we investigate the degradation pathways of triple-cation perovskite  $\text{Cs}_{0.05}(\text{FA}_{0.77}\text{MA}_{0.23})_{0.95}(\text{I}_{0.77}\text{Br}_{0.23})_3$  thin films, under controlled outdoor and indoor environments. Using a combination of XRD, SEM, UV-Vis, and XPS and PL analyses, we explored how high and low light intensities under inert, pure oxygen, and humidity conditions influence structural, morphological, and chemical stability. Results indicate distinct degradation pathways in outdoor and indoor conditions. Outdoor light exposure accelerates degradation via lead iodide formation and phase transitions to orthorhombic structures, while indoor lighting preserves the tetragonal phase with minimal degradation. Humidity was identified as a critical factor, causing severe structural breakdown and the formation of lead-based oxide and carbonate complexes. These findings underscore the promising potential for perovskite-based devices to achieve enhanced long-term stability under controlled, low-light environments, where degradation is significantly minimized compared to high-intensity or outdoor light exposure.



**Figure 1** Experimental framework for investigating stability in perovskite thin film

[1] D. Dou, H. Sun, C. Li, S. Gan, L. Li, “Perovskite-Based Indoor Photovoltaics and their Competitors” *Advanced Functional Materials* **2024**, *34*, 2314398.

[2] Y. Tang, Z. Zhang, H. Liu, M.H. Aldamasy, M. Bilal, F. Yang, J. Yang, C. Qin, Y. Yang, Z. Li, Y. Liu, M. Li, “Balancing bandgap and charge transport in triple-cation perovskite for efficient indoor photovoltaics” *Science China Materials* **2024**, *67*, 2611-2617.

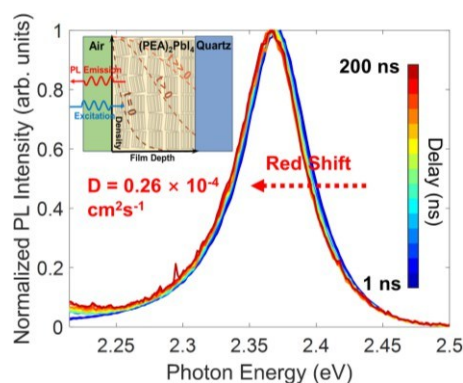
# INTER-LAYER DIFFUSION OF EXCITATIONS IN 2D PEROVSKITES REVEALED BY PHOTOLUMINESCENCE REABSORPTION

**Jiaxing Du,<sup>1</sup> Marcello Righetto,<sup>\*1</sup> Manuel Kober-Czerny,<sup>1</sup> Siyu Yan,<sup>1</sup> Karim A. Elmostekawy,<sup>1</sup> Henry J. Snaith,<sup>1</sup> Michael B. Johnston,<sup>1</sup> Laura M. Herz<sup>\*1</sup>**

<sup>1</sup>Department of Physics, University of Oxford, United Kingdom  
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Two-dimensional lead halide perovskites (2DPs) offer chemical compatibility with three-dimensional perovskites and enhanced stability, which are attractive for applications in photovoltaic and light-emitting devices.<sup>[1-2]</sup> However, such lowered structural dimensionality causes increased excitonic effects and highly anisotropic charge-carrier transport.<sup>[3-4]</sup> Determining the diffusivity of excitations, in particular for out-of-plane or inter-layer transport, is therefore crucial, yet challenging to achieve. Here, we demonstrate an effective method for monitoring inter-layer diffusion of photoexcitations in (PEA)<sub>2</sub>PbI<sub>4</sub> thin films by tracking time-dependent changes in photoluminescence spectra induced by photon reabsorption effects.<sup>[5]</sup> Through selective photoexcitation from either substrate- or air-side of the films we reveal differences in diffusion dynamics encountered through the film profile. We extract time-dependent diffusion coefficients from spectral dynamics through a one-dimensional diffusion model coupled with an interference correction for refractive index variations arising from the strong excitonic resonance of 2DPs.<sup>[5]</sup> Such analysis, together with structural probes, shows that minute misalignment of 2DPs planes occurs at distances far from the substrate, where efficient in-plane transport consequently overshadows the less efficient out-of-plane transport in the direction perpendicular to the substrate. Through detailed analysis, we determine a low out-of-plane excitation diffusion coefficient of  $(0.26 \pm 0.03) \times 10^{-4} \text{ cm}^2\text{s}^{-1}$ , consistent with a diffusion anisotropy of  $\sim 4$  orders of magnitude.<sup>[5]</sup>

**Figure:** Excitation diffusion in (PEA)<sub>2</sub>PbI<sub>4</sub> thin films tracked by the photon-reabsorption method



[1] Z. Wang, Q. Lin, F. P. Chmiel, N. Sakai, L. M. Herz, H. J. Snaith, *Nat. Energy* **2017**, 2, 17135.

[2] L. R. V. Buizza, T. W. Crothers, Z. Wang, J. B. Patel, R. L. Milot, H. J. Snaith, M. B. Johnston, L. M. Herz, *Adv. Funct. Mater.* **2019**, 29, 1902656.

[3] X. Lou, Y. Li, H. Lei, Y. Zhang, H. Zhou, E. Shi, H. Zhu, *ACS Nano* **2024**, 18, 20659.

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[5] J. Du, M. Righetto, M. Kober-Czerny, S. Yan, K. A. Elmostekawy, H. J. Snaith, M. B. Johnston, L. M. Herz, *Adv. Funct. Mater.* **2025**, 2421817.

# CRYSTALLIZATION VIA AEROSOL PROCESSING MITIGATES INTRINSIC QUANTUM CONFINEMENT EFFECTS AND BOOSTS OPTOELECTRONIC PERFORMANCE OF FAPbI<sub>3</sub> FILMS

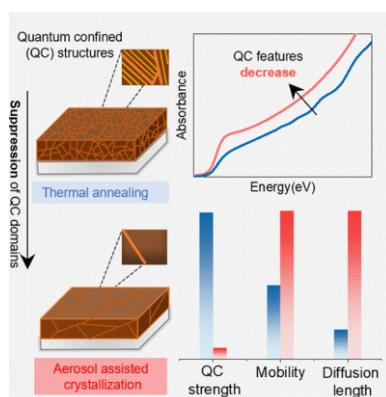
**Gurpreet Kaur,<sup>1</sup> Madsar Hameed,<sup>2</sup> Michael Johnston,<sup>1</sup> Joe Briscoe,<sup>2</sup> Laura Herz<sup>1</sup>**

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Formamidinium lead iodide (FAPbI<sub>3</sub>) is widely recognized as a benchmark perovskite absorber, offering great potential for efficient and scalable photovoltaic devices. However, its full potential is compromised by its inherent tendency to exhibit intrinsic quantum confinement (QC) effects, originating from the spontaneous formation of confined nanodomains in otherwise bulk films. The presence of these domains is distinctly identified as high energy features in the absorption spectrum and has been correlated with reduced photovoltaic efficiency. In this talk, I will present our recent efforts to address this challenge through the deployment of an aerosol-assisted crystallization (AAC) strategy. As unfolded by our experimental findings, this approach enables the fabrication of highly crystalline FAPbI<sub>3</sub> films while concurrently suppressing the formation of QC nanodomains. By leveraging a suite of complementary steady-state and time-resolved optical spectroscopic approaches, we further demonstrate that AAC processed films exhibit substantially reduced non-radiative recombination, higher charge-carrier mobilities, and extended carrier diffusion lengths compared to those prepared by conventional thermal annealing. The observed improvements in key optoelectronic metrics are driven by a synergistic effect of enhanced structural coherence and mitigation of quantum-confined regions. Taken together, these findings position AAC as a powerful strategy for overcoming persistent limitations in FAPbI<sub>3</sub> film fabrication, offering a clear pathway toward enhanced photovoltaic performance.



**Figure 1:** Suppression of QC effects in FAPbI<sub>3</sub> films prepared via aerosol-assisted crystallization enhances carrier mobility and diffusion length

## Acknowledgements:

[1] G. Kaur, M. Hameed, J. E. Lee, K. A. Elmostekawy, M. B. Johnston, J. Briscoe, L. M. Herz, *J. Phys. Chem. Lett.* **2025**, *16*, 9, 2212-2222.

# IN SITU INTERFACE FORMATION AND CHARACTERIZATION FOR INVERTED ARCHITECTURE PEROVSKITE SOLAR CELLS

**Karen Radetzky,<sup>1,2</sup> Alberto García-Fernández,<sup>3</sup> Birgit Kammlander,<sup>1</sup> Julia Prumbs,<sup>1,2</sup> Brian Rydgren,<sup>1,2</sup> Evelyn Johannesson,<sup>1,2</sup> Rahul Varma,<sup>1</sup> Håkan Rensmo,<sup>1</sup> Ute Cappel<sup>1,2</sup>**

<sup>1</sup>Department of Physics and Astronomy, Uppsala University, Sweden

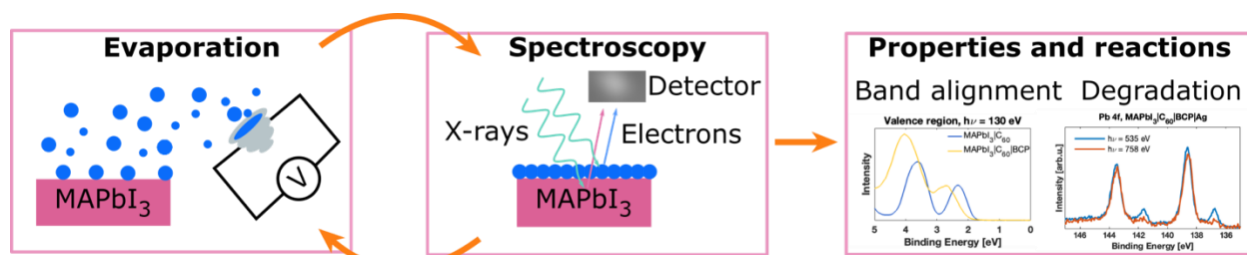
<sup>2</sup>Wallenberg Initiative Materials Science for Sustainability, Uppsala University, Sweden

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Organic inorganic lead halide perovskites are at the forefront of novel solar cell development due to their highly desirable optoelectronic properties. To approach facile scale-up, p-i-n architecture cells utilizing straightforward deposition techniques are increasingly investigated. In these devices, remaining charge losses are mainly associated with recombination at interfaces between the perovskite and charge transport layers.<sup>[1]</sup> Additionally, absorber phase decomposition under external stressors hinders commercialization as ion movement and chemical reactions drive deterioration within the material stack.<sup>[2]</sup> As a result, it is imperative to understand the interfaces present in the device, including energetic alignment, and reactions occurring during interface formation and operation. The presented research addresses the above by focusing on MAPbI<sub>3</sub> single crystals with consecutive in situ evaporation of charge transport layers and a silver back contact. Thereby, we fabricated a well-defined half-cell model system for an inverted perovskite solar cell.

We use X-ray photoelectron spectroscopy to attain quantitative, qualitative, and energetic information on the present species and reaction products.<sup>[3]</sup> In my talk, I will present high-quality synchrotron data from the above-described experiment. By tracking characteristic core levels, the energetic alignment between the different materials was determined including the observation of significant downwards band bending of C60 to BCP (Figure 1). This is suggested to benefit efficient charge extraction in a full device. Furthermore, ion movement is observed and followed in relation to the layer assembly. The permeability of the different materials to iodide ions becomes evident. Under illumination, we further observe the irreversible diffusion of Ag which results in perovskite degradation. Yet, the recorded data suggests that this can be mitigated by thicker passivation layers of BCP for which formation and coordination of Ag<sup>+</sup> is observed. Along these examples the talk will explain and demonstrate the great utility of in situ characterization methods for informed materials design to the perovskite community.



**Figure 1:** Scheme of the experimental procedure followed to fabricate and measure in situ interfaces.

[1] J. Warby et al., *Advanced Energy Materials* **2022**, 12(12).

[2] D. B. Khadka, *ACS Applied Energy Materials*, **2021**, 4(10).

[3] A. García-Fernández, *Materials Chemistry Frontiers*, **2024**, 8(21).

# EXPLORING PHOTOINDUCED PHASE SEGREGATION IN MIXED HALIDE PEROVSKITE POWDERS

**Markus Griesbach**,<sup>1</sup> **Fatemeh Haddadi Barzoki**,<sup>2</sup> **Tobias Siegert**,<sup>1</sup> **Anna Köhler**,<sup>1</sup> **Helen Grüninger**<sup>2</sup>

<sup>1</sup>*Soft Matter Optoelectronics, University of Bayreuth, Germany*

<sup>2</sup>*Inorganic Chemistry and Bavarian Center for Battery Technology (BayBatt), University of Bayreuth, Germany*  
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Mixed halide perovskites have emerged as leading contenders for multi-junction solar cells, thanks to their tunable band gaps—controlled by halide composition—and excellent optoelectronic properties. Yet, their potential is held back by a key weakness: phase instability. In compounds like MAPbI<sub>3-x</sub>Br<sub>x</sub>, exposure to light drives halide segregation, splitting the material into iodine- and bromine-rich domains that ultimately compromise device performance. Despite extensive research, the mechanisms behind this light-induced instability remain poorly understood, as they are shaped by a complex interplay of a multitude of different factors.

In this study, we synthesized a suite of MAPbI<sub>1.5</sub>Br<sub>1.5</sub> powders via mechanochemical routes<sup>[1]</sup> using different synthesis strategies, starting with precursor powders MAX and PbX<sub>2</sub> (X=I or Br) or parent perovskite powders MAPbI<sub>3</sub>/MAPbBr<sub>3</sub> as educts for the ball milling procedure. Additionally, we prepared mixed halide perovskite powders incorporating varying amounts of the ionic liquid BMIMBF<sub>4</sub>, which has been shown to act as a passivating agent.<sup>[2]</sup> We characterized the structural and optical properties of the samples using a range of complementary methods, such as SEM, X-ray diffraction (XRD), thermally stimulated luminescence (TSL) as well as photoluminescence and solid-state NMR spectroscopy. We found that the different synthesis approaches lead to systematic changes in crystallite size and defect density among otherwise compositionally similar powder samples.

To investigate phase segregation behavior, we performed in-situ XRD measurements under illumination. We find that the segregation kinetics are primarily governed by the defect density, whereas the extent of segregation, i.e. the thermodynamics, is dictated by crystallite size. In particular, in small crystallites the halides separate less, and we predict that segregation even completely ceases below a threshold of around 10-15 nm. The recovery behavior of the segregated samples in the dark, was governed by different factors than the segregation process. In particular, the presence of BMIMBF<sub>4</sub> decreases the segregation rate, yet enhances (re-)mixing rates.

Together, these findings provide more profound experimental insight on the kinetics and thermodynamics of halide segregation and its correlation to material structure, which might offer a pathway toward more stable perovskite materials for photovoltaic applications in the future.

## ***Acknowledgements:***

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[2] Ramming, P. et al., *J. Mater. Chem. C* **2021**, *9*, 11827-11837.

		<b>Town Hall</b>
<b>Session Chair</b>	<b>Lorenzo Malavasi, University of Pavia and INSTM, Italy</b>	
<b>Session Title</b>	<b>Poster Pitch Presentations (2 minutes each)</b>	
18:25	18:27	<b>Tianshan Xu</b> , University of Bayreuth, Germany <i>MAPbBr<sub>3</sub>-MAPbI<sub>3</sub> gradient films prepared at room temperature by Powder Aerosol Deposition (PAD) for controlled ion and electron transport</i>
18:27	18:29	<b>Qimu Yuan</b> , Oxford University, United Kingdom <i>Atomistic and photo-physical insights into vapour-deposited CsPbBr<sub>3</sub> and CsPbI<sub>3</sub> perovskites for emission and phase-stability enhancement</i>
18:29	18:31	<b>Allison Arber</b> , Oxford University, United Kingdom <i>Ion Migration and Dopant Effects in the Gamma-CsPbI<sub>3</sub> Perovskite Solar Cell Material: Atomistic Insights through Ab Initio and Machine Learning Methods</i>
18:31	18:33	<b>Ruohan Zhao</b> , Oxford University, United Kingdom <i>From solution to thin-film: approaches to improving the optoelectronic properties of halide perovskites</i>
18:33	18:35	<b>Lars Sonneveld</b> , AMOLF, The Netherlands <i>Resolving local structure in metal halide perovskites using SEM-EBSD by minimizing beam damage</i>
18:35	18:37	<b>Dilek Çırak</b> , Ege University Solar Energy Institute, Turkey <i>Unveiling the future of perovskite solar cells: the promising potential of additive for precursor stability</i>
18:37	18:39	<b>Amanda Covarelli</b> , University of Perugia, Italy <i>Additives in metal-halide perovskite solar cells: a computational study</i>
18:39	18:41	<b>Debrenda Prasad Panda</b> , University of Naples "Federico II", Italy <i>Suppressing the Stereochemically Active Lone Pair Expression in Tin Perovskite Solar Cells</i>
18:41	18:43	<b>Daphne Dekker</b> , AMOLF, The Netherlands <i>Greener and more stable mixed lead-tin halide perovskites using DMS</i>
18:43	18:45	<b>Maximilian Spies</b> , University of Bayreuth, Germany <i>Solvated PbI<sub>2</sub> clusters preceding the crystallization of lead halide perovskites – a UV/VIS in-situ study</i>
18:45	18:47	<b>Sebastian Hedwig</b> , FHNW Univ. of Applied Sciences and Arts Northwestern Switzerland, Switzerland <i>Indium and silver recovery from perovskite thin film solar cell waste by means of nanofiltration</i>
18:47	18:49	<b>Sevdiye Basak Turgut</b> , Ege University Solar Energy Institute, Turkey <i>Utilization of ionic liquids in triple-cation perovskite solar cells</i>
18:49	18:51	<b>Gulay Zeynep Gunel</b> , Ege University Solar Energy Institute, Turkey <i>Functionalized P-type triazatruxene-based self-assembly monolayers for perovskite solar cells</i>
18:51	18:53	<b>Müge Özdemir</b> , Ege University Solar Energy Institute, Turkey <i>Scalable fabrication of perovskite quantum dot layers with inkjet printing</i>
18:53	19:45	<b>POSTER SESSION &amp; SOCIAL APERITIVO</b>
19:45	20:00	<b>FREE TIME</b>
20:00	22:00	<b>WELCOME DINNER</b>

# MAPbBr<sub>3</sub>-MAPbI<sub>3</sub> GRADIENT FILMS PREPARED AT ROOM TEMPERATURE BY POWDER AEROSOL DEPOSITION (PAD) FOR CONTROLLED ION AND ELECTRON TRANSPORT

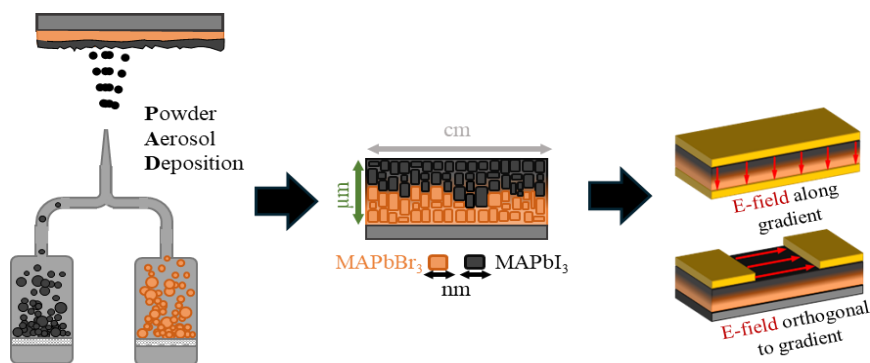
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In halide perovskites, the diffusion of ions, driven by an electric field, concentration gradients, or light, usually causes an electric field that impacts the motion of electrons. This coupling of ion and electron transport is undesired, leading, e.g. to hysteresis in solar cell structures due to the much slower ion motion than electron motion.<sup>[1]</sup> In this study, we report a novel approach to fabricate MAPbBr<sub>3</sub>-MAPbI<sub>3</sub> gradient films at room temperature using the Powder Aerosol Deposition method (PAD) [Figure 1], a solvent-free and scalable technique. This method enables the use of mechano-chemically synthesized powders to deposit dense films at room temperature, thereby decoupling the halide synthesis from film formation.<sup>[2,3]</sup> The resulting gradient films enable spatially resolved optical and electrical measurements, thus providing deeper insights into ion-electron interactions and field-dependent phenomena in complex perovskite systems.



**Figure 1:** Left: Schematic illustration of Powder Aerosol Deposition for fabricating a MAPbBr<sub>3</sub> (orange)-MAPbI<sub>3</sub> (black) vertical gradient film.<sup>[3]</sup> Middle: MAPbBr<sub>3</sub> (orange)-MAPbI<sub>3</sub> (black) vertical gradient film. Right: Electric field configurations for gradient film characterization.

SEM images of the PAD-gradient films show that a dense and nanocrystalline film structure is achieved. EDX mapping reveals a clear vertical distribution of bromide and iodide, indicating the formation of a compositional gradient within the film. The resulting gradient structure enables spatial control over halide composition, leading to tailored band alignment and improved separation of ion and electron transport. We investigated the effects of applying electric fields both along and perpendicular to the compositional gradient, focusing on how electric field orientation influences ionic and electronic transport properties—characterized by impedance spectroscopy—as well as optical behavior, probed by fluorescence lifetime microscopy (FLIM). This work highlights the potential of Powder Aerosol Deposition for engineering perovskite interfaces and advancing the design of high-efficiency, stable perovskite solar cells.

[1] C. Li et al., *Adv. Mater.* **2016**, 28, 2446-2454.

[2] S. Biberger et al., *Solar RRL* **2023**, 7, 2300261.

[3] F. Panzer et al., *Materials* **2016**, 9, 277.

# ATOMISTIC AND PHOTO-PHYSICAL INSIGHTS INTO VAPOUR-DEPOSITED CsPbBr<sub>3</sub> and CsPbI<sub>3</sub> PEROVSKITES FOR EMISSION AND PHASE-STABILITY ENHANCEMENT

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Vapour deposition is an established, solvent-free method well-suited for the uniform growth of metal-halide perovskites (MHPs) thin films, and their integration into optoelectronic devices.<sup>[1-2]</sup> In particular, all-inorganic MHPs of CsPbX<sub>3</sub> (X = Br or I) have garnered significant attention, owing to enhanced thermal durability and facile fabrication compared to the organic-inorganic counterparts. However, there currently lacks a detailed account of the crystallisation process of vapour-deposited inorganic perovskites, especially on both microstructural and atomistic scales. Therefore, we coupled photo-physical investigations with scanning transmission electron microscopy (STEM) and systematically scrutinised co-deposited  $\gamma$ -CsPbBr<sub>3</sub><sup>[3]</sup> and  $\gamma$ -CsPbI<sub>3</sub>.<sup>[4]</sup> For CsPbBr<sub>3</sub>, which is an ideal candidate for perovskite laser applications, we examined the impact on the amplified spontaneous emission (ASE) characteristics from varying precursor flux ratios of CsBr:PbBr<sub>2</sub> (Cs:Pb) from Cs-deficient (0.85:1) to Cs-rich (3:1). We obtained important insights on the thin-film growth: at both Cs-deficient and Cs-rich conditions, formation of CsPb<sub>2</sub>Br<sub>5</sub> and Cs<sub>4</sub>PbBr<sub>6</sub> impurity phases are consistently associated with a poor and incomplete crystallisation. With high Cs-excess ratios, presences of Ruddlesden-Popper (RP) planar defects act as major sources of non-radiative recombination centres which quench the photoluminescence (PL) emission. Nevertheless, a small amount of CsBr excess during co-evaporation (Cs:Pb=1.5:1) can significantly improve the resulting microstructures, achieving films with a homogenous, compact, and uniform morphology. We observed well-defined grains >500 nm in size with a highly oriented growth. Moreover, we elucidate that films with a Cs:Pb ratio of 1.5:1 exhibit relative suppression of both impurity phases and RP-defects, which all together attribute to enhanced absorption coefficient, PL intensity, and favourable ASE thresholds.<sup>[3]</sup> In the homologous CsPbI<sub>3</sub> system, achieving stable CsPbI<sub>3</sub> with an orthorhombic  $\gamma$ -phase from vapour deposition is currently a major challenge. Here, we underline the importance of excess Cs as a prerequisite for phase-stable  $\gamma$ -CsPbI<sub>3</sub> owing to the formation of RP planar faults and turning points, which both alleviate the internal lattice strain. However, increasing trap-mediated recombination dynamics are identified concurrently, with the density of RP-defects increasing linearly with the CsI:PbI<sub>2</sub> precursor molar ratio, which is detrimental to PL emission and charge-carrier lifetime. Therefore, for the incorporation of  $\gamma$ -CsPbI<sub>3</sub> as the active layer into efficient solar cells and optoelectronic devices, the degree of Cs-excess must be carefully fine-tuned for a balance of both phase-stability and optoelectronic performance.<sup>[4]</sup>

[1] Yuan. Q et al., *ACS Applied Material & Interfaces* **2022**, 15(1), 772–781.

[2] Zizlsperger, M., Nerreter, S., Yuan, Q et al., *Nature Photonics* **2024**, 18(9), 975-981.

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# ION MIGRATION AND DOPANT EFFECTS IN THE GAMMA-CsPbI<sub>3</sub> PEROVSKITE SOLAR CELL MATERIAL: ATOMISTIC INSIGHTS THROUGH AB INITIO AND MACHINE LEARNING METHODS

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Inorganic halide perovskites such as CsPbI<sub>3</sub> are attracting increasing attention for solar cell and optoelectronic applications. Ionic migration is known to be an important factor for perovskite behavior, but the impact of cation dopants on iodide diffusion in the room temperature orthorhombic gamma-CsPbI<sub>3</sub> is not fully understood, especially at the atomic level. Here, we investigate the effect on iodide migration of incorporating different cations (including Sn<sup>2+</sup>, Ba<sup>2+</sup>, and Cu<sup>2+</sup>) into gamma-CsPbI<sub>3</sub>, focusing on maintaining an inorganic phase rather than doping with molecular organic ions. Through a combination of ab initio and machine learning (ML) techniques, our results show that the simulated structure, band gap and ion migration energies are in good agreement with experimental data. We find that partial Pb-site substitution does not have a major suppressing effect on iodide ion transport, which is important in guiding future doping work. An ML interatomic potential model was derived, for the first time, for large-scale simulations (~80 ns) of the pristine and Sn-doped materials, which reveal iodide diffusion paths along the Pb-I octahedral edges with no correlated cation motion. Structural analysis indicates an ordered cation sublattice, but disorder in the anion sublattice indicative of high iodide ion mobility similar to fast-ion conductors.

# FROM SOLUTION TO THIN-FILM: APPROACHES TO IMPROVING THE OPTOELECTRONIC PROPERTIES OF HALIDE PEROVSKITES

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Metal halide perovskites have emerged as outstanding semiconductors for solar cells due to their excellent optoelectronic properties. Among these materials, formamidinium lead iodide (FAPbI<sub>3</sub>) is particularly notable as a competitive candidate for single-junction solar cells because of its optimal bandgap. However, a significant challenge is that the photoactive  $\alpha$ -phase FAPbI<sub>3</sub> can easily undergo phase transition to an undesired  $\delta$ -phase FAPbI<sub>3</sub> under ambient conditions.<sup>[1]</sup> Additionally, most highly efficient perovskite solar cells are achieved through the solvent- quenching technique, which is incompatible with large-scale production. Conversely, gas quenching is a potential deposition technique which can enable large-scale device fabrication,<sup>[2]</sup> yet using this method, perovskite thin-films fabricated from the traditional DMF/DMSO solvent system suffer from poor optoelectronic properties and stability.<sup>[3]</sup> In this context, achieving high- quality  $\alpha$ -FAPbI<sub>3</sub> via gas quenching is challenging, but it holds great promise for ensuring long- term stability. Here, we use a DMF/NMP solvent system for FAPbI<sub>3</sub> using the gas-quenching method and achieve a power conversion efficiency (PCE) of 21.0% and a steady-state efficiency of 20.3%, achieving the highest efficiency of additive-free FAPbI<sub>3</sub>-based inverted PSCs to date. The devices fabricated using the DMF/NMP solvent system show significantly higher efficiencies than those prepared from DMF/DMSO. We also introduce a bulk additive to modulate crystallisation kinetics and demonstrate that this additive effectively suppresses the formation of undesired hexagonal phase. Interestingly, we find that the additive influences the interactions of the precursor ink with NMP, which was not observed in the DMSO system. Additionally, this treatment prevents undesired phase formation and enhances crystallinity of the  $\alpha$ -FAPbI<sub>3</sub>, leading to improved absolute photoluminescence (PL), device efficiency, and long- term stability. We fabricated inverted-structured FAPbI<sub>3</sub> perovskite solar cells using the gas- assisted technique and show that the inclusion of this additive results in slightly improved device performance, achieving a PCE of 21.7% and a steady-state efficiency of 21.3%. Our findings illuminate the complex chemical interactions within precursor inks, offering valuable insights into their influence on crystallisation behaviour and, consequently, optoelectronic properties.

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[2] Yu, Y., Zhang, F., Hou, T., Sun, X., Yu, H. and Zhang, M., “A Review on Gas-Quenching Technique for Efficient Perovskite Solar Cells” *Solar RRL* **2021**, 5(10), .2100386.

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# RESOLVING LOCAL STRUCTURE IN METAL HALIDE PEROVSKITES USING SEM-EBSD BY MINIMIZING BEAM DAMAGE

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Understanding crystal grain orientation and surface termination is essential for optimizing the performance and stability of perovskite solar cells. While techniques like GIWAXS and XRD provide valuable macroscopic insights, they fall short of resolving crystallographic details at the grain level. Electron backscatter diffraction (EBSD) offers nanoscale resolution but has traditionally been limited in hybrid organic perovskites due to their sensitivity to electron beam-induced damage.

Recent advancements in detector technology and data processing have opened new possibilities for applying EBSD to these materials. In this work, we systematically explore key measurement parameters – such as beam current, accelerating voltage, spot size and exposure time – to understand their effects on both electron beam-induced degradation and signal-to-noise ratio. We introduce data analysis strategies that minimize electron dose, enabling higher-resolution mapping while mitigating damage. Additionally, we investigate local heating effects and demonstrate that operating at lower beam currents significantly reduces thermal degradation.

Our results highlight trade-offs between resolution and stability and provide practical guidelines for optimizing EBSD conditions in sensitive perovskite systems. This work supports the broader goal of enabling detailed microstructural analysis in perovskite research and accelerating the development of more efficient solar devices.

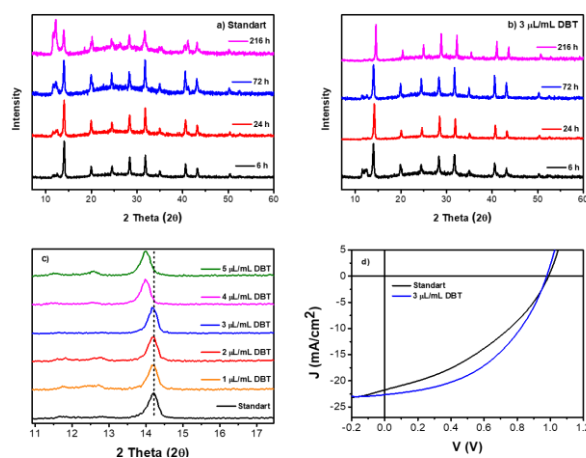
**Acknowledgements:** *We acknowledge the Dutch Research Council (NWO), Gatan (EDAX), Amsterdam Scientific Instruments (ASI) and CL Solutions for financing the project 'Achieving Semiconductor Stability From The Ground Up' (NWO project number 19459)*

# UNVEILING THE FUTURE OF PEROVSKITE SOLAR CELLS: THE PROMISING POTENTIAL OF ADDITIVE FOR PRECURSOR STABILITY

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In this study, 3,4-dibromothiophene (DBT) additive was added to the precursor solution to stabilize the precursor used in the production of solar cells. With the influence of external factors, they are exposed to during the process between synthesis and coating, perovskite precursor solutions exhibit aging effects that are an important roadblock to producing high-efficiency solar cells.<sup>[1]</sup> A thin film coated with fresh solutions after the synthesis of the precursor solutions creates a photoactive black phase, while films made with aged solutions create a non-photoactive yellow phase.<sup>[2]</sup> One of the most effective approaches to reducing these phase transitions is additive engineering. By adding a DBT additive to perovskite precursor solutions, we assume that phase changes would be avoided, and the storage time would be increased. It has been suggested that sulfur atoms in DBT will interact with lead, and bromine's steric effect will help to stabilize the perovskite. XRD, UV-VIS, and AFM analyses were performed to see the effects of additive and aging on the perovskite structure in fresh and aged precursor solutions with different amounts of additives added. According to our results 3  $\mu\text{L}/\text{mL}$  additive is the optimum amount for stabilization because it prevents the formation of the yellow phase without damaging the perovskite structure. In addition, solar cells were produced with the fresh precursor solutions synthesized and performance analyses were carried out.



**Figure 1:** a) XRD peaks of thin films prepared with standard solution and yellow phase formation with aging, b) XRD peaks of thin films prepared with DBT added solutions and suppression of the yellow phase, c) the shift in the XRD peaks due to the incorporation of the additive into the perovskite structure, and d)  $I$ - $V$  performances of solar cells prepared with and without additive solutions.

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[2] X. Wang et al., *Chem.* **2020**.

# ADDITIVES IN METAL-HALIDE PEROVSKITE SOLAR CELLS: A COMPUTATIONAL STUDY

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Perovskite solar cells (PSC) have gained attention in the last years because of their low-cost materials constituents, simple solution fabrication process,<sup>[1]</sup> high absorption coefficient in a wide wavelength range<sup>[2]</sup> and increasing power conversion efficiency (PCE), which has recently reached the value of 26.7 %.<sup>[3]</sup> However, long-term stability is still one of the key issues that impedes rapid commercialization.<sup>[4]</sup> To overcome this problem, different strategies for stabilizing the active layer have been explored, including compositional engineering, controlled morphology, grain size control, perovskite deposition techniques, interfacial engineering, and many others.<sup>[5]</sup> An easy-to-implement approach is the use of additives, which in small quantities fine-tune the materials properties and increase the stability of the devices<sup>[5]</sup>. In this work, I present the results of DFT calculations that have been conducted in this field, placing some additives on a PbI<sub>2</sub> terminated surface of a MAPbI<sub>3</sub> perovskite. The results include optimized geometries, adsorption energies, contact energies, molecular distortion energies, perovskite distortion energies and the PDOS of the systems. These results are important to evaluate the influence of the functional groups on the interactions with the surface: in particular, the final geometries show how the additives connect with the perovskite. The adsorption energy value of CO<sub>2</sub> on the surface of the perovskite obtained with DFT calculations (~ -0.22 eV) is in good agreement with the result obtained with molecular dynamics simulations (~ -0.15 eV). Moreover, all the data will be used to predict target properties of the perovskites, training a machine learning algorithm.

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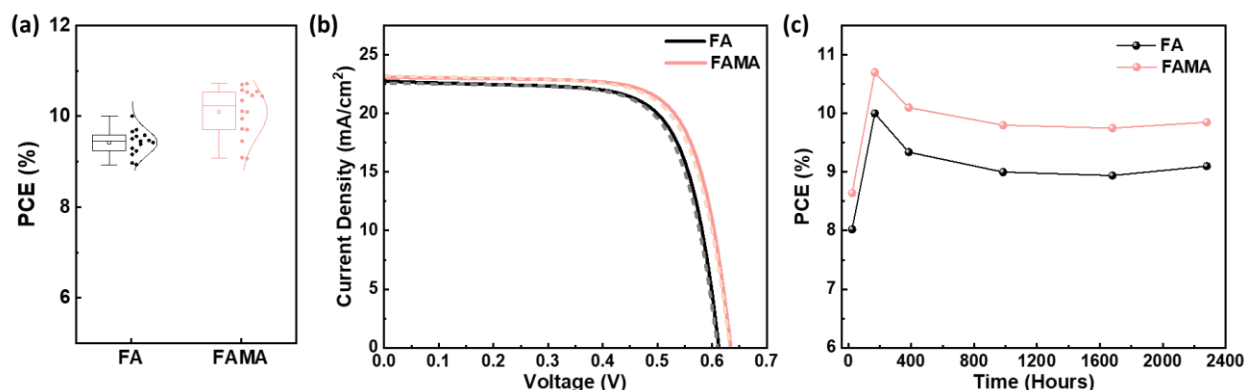
# SUPPRESSING THE STEREOCHEMICALLY ACTIVE LONE PAIR EXPRESSION IN TIN PEROVSKITE SOLAR CELLS

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The stereochemically active  $5s^2$  lone pair in  $\text{Sn}^{2+}$  exhibits stronger expression compared to  $\text{Pb}^{2+}$ , leading to local structural distortions in the perovskite lattice. This enhanced lone-pair activity contributes to emphasis, a dynamic off-centering of the Sn cation, which induces octahedral tilting and electronic disorder.<sup>[1]</sup> Such distortions can increase trap-assisted recombination and reduce charge transport efficiency in tin perovskite solar cells. To lower the emphasis effect, we performed A-site cation engineering, as smaller the A-site cation can reduce the lone-pair effect.<sup>[2]</sup> We substituted formamidinium cation ( $\text{FA}^+$ ) with methylammonium cation ( $\text{MA}^+$ ) as the later has smaller ionic radius. Since, DMSO is known to catalyse the deprotonation of  $\text{MA}^+$  cation,<sup>[3]</sup> we have employed a DMSO-free processing route, using an alternative solvent system. By introducing  $\text{MA}^+$  cation, the power conversion efficiency (PCE) significantly improved as shown in Figure 1a. Figure 1b illustrates the J-V curves of champion control and target devices showing a state-of-the-art PCE of 10.7% for DMSO-free tin perovskite was achieved after MA incorporation. It also improved the device stability, retaining  $\sim 92\%$  of maximum device PCE after 2400 hours of storage. The role of MA incorporation and its effect of reducing the lone-pair expression is well supported by both experimentally and theoretically.



**Figure 1:** (a) Statistical distribution of PCE and (b) J-V curves of champion FA- and FAMA-based tin perovskites. (c) Variation of PCE under storage in  $\text{N}_2$  atmosphere showing FAMA-based tin-PSC retains 92% of the maximum PCE for around 2400 hours.

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# GREENER AND MORE STABLE MIXED LEAD-TIN HALIDE PEROVSKITES USING DMS

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Owing to their low bandgap, mixed lead-tin halide perovskites have considerable potential both in high efficiency single junction solar cells and in all-perovskite tandem solar cells.<sup>[1]</sup> However, due to the facile oxidation of Sn<sup>2+</sup> to Sn<sup>4+</sup>, their stability is inferior to that of their pure lead counterpart, inhibiting this potential. While degradation through external factors can be controlled by proper encapsulation,<sup>[2]</sup> and several additives have successfully been used to prevent oxidation during the fabrication process,<sup>[3]</sup> some intrinsic instability remains.

The usage of dimethyl sulfoxide (DMSO) as a solvent has been identified as one of the culprits for this intrinsic instability. Because DMSO has a very high boiling point, some DMSO molecules remain in the perovskite film, even after annealing, where they can act as a source of oxygen for tin oxidation.<sup>[4]</sup> Some studies have addressed this issue by replacing DMSO by other solvents or additives. However, these often require the use of toxic or environmentally harmful solvents, like dimethylformamide (DMF).<sup>[5]</sup> Recently, Zuo et al. showed a fabrication method that uses DMSO as a solvent but efficiently extracts this from the film by replacing the antisolvent by dimethyl sulfide (DMS). This method improves both efficiency and stability of lead-based perovskite solar cells, while only using green solvents for the fabrication.<sup>[6]</sup>

In this study, we extend this method to mixed lead-tin perovskites. We compare films made using a DMF-based recipe to films made using only green (anti)solvents: DMSO, DMS, and anisole. By optimizing the fabrication, we can form dense, flat films with this recipe. By measuring the photoluminescence quantum yield and photoluminescence lifetime of these films at regular time intervals, we show the differences in their quality and stability. We hereby contribute to the advancement of lead-tin perovskite solar cells, both in terms of performance and stability, and potential for safer scalability.

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[5] G. Nasti, *ACS Energy Letters* **2022**, *7*, 3197-3203.

[6] W. Zuo, *Advanced Materials* **2023**, *35*, 2302889.

# SOLVATED PbI<sub>2</sub> CLUSTERS PRECEDING THE CRYSTALLIZATION OF LEAD HALIDE PEROVSKITES – A UV/VIS IN-SITU STUDY

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The solution-based fabrication of reproducible, high-quality lead iodide perovskite films demands a detailed understanding of the crystallization dynamics, which is mainly determined by the perovskite precursor solution and its processing conditions. We conducted a systematic in-situ study during the critical phase before the nucleation in solution to elucidate the formation dynamics of lead iodide perovskite films. Using UV absorption spectroscopy during spin coating allows us to track the evolution of iodoplumbate complexes present in the precursor solution. We find that prior to film formation, a novel absorption signature at 3.15 eV arises. We attribute this to the emergence of a PbI<sub>2</sub>-DMF solvated (PDS) phase. The amount of PDS phase is closely connected to the concentration of the solution layer during spin coating. We also propose that PDS clusters are a predecessor of crystalline perovskite phases and act as nucleation seeds in the precursor solution. In this way, our work provides insights into the early stages of perovskite crystallization.

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

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The rapid deployment of perovskite solar cells (PSCs) poses challenges for sustainable raw material supply and waste management of the future, particularly due to their use of precious raw materials such as indium (In) and silver (Ag).<sup>[1]</sup> This study presents a novel and environmentally benign process for the recovery of PbI<sub>2</sub>, In and Ag from end-of-life PSCs, integrating hydrometallurgical extraction and advanced nanofiltration (NF) technologies.

Following mechanical dismantling and aqueous PbI<sub>2</sub> recovery,<sup>[2]</sup> In and Ag were extracted using nitric acid, achieving recovery efficiencies of 87 ± 7% for both metals.<sup>[3]</sup> To separate and concentrate these elements from the acidic leachate, we employed a custom-built layer-by-layer (LbL) NF membrane. The LbL membrane demonstrated near-complete In retention (96.9 ± 0.4%) and negligible Ag retention, resulting in a concentrated In stream and a dilute Ag permeate. Compared to a commercial acid-resistant NF membrane, the LbL membrane achieved similar separation performance with significantly lower pressure (5 bar vs. 25 bar) and higher flux (30 L/m<sup>2</sup>h vs. 6 L/m<sup>2</sup>h), reducing energy consumption by over 85%. By modifying their composition, the LbL membranes gained stability towards a number of highly concentrated inorganic acids, expanding their range of applications beyond In / Ag recovery from PSC.<sup>[4]</sup>

Life cycle assessment confirmed the environmental benefits of the processes in comparison to primary raw material extraction, especially when acid reuse strategies were considered. Hence, the hydrometallurgical recovery of Pb, In and Ag offers a scalable and environmentally benign solution for material recycling from next-generation photovoltaics.<sup>[3,4]</sup>

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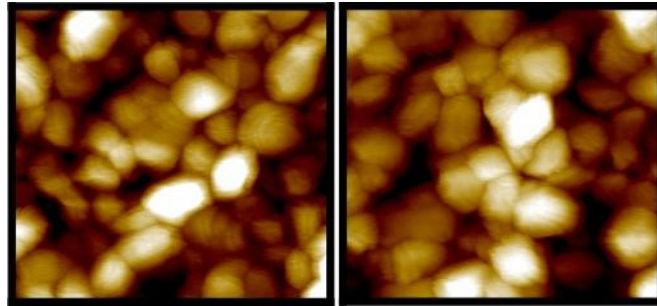
# UTILIZATION OF IONIC LIQUIDS IN TRIPLE-CATION PEROVSKITE SOLAR CELLS

**Sevdiye Basak Turgut,<sup>1</sup> Sirin Siyahjani Gultekin,<sup>1</sup> Saliha Özdemir,<sup>2</sup> Burak Gultekin,<sup>1</sup> Canan Varlikli<sup>3</sup>**

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**Figure 1:** AFM micrographs of pristine perovskite and IL doped perovskite film, respectively.

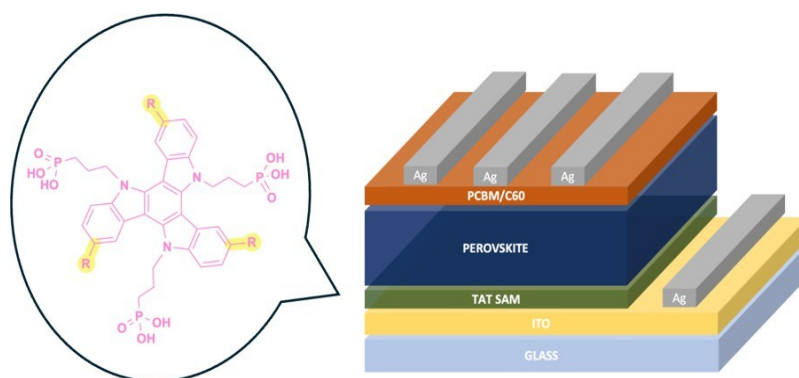
The functional design of ionic liquid (IL) additives provides a versatile strategy to enhance the morphological quality and long-term stability of perovskite solar cells. In this study, we examine the influence of structurally distinct ammonium-based ILs on triple-cation perovskite films. By exploring variations in their functional groups, we reveal significant improvements in film morphology and interface quality. Morphological and optical characterizations show that IL incorporation enhances grain size, improves grain boundary connectivity, and reduces surface roughness, all contributing to more efficient charge transport. IL additive PSC achieved the highest power conversion efficiency (PCE) of 17.65%, while the pristine perovskite film, without any additive, exhibits a PCE of 16.38%. These results underscore the potential of tailored IL additives to optimize perovskite film formation and enable more stable and efficient photovoltaic devices.

# FUNCTIONALIZED P-TYPE TRIAZATRUXENE-BASED SELF- ASSEMBLY MONOLAYERS FOR PEROVSKITE SOLAR CELLS

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In recent years, self-assembled monolayer (SAM)-based hole-selective layers have been proposed as an alternative to conventional HTLs in perovskite solar cells, offering advantages such as reduced material use, simplified fabrication, and lower costs.<sup>[1]</sup> A planar  $\pi$ -conjugated triazatruxene-based self-assembly monolayers (TAT-SAMs) was synthesized with three anchoring groups for covalent binding to the transparent electrode surface, enabling a tripodal attachment and controlled molecular orientation. The tripodal binding motif facilitates robust surface coverage and stable integration of the SAM layer. Thin-film characterization was conducted through UV–Vis absorption spectroscopy, photoluminescence lifetime measurements, and surface morphology analysis with AFM and SEM. Electrochemical properties and energy level alignment were evaluated using cyclic voltammetry (CV) and Kelvin probe measurements to assess charge extraction and transport efficiency at the perovskite interface. The TAT-SAM was implemented as an interfacial layer in inverted perovskite solar cells, resulting in a 5% increase in power conversion efficiency compared to conventional MeO-2PACz and 2PACz materials.



**Figure 1:** Schematic illustration of the *p-i-n* perovskite solar cell architecture incorporating the synthesized SAMs as the hole-selective contact. *R* = Br, MeO, and MeOPh

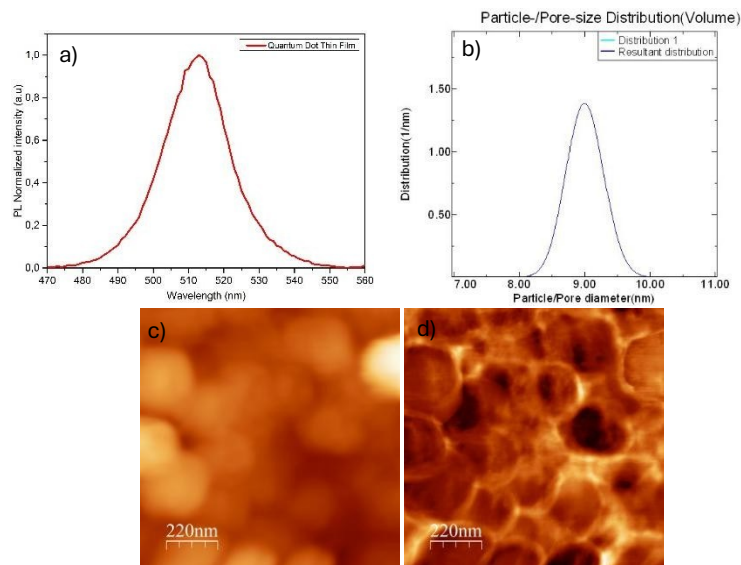
[1] Wang, S., Guo, H., & Wu, Y., “Advantages and challenges of self-assembled monolayer as a hole-selective contact for perovskite solar cells” *Materials Futures* **2023**, 2(1). <https://doi.org/10.1088/2752-5724/>

# SCALABLE FABRICATION OF PEROVSKITE QUANTUM DOT LAYERS WITH INKJET PRINTING

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In this study, inkjet printing studies of CsSn<sub>0.5</sub>Pb<sub>0.5</sub>Br<sub>3</sub> quantum dots (QDs) and their SiO<sub>2</sub>-coated core-shell derivatives as active layers in photovoltaic devices were carried out. The QDs are pre-crystallized and dispersed in a stable ink formulation, eliminating the need for post-deposition crystallization steps such as antisolvent or inert gas treatments; only mild thermal annealing is applied.<sup>[1]</sup> Surface modification with (3-aminopropyl)triethoxysilane (APTES) replaces oleylamine ligands, improving ink-substrate interaction and enabling uniform droplet spreading.<sup>[2]</sup> Atomic force microscopy (AFM) measurements reveal smooth surfaces with low root-mean-square roughness of 13.9 nm (Figure 1c-d). Small-angle X-ray scattering (SAXS) measurements performed in solution phase confirm preserved nanocrystal structure, with an average radius of ~9 nm (Figure 1b). Photoluminescence (PL) analysis shows a strong emission peak centered at ~513 nm (Figure 1a), indicating minimal quenching and retained optical quality. These findings demonstrate the potential of APTES-capped QDs for uniform, scalable inkjet-printed active layers in perovskite quantum dot photovoltaics.

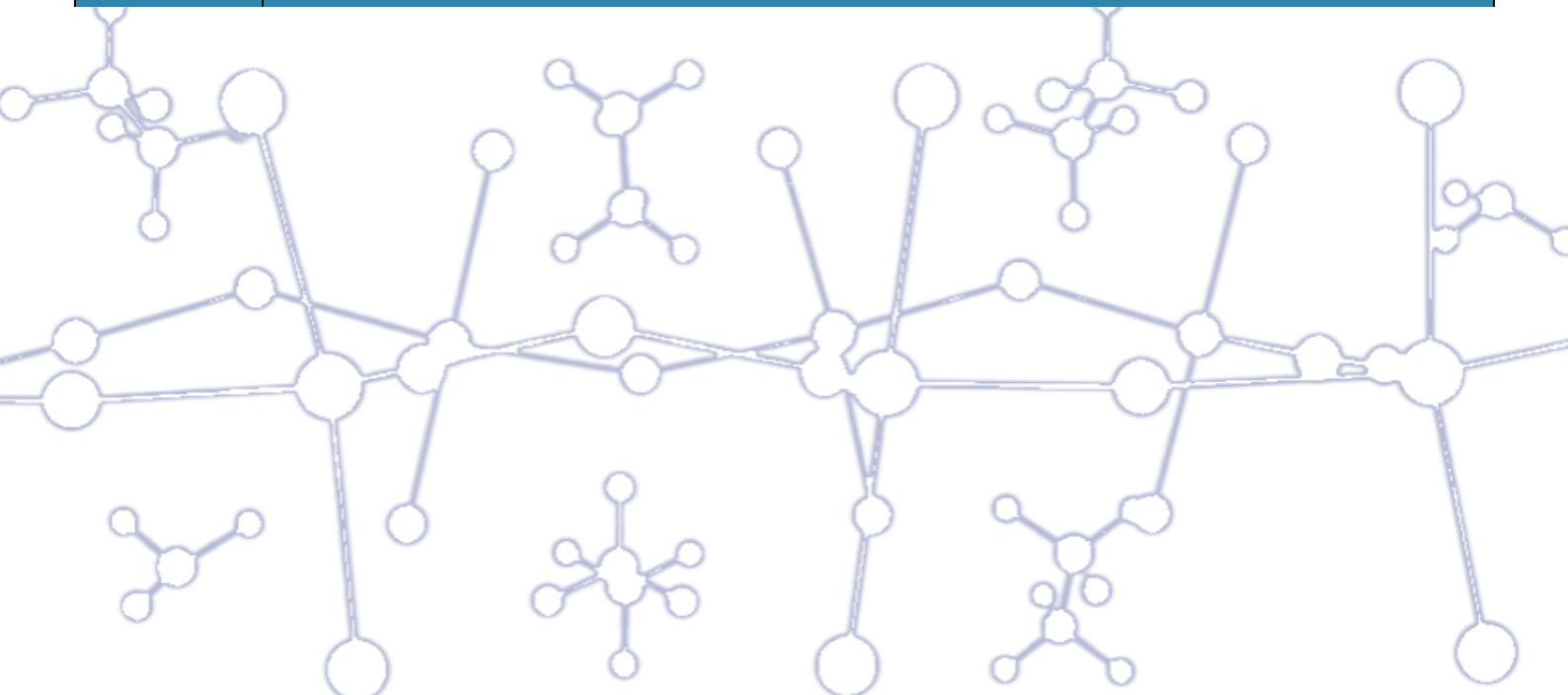


**Figure 1:** a) Photoluminescence Spectra of CsSn<sub>0.5</sub>Pb<sub>0.5</sub>Br<sub>3</sub> Quantum Dot Thin film b) Pore Size Distribution of CsSn<sub>0.5</sub>Pb<sub>0.5</sub>Br<sub>3</sub> Quantum Dot SAXS curve c, d) CsSn<sub>0.5</sub>Pb<sub>0.5</sub>Br<sub>3</sub> Quantum Dot AFM Images

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**Day 2 - Tuesday, September 16th 2025**

<b>Session Chair</b> <b>Session Title</b>	<b>Town Hall</b> <b>Saiful Islam, Oxford University, United Kingdom</b> <b>Session 1 – Invited Lectures</b>
<b>08:45 09:00</b>	<b>CONFERENCE DESK</b>
09:00 09:25	7° INVITED LECTURE - <b>Steve Albrecht</b> , Helmholtz-Zentrum Berlin, Germany <i>Integrating metal halide perovskite top cells with bottom cells formed by crystalline silicon or low band gap</i>
09:25 09:50	8° INVITED LECTURE - <b>Martin Stollerfoht</b> , The Chinese University of Hong Kong, Hong Kong <i>Understanding and improving the stability of perovskite solar cells based on their ionic properties</i>
09:50 10:15	9° INVITED LECTURE - <b>Shuzi Hayase</b> , The University of Electro-Communications, Japan <i>Tin-based perovskite solar cells Mechanism of degradation and direction to enhance stability</i>
10:15 10:40	10° INVITED LECTURE - <b>Selina Olthof</b> , University of Wuppertal, Germany <i>Investigation of the electronic structure of 3D halide perovskites as well as 3D/2D interfaces</i>
10:40 10:45	3° SPONSOR SPEACH - QYB
10:45 10:50	4° SPONSOR SPEACH – Korea Kiyon
<b>10:50 11:20</b>	<b>COFFEE BREAK AM</b>
<b>Session Chair</b> <b>Session Title</b>	<b>Town Hall</b> <b>Annamaria Petrozza, Istituto Italiano di Tecnologia, Italy</b> <b>Session 2 – Invited Lectures</b>
11:20 11:45	11° INVITED LECTURE – <b>Henry Snaith</b> , Oxford University, United Kingdom <i>Understanding Degradation and Enhancing Efficiency in Perovskite Solar Cells</i>
11:45 12:10	12° INVITED LECTURE - <b>Linn Leppert</b> , University of Twente, The Netherlands <i>Excitons in low-dimensional halide perovskites from first-principles calculations</i>
12:10 12:35	13° INVITED LECTURE - <b>Dewei Zhao</b> , Sichuan University, China <i>All-perovskite tandem solar cells</i>
12:35 12:45	Prof. Luca Gammaitoni for VITALITY Project
<b>12:45 14:00</b>	<b>LIGHT BUFFET LUNCH</b>



# INTEGRATING METAL HALIDE PEROVSKITE TOP CELLS WITH BOTTOM CELLS FORMED BY CRYSTALLINE SILICON OR LOW BAND GAP

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Perovskites into monolithic tandem devices have recently attracted increased attention due to the high efficiency potential and application relevance of these cell architectures. Here we present our recent results on monolithic tandem combinations of perovskite top-cells with crystalline silicon, and Sn-Pb perovskites as well as tandem relevant aspects of perovskite single junction solar cells. In 2020, we have shown that self-assembled monolayers (SAM) could be implemented as appropriate hole selective contacts. The implementation of new generation SAM molecules enabled further reduction of non-radiative recombination losses with high open circuit voltages and fill factor. By fine-tuning the SAM molecular structure even further, the photostability of perovskite composition with tandem-ideal band gaps of 1.68 eV could be enhanced by reduction of defect density and fast hole extraction. That enabled a certified efficiency for perovskite/silicon tandems at 29.15%.

By optical optimizations, we could further improve this value to 29.80% in 2021. Periodic nanotextures were used that show a reduction in reflection losses in comparison to planar tandems, with the new devices being less sensitive to deviations from optimum layer thicknesses. The nanotextures also enable a greatly increased fabrication yield from 50% to 95%. Moreover, the open-circuit voltage is improved by 15 mV due to the enhanced optoelectronic properties of the perovskite top cell on top of the nanotexture.

In the end of 2022, we enabled a new world record for perovskite/silicon tandem solar cells at 32.5% efficiency. We demonstrated that an additional surface treatment strongly reduces interface recombination and improves the band alignment with the C60 electron transporting material. With these modifications, single junction solar cells show high open circuit voltages of up to 1.28 V in a p-i-n configuration, and we achieve 2.00 V in monolithic tandem solar cells. A comparable surface treatment was also applied to 1.80 eV band gap perovskites to enable Voc values of 1.35 V and these were integrated into monolithic all-perovskite tandem solar cells enabling a certified efficiency of 27.5%.

In addition to the experimental material and device development, also main scientific and technological challenges and empirical efficiency limits as well as advanced analysis methods will be discussed for perovskite based tandem solar cells. In addition, results on upscaling and stability of these industrial relevant tandem solar cells by thermal evaporation will be shown

# UNDERSTANDING AND IMPROVING THE STABILITY OF PEROVSKITE SOLAR CELLS BASED ON THEIR IONIC PROPERTIES

**Martin Stolterfoht**,<sup>1</sup>**Nikhil Kalasariya**,<sup>1</sup> **Paria Forozi Sowmeh**,<sup>2</sup> **Sahil Shah**,<sup>3</sup> **Felix Lang**<sup>2</sup>

<sup>1</sup>*Electronic Engineering Department, The Chinese University of Hong Kong, Shatin, N.T. 999077, Hong Kong SAR*

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Improving the stability of perovskite-based tandem solar cells is the last major scientific and technical challenge to be overcome before commercialization. In this context, mobile ions play a significant role, yet their exact impact on the overall performance and stability of perovskite-based photovoltaics remains not well understood. We recently found that an increasing bulk and interfacial trap midgap trap density is apparently not the most decisive factor for perovskite solar cell degradation. Instead, it is the generation of an increasing number of mobile ions under external stressors, which progressively screen the built-in field, leading to charge extraction losses.<sup>1–3</sup> In this talk, I will discuss our recent understanding of how ion migration influences the performance and stability of various perovskite solar cells, including Si/perovskite and all-perovskite tandem solar cells,<sup>4</sup> as well as single junctions with 2D perovskite capping layers, which substantially influence the ionic properties and device stability.<sup>5</sup> I will also discuss the intriguing correlation between halide segregation and ionic losses in wide-bandgap perovskite solar cells, which suffer from very large ionic losses that can reduce the steady-state current by over 10 mA/cm<sup>2</sup>. I will then address how performance recovery - a crucial factor for operational device stability - relates to ionic loss and ion density recovery. Finally, I will elaborate on several strategies to mitigate mobile ion-induced performance degradation for stable next-generation perovskite-based solar cells.

## *Acknowledgements: (Optional)*

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# TIN-BASED PEROVSKITE SOLAR CELLS MECHANISM OF DEGRADATION AND DIRECTION TO ENHANCE STABILITY

**Shuzi Hayase**

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The Sn-based PVK is the best light-harvesting material among halide perovskites as single junction solar cells and tandem solar cells. The highest efficiency of the former and the latter is 17.1% and 24.5% respectively. To improve the efficiency of Sn-based perovskite solar cells, reducing Sn<sup>4+</sup> impurity and bandgap offset, suppressing strain at the interface, decreasing defect densities are the direction for the research. We have reported 15.3% and 23.3% respectively<sup>1-3</sup>. An alternative way to enhance efficiency is to fabricate all-perovskite tandem solar cells. They are composed of the top cell (Pb-PVK-PV with 1.77 eV bandgap), the bottom cell (SnPb-PVK- PV with 1.25 eV bandgap), and interconnecting layer, and the efficiency is 30.1%. We have reported 26.8% by optimizing the interconnection layer<sup>4,5</sup>. In addition, we demonstrated the Pb- free perovskite tandem cells composed of wide bandgap Sn-PVK/CIGS cells<sup>6</sup>.

The most serious concern is the stability of the bottom cell. We focus on the stability against heat exposure (85 °C) and xenon lamp exposure consisting of UV light. The thermal stability of Sn-based PVK PV was improved by introducing inorganic layer such as GeOx and ALD SnOx as the ion blocking layer against H<sup>+</sup> and I<sup>-</sup> or by avoiding ion-sources such as PEDOT-PSS. DMSO in the perovskite precursor ink damages the Sn-based PVK-PV. We will show one of the approaches to preparing DMSO-free ink. In addition, we found that carbazole-free SAM (ethylenediamine tetramethyl phosphonic acid: EDTMP) gave efficiency over 20% similar to conventional 2PACz with carbazole group, and unexpectedly improved light exposure stability. Less damage against UV exposure, weak proton acidity, high surface coverage of EDTMP may explain the high stability against light exposure. The reaction mechanism of degradation would be discussed by the analysis of the damaged solar cells. We expect further stability improvement, according to the direction obtained by our research.

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# INVESTIGATION OF THE ELECTRONIC STRUCTURE OF 3D HALIDE PEROVSKITES AS WELL AS 3D/2D INTERFACES

**Selina Olthof**

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Two-dimensional (2D) halide perovskites have gained significant attention for enhancing both the performance and stability of perovskite devices. While band gap changes and crystal structure variations are well established, the energy level positions and band alignments at interfaces remain less understood. To address this, we systematically investigate alkylammonium-based Ruddlesden–Popper perovskites ( $n = 1, A'_2\text{PbI}_4$ ) with varying alkyl chain lengths (from propylammonium  $\text{C}_3$ , to decylammonium  $\text{C}_{10}$ ) using X-ray diffraction (XRD), optical analysis and ultraviolet photoelectron spectroscopy (UPS).<sup>[1]</sup> UPS reveals systematic changes in the density of states (DOS), depending on the length of these spacer cations. These variations can be well explained by comparison to calculations of the density of states done by density functional theory (DFT) when considering the low probing depth of UPS. Surprisingly, the ionization energy (i.e., VB position) remains nearly constant across all samples, and are in a similar range as the 3D forming  $\text{MAPbI}_3$ , suggesting that the increase in band gap for 2D perovskites seems predominantly due to an upward shift in the conduction band.

When performing photoluminescence and reflection spectroscopy measurements on these various 2D layers, only minor band gap variations (up to 90 meV) are observed as a function of spacer cation length. Here, no linear trend is found, rather an intriguing odd-even effect emerges, where perovskites with odd-numbered alkyl chains exhibit a blue-shifted absorption onset compared to their even-numbered counterparts. DFT simulations attribute this effect to Pb-I-Pb bond distortions within the inorganic framework, influenced by the packing efficiency of the alkyl chains.

Finally, I will present reflection electron energy loss spectroscopy (REELS) measurements, which probe inelastic electron scattering to provide insights into electronic transitions from conduction to valence band states. By tuning the excitation energy, it is possible to adjust the probing depth from  $\sim 1$  to 10 nm, enabling us to assess surface modifications and their impact on the optical gap. This is particularly relevant for investigating 2D perovskite formation on 3D layers, for which I will present several examples.

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# UNDERSTANDING DEGRADATION AND ENHANCING EFFICIENCY IN PEROVSKITE SOLAR CELLS

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Perovskite solar cells are efficient in single junction devices, very efficient in two junction tandem cells, especially when combined with silicon, and commercial products are starting to be deployed. However, there remains a need to understand and further mitigate degradation under a range of environmental stress conditions, and specifically under the combined stress of heat and light. Here I will present a range of different studies upon understanding degradation and improving stability for perovskite solar cells. In addition, although single junction cells and tandems with silicon are already approaching their feasible efficiency limits, the potential for even higher efficiencies with 3 to 5 junction perovskite solar cells remains. The key challenges here are how do we obtain comparably high voltages from very wide band gap perovskite solar cells? and how do we stabilize our very wide band gap cells against issues such as halide-segregation, compositional inhomogeneities, and surface/interface defects? I will present some work related to this topic.

# EXCITONS IN LOW-DIMENSIONAL HALIDE PEROVSKITES FROM FIRST-PRINCIPLES CALCULATIONS

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Excitons, neutral quasiparticles formed by electron-hole pairs, play a key role in the optoelectronic properties of semiconductors. Understanding their formation, transport, and dissociation is essential for interpreting experiments, predicting material behavior, and designing new materials for targeted applications. Low-dimensional halide perovskite semiconductors provide a versatile platform for studying excitons due to their structural tunability and facile fabrication. Quasi-two-dimensional (2D) halide perovskites, consisting of metal-halide octahedral layers separated by organic spacers, are particularly promising. Their unique structure, which disrupts octahedral connectivity in one direction, results in anisotropic charge-carrier masses and dielectric screening, promoting the formation of strongly bound excitons. First-principles calculations of excitonic properties in these materials have been limited by the large unit-cell sizes of most experimentally synthesized quasi-2D perovskites. However, recent advances in hardware and many-body perturbation theory methods, such as the *GW* and Bethe-Salpeter Equation approaches, now enable detailed insights into these systems. In this presentation, I will showcase how these methods allow for a microscopic understanding of the emergence of intra-, interlayer and charge-transfer excitons and their coupling to lattice degrees of freedom in low-dimensional halide perovskites. Our calculations provide predictive accuracy, explain experimental observations, and open pathways for tuning excitonic properties in these complex, heterogeneous materials.

# ALL-PEROVSKITE TANDEM SOLAR CELLS

**Dewei Zhao,<sup>1</sup> Cong Chen<sup>1</sup>, Jingwei Zhu<sup>1</sup>, Yuliang Xu<sup>1</sup>, Yi Luo<sup>1</sup>**

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Tandem solar cells using all metal-halide perovskite thin films show great promise for next-generation solar cells in terms of reduced cost, flexibility, and high efficiency, an effective way to break the Shockley-Queisser limit of single-junction cells. Low-bandgap mixed tin (Sn)-lead (Pb) and wide-bandgap perovskite solar cells, as the key to make highly efficient all-perovskite tandem solar cells, have been gaining extensive interest due to their appropriate bandgaps and promising application to build efficient all-perovskite tandem cells. Growth process of perovskites plays a crucial role in the formation of high-quality perovskites. We will present perovskite crystallization regulation strategies such as universal close space annealing (CSA) and buried interface-assisted growth, etc to increase grain size, enhance crystallinity, and prolong carrier lifetimes in low-bandgap (~1.25 eV) and wide-bandgap (~1.75-1.80 eV) perovskite films, leading to high-quality perovskite absorber layers. We will also present new self-assembly monolayer (SAM) materials for efficient wide-bandgap perovskite subcells and their mechanisms for reducing interfacial charge non-radiative recombination losses. We will also discuss the design and optimization of interconnecting layers for all-perovskite tandems.

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<b>Session Chair</b>		<b>Town Hall</b>	
<b>Session Title</b>		<b>Henry Snaith, Oxford University, United Kingdom</b>	
		<b>Session 3 – Invited Lectures</b>	
14:00	14:25	14° INVITED LECTURE - <b>Hou Yi</b> , National University Singapore, Singapore <i>Unlocking the Potential of Perovskite Solar Cells: from Single-Junction to Tandem</i>	
14:25	14:50	15° INVITED LECTURE - <b>Maria Vasilopoulou</b> , University of Athens, Greece <i>Solving perovskite instability at its source next-generation photonic devices and solar cells</i>	
14:50	15:00	<b>COMFORT BREAK</b>	
<b>Session Chair</b>		<b>Town Hall</b>	<b>Trumpet</b>
<b>Session Title</b>		<b>Maria Vasilopoulou, University of Athens, Greece</b>	<b>Selina Olthof, University of Wuppertal, Germany</b>
		<b>Session 1A – Engineering PV</b>	<b>Session 1B – Computational Insight</b>
15:00	15:12	<b>Liam Van Gaal</b> , KU Leuven, Belgium <i>Sn-Induced phase stabilization of CsPbI<sub>3</sub> quantum dots for stable red light-emitting diodes</i>	<b>James McQueen</b> , Oxford University, United Kingdom <i>Multiscale Modelling of Perovskite Solar Cell Interfaces to Optimise Efficiency and Durability</i>
15:12	15:24	<b>Kasparas Rakstys</b> , Kaunas University of Technology, Lithuania <i>Molecular engineering of functional components towards high performance perovskite solar cells</i>	<b>Max Grischek</b> , Helmholtz-Zentrum Berlin, Germany <i>Predicting the stability of inorganic perovskite solar cells based on the influence of mobile ions</i>
15:24	15:36	<b>Thomas Gomes</b> , CEA, France <i>Cesium chloride additive for enhanced illumination stability: mechanisms and tandem integration</i>	<b>Pradeep Nair</b> , Indian Institute of Technology Bombay, India <i>Modeling of Perovskite Optoelectronics: from Photoluminescence and Recombination kinetics to Solar Cells and LEDs</i>
15:36	15:48	<b>Dane deQuilettes</b> , Optigon, Inc., United States <i>Rapid, Automated, Multimodal Characterization and Device Parameter Prediction of Perovskite Photovoltaics</i>	<b>Ana Palacios Saura</b> , Helmholtz-Zentrum Berlin, Germany <i>FAPbI<sub>3</sub>: the dynamic material</i>
15:48	16:00	<b>Larissa van de Ven</b> , University of Groningen/AMOLF, The Netherlands <i>Understanding the tin and lead arrangement in the atomic lattice of all inorganic tin-lead perovskites</i>	<b>Zhen Li</b> , Northwestern Polytechnical University, China <i>Efficient and robust flexible perovskite solar cells for space applications</i>
16:00	16:12	<b>Tom Savenije</b> , TU Delft, The Netherlands <i>Additive-free sequential thermal evaporation of nearintrinsic low bandgap perovskites: from thin film to device fabrication</i>	<b>Pabitra Kumar Nayak</b> , Indian Institute of Technology Delhi, India <i>Optimizing excited charge dynamics in layered halide perovskites through compositional engineering</i>

# UNLOCKING THE POTENTIAL OF PEROVSKITE SOLAR CELLS: FROM SINGLE-JUNCTION TO TANDEM

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Perovskite solar cells (PSCs) hold great promise as either standalone technology or in conjunction with silicon in tandem configurations. However, the commercialization of state-of-the-art PSCs faces two primary challenges: interface recombination losses and degradation. To address these hurdles, we've focused on developing novel interface materials and innovative device design concepts. During this presentation, I'll delve into the rationale behind inverted perovskite design and shed light on how we plan to unlock the vast potential of this technology in different tandem devices. I'll highlight its advantages and prospects for future advancements. Additionally, I'll discuss the rationale behind wide-bandgap perovskite design for achieving record performance in perovskite, perovskite/organic, perovskite/Si, and triple-junction perovskite/perovskite/Si tandems. I'll explain how perovskite-based tandem solar cells have attained high efficiencies and unveil the immense potential of this technology. The advances reported herein show that it is possible and powerful to marry the traditional PVs and perovskite technologies in tandems.

# SOLVING PEROVSKITE INSTABILITY AT ITS SOURCE NEXT-GENERATION PHOTONIC DEVICES AND SOLAR CELLS

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Despite remarkable progress in perovskite optoelectronics, the long-term operational stability of these devices remains a critical bottleneck, fundamentally limiting their commercial deployment. Here, we identify the origin of perovskite instability as the rapid formation of atomic planes with high planar density during crystallization, which act as preferential sites for defect accumulation, dislocation formation, and phase degradation. In contrast, our investigations reveal that crystallographic planes with low atomic density inherently promote smooth, homogeneous surfaces that encapsulate perovskite grains and interfaces, functioning as self-assembled nanomembranes. These atomically thin, low-density planes serve as intrinsic barriers, effectively isolating the perovskite lattice from environmental stressors and suppressing the propagation of defects.

Building on this mechanistic understanding, we introduce a targeted in-situ engineering strategy that selectively modulates the crystallization pathway, favoring the growth of low-density encapsulating planes while suppressing the rapid emergence of high-density, defect-prone planes. The resulting perovskite films exhibit a dramatic reduction in defect density, extended charge carrier lifetimes, and exceptional morphological uniformity. These self-encapsulated structures also display robust resistance to humidity and thermal stress, maintaining structural and optoelectronic integrity under 85% relative humidity at 85 °C.

Engineered perovskites enable photoluminescence quantum yield approaching unity and high temperature superradiance opening the path towards room temperature superradiance lasers. Photovoltaic devices achieve a certified power conversion efficiency of 26.14%, while retaining over 95% of their initial efficiency during extended operational testing. This work not only elucidates the crystallographic origin of perovskite instability but also establishes a new paradigm for self-protection through the deliberate engineering of low-density nanomembrane planes, paving the way for the next generation of durable, high-performance perovskite photovoltaic technologies.

## ***Acknowledgments***

*This work is funded from the European Innovation Council (EIC), project SUPELASER under grant agreement No. 101162503. The EIC receives support from the European Union's Horizon Europe research and innovation program. This work is also partially funded by the National Foundation for Research and Innovation, Greece (project: DATA4SOLAR, No. 61401500).*

# Sn-INDUCED PHASE STABILIZATION OF CsPbI<sub>3</sub> QUANTUM DOTS FOR STABLE RED LIGHT-EMITTING DIODES

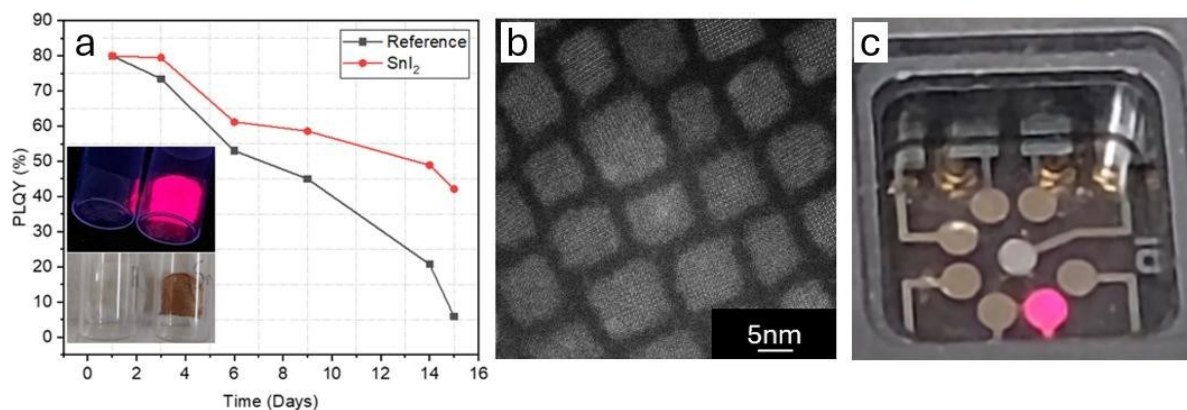
**Liam Van Gaal,<sup>1</sup> Irina Skvortsova,<sup>2</sup> Bapi Pradhan,<sup>1</sup> Sara Bals,<sup>2</sup> Johan Hofkens<sup>1</sup> and Elke Debroye<sup>1</sup>**

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Strain engineering, potentially by chemical doping, is a key strategy to enhance both the structural stability and optoelectronic performance of halide perovskites.<sup>[1]</sup> In particular, partial substitution of Pb<sup>2+</sup> with Sn<sup>2+</sup> in CsPbI<sub>3</sub> introduces a subtle amount of lattice strain due to the smaller ionic radius of Sn<sup>2+</sup>. This not only stabilizes the photoactive black phase but also reduces toxicity, addressing key environmental concerns. While Pb–Sn alloyed perovskites have been extensively explored for photovoltaics, their potential for light-emitting applications remains largely untapped. In this presentation, I will demonstrate a systematic approach to develop Sn-alloyed CsPbI<sub>3</sub> quantum dots (QDs) tailored for light-emitting diodes (LEDs). We first optimized the hot-injection synthesis by carefully considering the trade-off between quantum dot size and monodispersity, achieving small QDs with narrow size distributions and high photoluminescence quantum yields (PLQYs). Subsequently, deliberate SnI<sub>2</sub> incorporation enabled improved phase stability without compromising optical properties. A wide range of complementary techniques, including transmission electron microscopy and time-resolved spectroscopy, were employed to investigate the structural and photophysical effects of Sn-incorporation. Proof-of-concept LEDs fabricated with these QDs exhibit a significantly enhanced performance. These findings (manuscript submitted) build on our previous efforts in perovskite stabilization for LEDs,<sup>[2]</sup> and underscore the promise of Sn-alloyed perovskites for next-generation optoelectronic devices



**Figure 1 :** a) Stability tests of reference CsPbI<sub>3</sub> and SnI<sub>2</sub>-alloyed QD samples (stored as spincoated films in a desiccator with constant humidity of 75%). b) HAADF-STEM image of a purified SnI<sub>2</sub> sample. c) Picture of working LED device

[1] J. Teunissen, E. Debroye et al., *J. Phys. Chem. C* **2023**, *127*, 48, 23400–23411.

[2] H. Bhatia, L. Van Gaal et al., *ACS Appl. Opt. Mater.* **2023**, *1*, 6, 1184–1191.

# MULTISCALE MODELLING OF PEROVSKITE SOLAR CELL INTERFACES TO OPTIMISE EFFICIENCY AND DURABILITY

**James McQueen,<sup>1,2</sup> Vikram,<sup>1</sup> Amit Kumar,<sup>2</sup> Henry J. Snaith,<sup>2</sup> M. Saiful Islam,<sup>1</sup> Ruy S. Bonilla<sup>1</sup>**

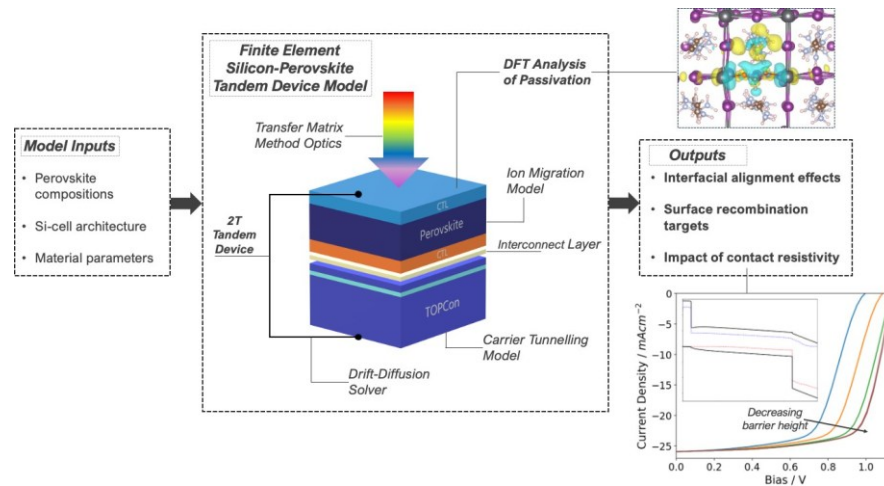
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Engineering interfaces in perovskite solar cells has driven recent advances in stability and efficiency. Interactions between surface defects in the perovskite and passivating material can suppress undesirable phase transitions, and non-radiative recombination. Accordingly, many different approaches, including molecular layers and 2D/3D heterojunctions, have been shown to enable these improvements. However, experimentally identifying the most important defect interactions for loss mitigation has proven prohibitively expensive and challenging, impeding a consensus on the most effective strategy. Here we exploit a suite of simulation techniques to overcome these difficulties.

In this work, we explore perovskite solar cells *in-silico* at a range of length-scales, revealing which interfaces most significantly affect efficiency and durability. We have developed a state-of-the-art perovskite-silicon tandem device model including transfer matrix method and raytracing optics, carrier tunnelling, and ion migration, coupled with a widely used drift-diffusion solver.<sup>[1]</sup> Starting with an industrially relevant perovskite-on-TOPCon architecture, we quantify potential performance improvements from interface passivation throughout the device. We then move down the length-scales to ab-initio modelling, elucidating the atomistic mechanisms driving improved efficiency and stability in a novel interface passivation scheme demonstrated experimentally. A clear strategy for ameliorating the most critical interface identified by the device model hence emerges. Our methodology uniquely provides deep physical insight, whilst remaining broadly applicable to a range of device architectures.



**Figure 1:** Overview of simulation scheme. The underlying models and input parameters are presented, with examples of outputs including J-V curve optimisation, and DFT exploration of interface passivation strategies.

[1] Burgelman, et al., *Thin solid films* **2000**, 527-532, 361

# MOLECULAR ENGINEERING OF FUNCTIONAL COMPONENTS TOWARDS HIGH PERFORMANCE PEROVSKITE SOLAR CELLS

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Perovskite solar cells (PSCs) with certified power conversion efficiency (PCEs) over 27% show great promise for scale-up and future commercialization due to relatively simple fabrication methods. For any solar cell technology to be successful, three milestones must be fulfilled: low-cost, high efficiency, and long-term stability. Although PSCs have climbed to commercially attractive PCE values, much-needed long-term stability hasn't been matched yet due to the degradation of individual layers and undesired processes at interfaces. In this talk, novel molecular approaches and innovations that are currently unpublished will be presented towards highly efficient and stabilized PSCs including novel small cations for three-dimensional (3D) perovskite compositions, passivating organic cations sandwiching 3D perovskite layer to obtain defectless interfaces that prevent lead leakage caused environmental risks, and hole selective self-assembled monolayers with dual functionality.

First, a novel approach using a simple organic fluorinated methylammonium cation to replace the widely used methylammonium cation will be presented. With the addition of a novel small cation perovskite compositions are thermally more stable and enables more reproducible device performance achieving a power conversion efficiency (PCE) of 25.67%. Importantly, the long-term operational stability for 2000 h is demonstrated.

Secondly, the energy barrier of 2D perovskite formation from *ortho*-, *meta*- and *para*-isomers of (phenylene)di(ethylammonium) iodide (PDEAI<sub>2</sub>) that were designed for tailored defect passivation was studied.<sup>[1]</sup> Treatment with the most sterically hindered *ortho*-isomer not only prevents the formation of surficial 2D perovskite film, even at elevated temperatures but also maximizes the passivation effect on both shallow- and deep-level defects. The ensuing PSCs achieve PCE of 23.9% with long-term operational stability showing a great prospect of a simple passivation strategy forming a thin organic salt layer instead of a surficial 2D perovskite layer.

Thirdly, a series of unpublished isothiuronium agents for PSCs were molecularly engineered to study their passivation effect for the first time. In comparison to traditional ammonium salt passivation, a novel approach improved charge transport and significantly enhanced overall performance reaching a PCE over 26% for sandwich-passivated PSCs.

Lastly, unpublished tailored hole selective self-assembling monolayers (SAMs) will be presented, which are developed with optimized dipole moment and functional anchoring groups maximizing transport properties. Such SAMs not only efficiently extract and transport charges but also interact with the perovskite layer from degradation by interfacially stitching with the 3D perovskite layer forming a protective layer under the perovskite absorber in order to improve the perovskite/HSL interface.

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[1] C. Liu, Y. Yang, K. Rakstys et al., *Nat. Commun.* **2021**, *12*, 6394

# PREDICTING THE STABILITY OF INORGANIC PEROVSKITE SOLAR CELLS BASED ON THE INFLUENCE OF MOBILE IONS

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Felix Lang,<sup>2</sup> Dieter Neher,<sup>2</sup> Martin Stolterfoht,<sup>3</sup> Steve Albrecht<sup>1</sup>**

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Long-term operational stability is essential for the commercialisation of perovskite solar cells. This operational stability has been shown to be limited by the influence of mobile ions.<sup>[1]</sup> Mobile ions likely accumulate at the interfaces with the charge transport layers (CTL).<sup>[2-3]</sup> This results in accumulation of photogenerated charges and therefore in increased non-radiative recombination and decreased operational stability<sup>[2], [3]</sup>. Inorganic CsPbI<sub>3</sub> perovskite solar cells achieve a high operational stability and efficiencies of up to 21.75 %, which corresponds to 75 % of the radiative limit for the band gap of 1.72 eV.<sup>[4]</sup> However, there is a lack of comparative studies of stability and the role of mobile ions for a range of other inorganic perovskite compositions.

This study investigates the influence of mobile ions on the operational stability for CsPbI<sub>x</sub>Br<sub>(3-x)</sub> inorganic perovskite solar cells with band gaps ranging from 1.7 eV to 2 eV. First, the peak hysteresis and the ionic losses are quantified in fast hysteresis measurements by measuring *J-V* curves with a wide range of scan speeds as presented in a previous publication.<sup>[5]</sup> Second, the operational stability is measured by tracking the power conversion efficiency of the solar cells at maximum power point for 1500 hours. Third, these findings are generalised using measurements on organic-inorganic perovskite solar cells with a wide range of band gaps.

As a result, the operational stability is strongly dependent on the peak hysteresis, which is a measure of the influence of mobile ions. Increasing the Br content from CsPbI<sub>3</sub> to CsPbI<sub>1.4</sub>Br<sub>1.6</sub> leads to an increase in peak hysteresis index from 0.15 to 0.71 and to a decrease in T<sub>80</sub> from 850 h to 28 h. In addition, fast hysteresis measurements before and after the aging experiment reveal that the J<sub>SC</sub> and PCE loss caused by mobile ions is significantly increased. These ionic losses can be quantified as the difference between the static-ion PCE and the steady-state PCE. The static-ion PCE is measured when the scan speed is fast enough to measure a reverse and forward *J-V* curve before mobile ions start moving. The steady-state PCE is measured when the scan speed is slow enough for all mobile ions to accumulate at a CTL during the reverse scan. In these cases, the influence of mobile ions on the reverse and forward scans is identical and no hysteresis is observed. These results further strengthen our findings of a general dependency of operational stability on the peak hysteresis index, allowing for a prediction of the T<sub>80</sub> based on the peak hysteresis index.

**Acknowledgements:** Thomas Gries, Markus Johannes Beckedahl

[1] J. Thiesbrummel et al., *Nat. Energy* **2024**, 9, 664–676.

[2] G. Richardson et al., *Energy Environ. Sci.* **2016**, 9, 1476–1485.

[3] T. S. Sherkar et al., *ACS Energy Lett.* **2017**, 2, 1214–1222.

[4] H. Zhang et al., *Adv. Mater.* **2023**, 35, 2301140.

[5] V. M. Le Corre et al., *Sol. RRL* **2022**, 6, 2100772.

# CESIUM CHLORIDE ADDITIVE FOR ENHANCED ILLUMINATION STABILITY: MECHANISMS AND TANDEM INTEGRATION

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Despite the rapid advances of the perovskite-based devices record efficiencies, especially silicon-perovskite tandem cells, some obstacles remain before the technology reaches maturity, such as device instability under many different stresses, such as moisture, high temperature or illumination.

This work aims at implementing CsCl as a passivating additive, to improve stability by targeting two key factors in degradation mechanisms: point defects and ion migration. CsCl offers flexibility, in that it allows for different mechanisms depending on the conditions: passivation by free CsCl or passivation by an inorganic 2D perovskite  $\text{Cs}_2\text{PbI}_2\text{Cl}_2$ , formed by reaction between CsCl and  $\text{PbI}_2$ . This second mechanism is of particular interest to us, because while the free CsCl would mainly passivate point defects, the formation of the 2D phase would also participate more efficiently in limiting the ion migration.<sup>[1,2]</sup>

Here, we show an optimized protocol for CsCl integration in a 1 cm<sup>2</sup> single junction perovskite cell mimicking a silicon-perovskite tandem, with a silicon heterojunction-like substrate, allowing for easy transfer to tandem after development of the process. The CsCl treatment yields enhanced stability under continuous illumination at open circuit voltage, notably with no  $V_{oc}$  losses after 72 h while the untreated reference loses 10% of its initial  $V_{oc}$ .  $J_{sc}$  and FF also show improved stability, resulting in a 20% PCE loss in 72 h under such stress against 48% for the reference cell. The promising results obtained on the model single junction were transferred to 1 cm<sup>2</sup> and 9 cm<sup>2</sup> silicon-perovskite tandem cells, to reproduce the early results in continuous illumination, and to extend them with ISOS protocol stability tests,<sup>[3]</sup> mainly light cycling (ISOS-LC) and outdoor aging (ISOS-O).

The improvement observed with the CsCl treatment shows an impact of the additive on the perovskite, but the nature and the location of said impact are still unclear. To decipher the mechanisms involved, advanced characterizations were used. The additive behavior was studied by probing the chlorine chemical environment and spatial distribution, respectively by X-ray Absorption Spectroscopy (XAS) and Nanoscale Secondary Ion Mass Spectroscopy (NanoSIMS). It was found that the chlorine environment hints at an intermediate mechanism between the free CsCl and the formation of the 2D perovskite  $\text{Cs}_2\text{PbI}_2\text{Cl}_2$ , suggesting the observed effects might be linked to both point defect passivation and ion migration hindrance. Meanwhile, the spatial distribution seems rather homogeneous laterally for the resolution used, as there doesn't seem to be a clear correlation between chlorine accumulation and grain boundaries. However, the depth profiles show an accumulation of chlorine at both interfaces of the films, with a constant baseline in the whole film. This result suggests that the main impact of the additive could be located near the surface of the film, although more characterizations would be needed to verify that, either by assessment of the ion migration dynamics or by monitoring defect densities in the CsCl-treated film.

[1] Z. Li et al., *J. Phys. Chem. Lett.* **2020**, *11*, 4138.

[2] X. Zhao et al., *Science* **2022**, *377*, 307.

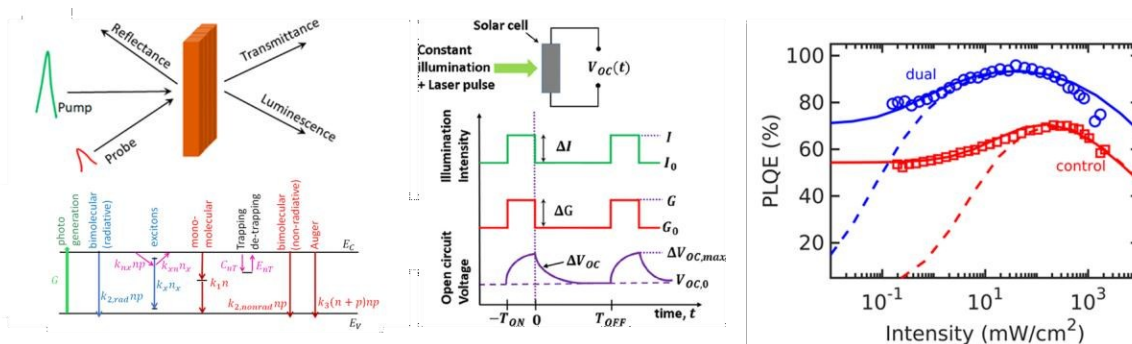
[3] M. Khenkin et al., *Nature Energy* **2020**, *5*, 1, 35.

# MODELING OF PEROVSKITE OPTOELECTRONICS: FROM PHOTOLUMINESCENCE AND RECOMBINATION KINETICS TO SOLAR CELLS AND LEDs

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The performance of optoelectronic devices like solar cells and LEDs critically depends on the recombination processes. Hence, it is crucial that the associated parameters are self-consistently estimated both at the material and device level. While optical spectroscopy techniques are used at a material level, transient switching characteristics are widely used at a device level (see Fig. 1). Often, several of these techniques are used in isolation which leads to inconsistency among the parameter sets obtained through such methods. In addition, several lacunae are evident in the analysis of experimental data – both systemic as well as conceptual. For example, (i) transients are often analyzed and interpreted in terms of exponential decays while the underlying trends are clearly non-exponential (i.e., power law or logarithmic), (ii) excitonic effects are wrongly attributed to monomolecular recombination rates, (iii) parameters back extracted from PL transients are seldom cross verified against steady-state PL, (iv) the influence of traps on transients is not elucidated in a quantitative manner, and (v) lack of coherent analysis of multiple characterization schemes to assure self-consistency of back extracted recombination parameters. Much of the above-mentioned issues stem from the lack of availability of hierarchically compact analytical models to analyze material/device characterization schemes. Through a series of recent publications, we have tried to bridge this gap<sup>[1-6]</sup> and we aim to present the same to a broader community in this presentation. Specifically, we explore – (i) the origin of logarithmic or power-law transients in pump-probe spectroscopy, (ii) influence of excitons in PL transients, (iii) prediction of intensity dependent PLQE using parameters back extracted from PL transients, and (iv) analysis of VOC transients to back extract recombination parameters at a device level.



**Figure 1:** Material/Device characterization for Perovskite optoelectronics. Left panel depicts a pump-probe spectroscopy scheme with free carrier-exciton dynamics. Middle panel shows open circuit transient measurements to back extract recombination parameters. Right panel shows PL Quantum Efficiency comparisons.

- [1] P. R. Nair, *Journal of Physical Chemistry C*, **2023**.
- [2] P. R. Nair, *Journal of Applied Physics*, **2024**.
- [3] Hossain et al., *ACS Energy Letters*, **2024**.
- [4] Chittiboina et al., *ACS Energy Letters*, **2023**.
- [5] P. R. Nair et al., under review (<https://arxiv.org/pdf/2412.19572>).
- [6] Raithani et al., under review (<https://arxiv.org/pdf/2502.05465>).

# RAPID, AUTOMATED, MULTIMODAL CHARACTERIZATION AND DEVICE PARAMETER PREDICTION OF PEROVSKITE PHOTOVOLTAICS

**Dane W. deQuilettes**,<sup>1</sup> **Minhal Hasham**,<sup>1</sup> **Brandon Motes**,<sup>1</sup> **Anthony Troupe**,<sup>1</sup> **James Motes**,<sup>1</sup>  
**Arav Agarwal**

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As perovskite photovoltaic (PV) and optoelectronic technologies begin to be deployed at commercial scales, fundamental challenges remain to push these materials and devices toward their theoretical maximum efficiencies. Specifically, as iterative development and manufacturing processes seek to converge on optimal conditions to increase device stability, characterization remains a bottleneck to rapidly assess the effects of these variations, taking up to 50% of the total device fabrication time.<sup>[1]</sup> Here, we showcase Prism, a rapid, multimodal, and automated characterization platform capable of measuring and extracting key material parameters diagnostic of PV device performance. Using transmission and both spectrally- and temporally-resolved photoluminescence measurements, we determine absorption coefficients, carrier mobilities, and charge carrier lifetimes in perovskite PVs, within a few milliseconds, key metrics which have been shown to be indicative of overall device performance.<sup>[2]</sup> We measure half-completed device stacks which go on to full device fabrication and demonstrate that predictions of open-circuit voltage ( $V_{oc}$ ) from material parameters extracted *via* our measurements are >90% accurate.<sup>[3]</sup> Further, our in-house machine learning models achieve >95% prediction accuracy over key PV metrics:  $V_{oc}$ , short-circuit current ( $J_{sc}$ ), Fill Factor, and Power Conversion Efficiency (PCE), using only thin-film optical properties measured from half-stacks of devices which were subsequently completed. Harnessing the ability to rapidly characterize these materials in Prism, we measure 368 unique heterostructured devices, with extracted material parameters used to train a neural network using to ultimately predict photovoltaic properties.<sup>[4]</sup> Finally, we demonstrate that our models are able to rank the importance of specific material parameters, directly linking the most impactful physically interpretable optoelectronic properties to overall device performance. These rapidly determined property-function correlations provide researchers with direct insight on the most impactful process parameters to achieve maximal device efficiency, allowing for R&D pipelines to quickly identify key variables which have outsized contributions on overall device performance. Taken together, Prism as an automated, multimodal characterization tool in tandem with our analysis and machine learning workflows accelerates perovskite PV characterization, process optimization, and allows for efficient iteration by leveraging large datasets connected to machine learning models.

**Acknowledgements:** *This material is based upon work supported by the United States Department of Energy, Office of Science, Office of Energy Efficiency and Renewable Energy (EERE) under the Solar Energy Technologies Office Award Number DE-SC0024014.*

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[3] Louks, A.E., Motes, B.T., Troupe, A.T, Palmstrom, A.F., Berry, J.J., deQuilettes, D.W., *In preparation* **2025**.

[4] Zhang, R., Motes, B., Tan, S., Lu, Y., Shih, M.-C., Hao, Y., Yang, K., Srinivasan, S., Bawendi, M.G., Bulovic, V., *ACS Energy Lett.* **2025**, 10.

# FAPbI<sub>3</sub>: THE DYNAMIC MATERIAL

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<sup>2</sup>Freie Universität Berlin, Germany

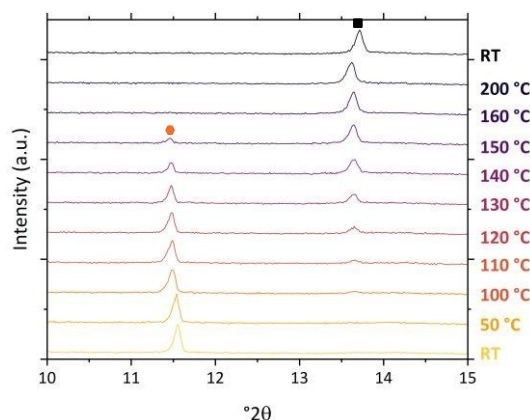
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Hybrid halide perovskites (HHPs) have drawn the attention of the scientific community due to the outstanding power conversion efficiency (up to 27%)<sup>[1]</sup> of HHP-based solar cells as well as their low-cost solution-based processing methods.

One of the HHPs which has been extensively studied is formamidinium lead iodide (FAPbI<sub>3</sub>), which is known to undergo a phase transition from the not photoactive non-perovskite 2H phase, which is stable at room temperature; to the photoactive perovskite  $\alpha$ -phase (cubic), which is stable over 150°C.<sup>[2]</sup> However, the temperature at which this structural phase transition occurs has not yet been determined. For this reason, we investigated the crystal structure of FAPbI<sub>3</sub> from room temperature up to 200°C, in order to determine at which temperature the phase transition takes place.

FAPbI<sub>3</sub> was synthesised following the inverse temperature crystallisation method,<sup>[3]</sup> by mixing the precursors FAI and PbI<sub>2</sub> in GBL. The obtained FAPbI<sub>3</sub> powder was thoroughly investigated by *in-situ* temperature dependent X-ray diffraction (XRD) from room temperature (RT) up to 200°C (Figure 1). We found, that the phase transition starts at 106 – 108 °C, where both phases, the 2H-phase and the cubic perovskite phase, coexist over a certain temperature range. The phase transition is completed at about 160°C.

We also show that once FAPbI<sub>3</sub> adopts the cubic perovskite structure, it does not change back to the 2H phase immediately upon cooling. When cubic FAPbI<sub>3</sub> is left under N<sub>2</sub> atmosphere for a prolonged period of time (e.g. 2 days), the  $\alpha$ -phase stabilises up to 6 days. Hence N<sub>2</sub> seems to have a stabilising effect on the cubic phase of FAPbI<sub>3</sub>.



**Figure 1:** Exemplarily *in-situ* XRD pattern of FAPbI<sub>3</sub> showing the phase transition from the 2H-phase (100 Bragg peak, orange hexagon) to the  $\alpha$ -phase (100 Bragg peak, black square).

[1] NREL Best Research-Cell Efficiency Chart, <https://www.nrel.gov/pv/cell-efficiency.html>

[2] M. Simenas et al., *Chem. Rev.* **2024**, *124*, 2281 – 2326

[3] M. I. Saidaminov et al., *Nat. Commun.* **2015**, *6*, 7586

# UNDERSTANDING THE TIN AND LEAD ARRANGEMENT IN THE ATOMIC LATTICE OF ALL INORGANIC TIN-LEAD PEROVSKITES

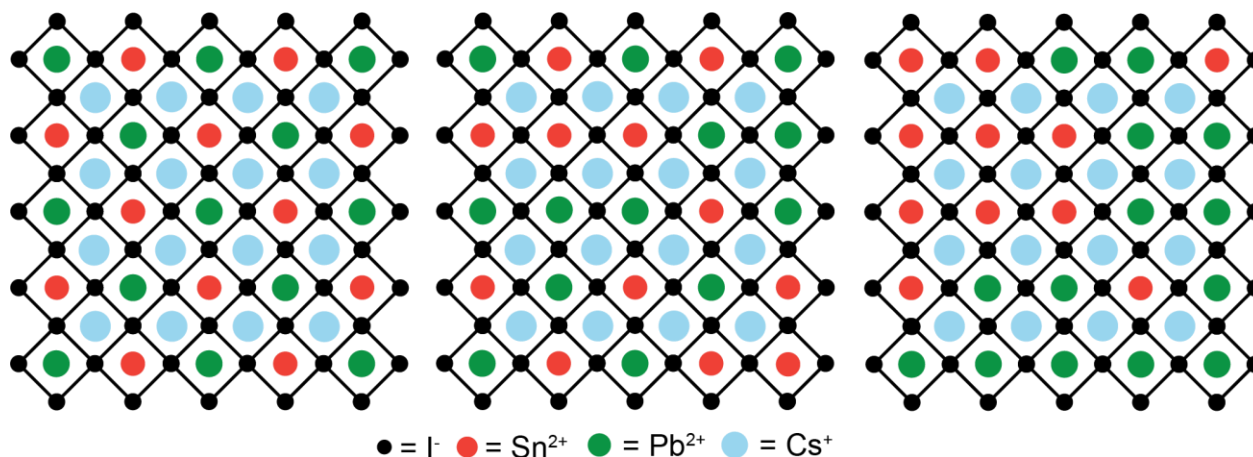
Larissa van de Ven,<sup>1,2</sup> Alessia Lasorsa,<sup>1</sup> Igor Hoogsteder,<sup>2</sup> Wiebke Albrecht,<sup>2</sup> Patrick van der Wel,<sup>1</sup> Maria Loi,<sup>1</sup> Bruno Ehrler<sup>1,2</sup>

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In the progress towards all-perovskite tandem solar cells, significant effort is focused on optimizing half-tin–half-lead perovskites. However, their structure–property relationships remain underexplored, largely due to the difficulty in probing short- versus long-range ordering of tin and lead atoms in the lattice. The tin and lead arrangement has been suggested to impact defect density, oxidation resistance, band gap variations, and has recently become a particularly hot topic, as many record-efficiency tin–lead solar cells have been reported to achieve high performance by mitigating clustering of lead and tin.<sup>[1–6]</sup> It thus deserves more attention. We investigate the presence of larger-scale lead and tin clusters in  $\text{CsSn}_x\text{Pb}_{1-x}\text{I}_3$  through energy-dispersive X-ray spectroscopy. Under the spatial resolution of 100 nm, none are observed. To probe the short-range order in the atomic lattice we employ solid-state nuclear magnetic resonance on the full series ranging from  $\text{CsPbI}_3$  to  $\text{CsSnI}_3$ .  $^{133}\text{Cs}$  NMR indicates the formation of a fully-mixed, random solid. To further investigate local atomic structure, we employ atomic resolution scanning transmission electron microscopy on  $\text{CsSn}_{0.5}\text{Pb}_{0.5}\text{I}_3$ .



**Figure 1:** Possible lattice configurations of cesium tin-lead perovskites: a perfect alloy with alternating tin and lead (left), a fully-mixed but random solid (middle), and nanodomains of pure tin and lead (right).

- [1] T. Leijtens, *ACS Energy Letters* **2017**, 2, 2159-2165.  
[2] W. Zhang, *Advanced Materials* **2023**, 35, 2303674.  
[3] T. Zhang, *Applied Physics Reviews* **2023**, 10, 041417.  
[4] J. Zhou, *Nature Communications* **2024**, 15, 2324.  
[5] Y. Zhang, *Nature Communications* **2024**, 15, 6887.  
[6] H. Gao, *Science Advances* **2025**, 11, 4038.

# EFFICIENT AND ROBUST FLEXIBLE PEROVSKITE SOLAR CELLS FOR SPACE APPLICATIONS

**Zhen Li,<sup>1</sup> Zhihao Li,<sup>1</sup> Chunmei Jia<sup>1</sup>**

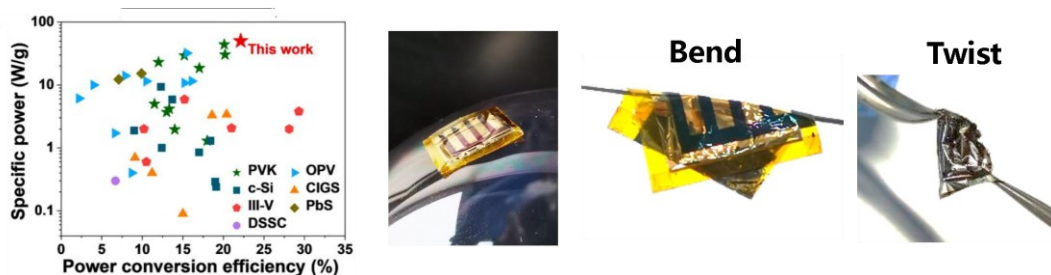
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Flexible perovskite solar cells (FPSCs) have great potential in space applications due to their low cost, light weight and irradiation resistance. However, the efficiency of FPSCs is still lagging behind their rigid counterparts. Extra research efforts are needed to address several stability issues facing extreme space environment, such as vigorous vibration, high vacuum and large temperature variation. In this presentation, I will discuss our recent developments in fabricating efficient and robust FPSCs for space applications.

Firstly, ultra-thin FPSCs were fabricated using color-less polyimide (CPI) thin films with thickness of 10  $\mu\text{m}$ . The ultra-thin FPSCs achieve a power conversion efficiency (PCE) of 22% and an outstanding specific power density of 50 W/g, surpassing most existing solar cells.<sup>[1]</sup> The ultra-thin FPSCs demonstrated exceptional mechanical robustness, maintaining performance even under rigorous bending and twisting. Moreover, CPI exhibited better thermal expansion matching with perovskite and demonstrated enhanced stability under low-temperature conditions and thermal cycling.

Secondly, a highly adhesive polyamide-amine-based hyperbranched polymer (HBP) was developed to reinforce the interface of FPSCs. The abundant functional end groups of HBPs provide strong adhesion between  $\text{SnO}_2$  and perovskite layers, increasing the interface toughness ( $G_c$ ) of ETL/perovskite interface from 1.08 to 2.13  $\text{J}\cdot\text{m}^{-2}$ , and enhance the stability during repeat bending.<sup>[2]</sup> Furthermore, a mussel-inspired HBP with dopamine end-groups was introduced into the perovskite thin films to enforce the grain boundaries and passivate defects, resulting a FPSC with PCE of 24.43%.<sup>[3]</sup>

Thirdly, to address the issues of vacuum induced degradation, initiating from perovskite decomposition at grain boundaries, we developed an grain boundary (GB) strengthen strategy through *in-situ* polymerization at perovskite GBs. The polymer network blocks gas releasing pathways at GBs. Together with a conductive oxide electrode and polymer/oxide composite flexible encapsulation layers, we achieved a 10-fold reduction of vacuum-induced PCE decay.



**Figure 1:** Ultra-thin FPSCs with light-weight and its robustness against vigorous mechanical deformation

[1] C. Jia, *Nano Energy* **2024**, 131A,110259.

[2] Z. Li, *Nat. Comm.* **2023**, 14, 6451.

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# ADDITIVE-FREE SEQUENTIAL THERMAL EVAPORATION OF NEAR-INTRINSIC LOW BANDGAP PEROVSKITES: FROM THIN FILM TO DEVICE FABRICATION

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Reinder K. Boekhoff,<sup>2</sup> Lars J. Bannenberg,<sup>3</sup> Arno H.M. Smets<sup>2</sup>

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Single-junction perovskite solar cells (PSCs) are nearing the maximum efficiency attainable with a single absorber layer. To exceed this limit, tandem cells are utilized. These architectures necessitate low bandgap materials, achieved by partially substituting lead(II) ( $\text{Pb}^{2+}$ ) with tin(II) ( $\text{Sn}^{2+}$ ) in the perovskite structure. In this study, we present the sequential thermal evaporation (sTE) of the low bandgap formamidinium lead-tin iodide ( $\text{FAPb}_{0.5}\text{Sn}_{0.5}\text{I}_3$ ). An alloy of  $\text{SnI}_2$  and  $\text{PbI}_2$  is prepared by heating and evaporated in vacuum, followed by the deposition of FAI. This layer-by-layer technique yields highly oriented, compact, and crystalline thin films with continuous grains averaging over 1  $\mu\text{m}$  in size throughout the film thickness. Photoconductance measurements reveal mobilities exceeding 60  $\text{cm}^2/(\text{Vs})$  and lifetimes surpassing 2  $\mu\text{s}$ . Most interestingly structural analysis indicates that precursor interdiffusion readily occurs at room temperature, resulting in a mixed amorphous material. Complete crystallization into the perovskite phase requires annealing at 200°C. In contrast to findings with pure lead perovskites,<sup>[1]</sup> sTE of mixed lead tin perovskites allows the fabrication of 750 nm thick films in a single cycle. A comparison between the sTE films and spin-coated samples of the same composition shows the superior photoconductance of the sTE films without the need for any additives such as  $\text{SnF}_2$ . PSCs produced using this method, with the architecture ITO/PEDOT/ $\text{FAPb}_{0.5}\text{Sn}_{0.5}\text{I}_3/\text{C}_{60}/\text{BCP}/\text{Ag}$ , reach efficiencies over 10%. Overall, this study highlights the potential of sTE in producing high-quality low bandgap perovskite materials and solar devices.<sup>[2]</sup>

[1] J. Yan et al., “Crystallization Process for High-Quality  $\text{Cs}_{0.15}\text{FA}_{0.85}\text{PbI}_{2.85}\text{Br}_{0.15}$  Film Deposited via Simplified Sequential Vacuum Evaporation” *ACS Appl. Energy Mat.* **2023**, 6, 110265.

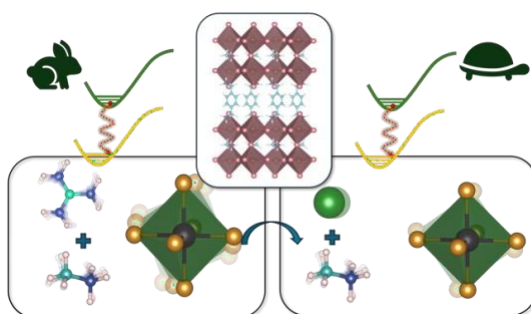
[2] L.M. van der Poll et al., “Small Methods Additive-Free Sequential Thermal Evaporation of Near-Intrinsic Pb-Sn Perovskites” **2024**, 2401246.

# OPTIMIZING EXCITED CHARGE DYNAMICS IN LAYERED HALIDE PEROVSKITES THROUGH COMPOSITIONAL ENGINEERING

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Dion-Jacobson phase multi-layered halide perovskites (MLHPs) improve carrier transport and optoelectronic performance thanks to their shorter interlayer distance, long carrier lifetimes, and minimized nonradiative losses. However, limited atomistic insights into dynamic structure-property relationships hinder rational design efforts to further boost their performance. Here, we employ nonadiabatic molecular dynamics, time-domain density functional theory, and unsupervised machine learning, uncovering the impact of A-cation mixing on controlling the excited carrier dynamics and recombination processes in MLHPs. Mixing smaller-sized Cs with methylammonium in MLHP weakens electron-phonon interactions, suppresses the nonradiative losses, and slows down intra-band hot electron relaxations. On contrary, larger-sized guanidinium incorporation accelerates non-radiative relaxations. The mutual information analyses reveal the importance of interlayer distances, intra and inter-octahedral angle dynamics, and A-cation motion in extending the excited carrier lifetime by mitigating non-radiative losses in MLHPs. Our work provides a guideline for strategically choosing A-cations to boost optoelectronic performance of layered halide perovskites.<sup>[1]</sup>



**Figure 1:** Schematic of strategic A-cation mixing in layered halide perovskites (LHPs) for enhanced charge carrier dynamics. Unlike mixing small fractions of large-sized guanidinium (GA), fractional mixing of inorganic Cs with methylammonium in LHP weakens electron-phonon interactions, suppresses the band-to-band nonradiative losses, and slows down intra-band hot electron relaxations.

## **Acknowledgements:**

[1] Nayak, P. K., & Ghosh, D. *Nano Letters*, **2025**, 25(13), 5520–5528.

16:12 16:45		COFFEE BREAK PM	
		Town Hall	Trumpet
Session Chair		<i>Hou Yi, National University Singapore, Singapore</i>	<i>Daniele Cortecchia, University of Bologna, Italy</i>
Session Title		<b>Session 3A – Advanced Perovskite Technologies</b>	<b>Session 3B – Characterization 2</b>
16:45 16:57	<b>Markus Lenz</b> , FHNW, Switzerland <i>PERCENT- An open access tool to predict environmental Pb concentrations and their possible impacts on soils.</i>	<b>Chuanxiao Xiao</b> , Ningbo Institute of Materials Technology & Engineering, Chinese Academy of Sciences, China <i>Characterization technique development and failure analysis of perovskite solar cells</i>	
16:57 17:09	<b>Weilun Li</b> , Monash University, Australia <i>Connecting atomic structure to performance of perovskite solar cells</i>	<b>Sander Heester</b> , Zernike Institute for Advanced Materials, The Netherlands <i>The Red, White &amp; Blue: Identifying the dominant recombination loss mechanism in perovskite solar cells</i>	
17:09 17:21	<b>Marco Moroni</b> , University of Pavia, Italy <i>3D chiral hybrid perovskite derivatives: structural and functional insights</i>	<b>Rebecca Belisle</b> , Wellesley College, United States <i>Photodriven iodine expulsion and its impacts on microscale heterogeneity</i>	
17:21 17:33	<b>Inna Ivashchenko</b> , Cracow University of Technology, Poland <i>Compositional design approach for pe-LED production based on 3D lead-free halide double perovskites</i>	<b>Nada Mrkyvkova</b> , CEMEA Slovak Academy of Sciences, Slovakia <i>Complete operando study tracking perovskite solar cells degradation</i>	
17:33 17:45	<b>Xinyu Shen</b> , Oxford University, United Kingdom <i>Rational design of phosphine oxide for efficient perovskite light-emitting diodes</i>	<b>Iwan Zimmermann</b> , IPVF, France <i>Large scale deposition of uniform perovskite films in ambient atmosphere by combining slot-die coating and vacuum flash quenching</i>	
17:45 17:57	<b>Zhongcheng Yuan</b> , Oxford University, United Kingdom <i>Applications of perovskite LEDs in multifunctional display and light communication system</i>	<b>Elnaz Ghahremani Rad</b> , The University of British Columbia, Canada <i>Exploring charge collection efficiency losses of perovskite solar cells using hysteresis and impedance measurements</i>	
17:57 18:09	<b>Marcel Kouwenhoven</b> , AMOLF, The Netherlands <i>Writing with light: optical excitation-induced memory in mixed halide perovskites</i>	<b>Federico Ventosinos</b> , ICMOL - Universidad de Valencia, Spain <i>Unraveling ion transport and electronic states in perovskite thin films using moving grating techniques</i>	
18:09 18:21	<b>Yasuhiro Yamada</b> , Chiba University, Japan <i>Anti-stokes optical cooling in CsPbBr<sub>3</sub>/Cs<sub>4</sub>PbBr<sub>6</sub> Dot-in-crystal perovskites: exploring the potential and fundamental limits</i>	<b>Roel Vanden Brande</b> , KU Leuven, Belgium <i>Chemical vapor deposited highly crystalline CsPbBr<sub>3</sub> films for enhanced broad-range photodetection with ultra low dark current</i>	
18:21 18:33	<b>Sownder Subramaniam</b> , imec, Belgium <i>Energetics and defect landscape of soft-sputtered SnO<sub>x</sub>: implications for perovskite solar cells and lowleakage photodetectors</i>	<b>Yudi Wang</b> , Dalian University of Technology, China <i>Graphene oxide doping boosts efficiency of perovskite solar cells with carbon electrode towards 24%</i>	
18:33 20:00	<b>POSTER SESSION</b>		
20:00 20:30	<b>FREE TIME</b>		
20:30 22:30	<b>SOCIAL DINNER</b>		

# PERCENT- AN OPEN ACCESS TOOL TO PREDICT ENVIRONMENTAL Pb CONCENTRATIONS AND THEIR POSSIBLE IMPACTS ON SOILS

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Although a possible environmental risk (i.e. probability  $\times$  impact) of lead (Pb) leaching from perovskite solar cells (PSCs) is frequently highlighted, it is seldomly quantified. The possible negative environmental impact on protected entities will depend on the concentration of Pb, as well as its speciation<sup>1</sup> and the transfer within the exposure pathway considered.<sup>2</sup> Obviously, there is a physical limit to thickness of the perovskite layer in photovoltaics and thus a limit to the amount of Pb that can leach and enter surface waters, sediments soils, and ultimately biota. We have come across several studies that use unrealistic assumptions about leaching, which end up misrepresenting the actual Pb concentrations and impacts.

To realistically assess potential environmental risks, we have developed an open-access web tool called "PERCENT" (PERovskite leaChing assEssmeNt Tool). This tool allows both professionals and the public to interactively estimate the predicted environmental concentrations (PECs) of Pb in soils. The tool allows the user to set factors such as PSC composition, Pb layer thickness, module area and soil volume affected. Based on the PECs calculated, the user is provided with a context menu to explain possible impacts to be expected at such Pb soil concentrations. These are based on regulations of Swiss soil protection, which are well detailed, documented and publicly available. All assumptions and calculations are documented, which offers a transparent approach to address potential concerns of the public as well as to verify and modify own assumptions by the perovskite community.

We demonstrate the tool using different scenarios on perovskite composition and extent of leaching. We then put the calculated PECs as well as indicated impacts into perspective in terms of soil fertility as well as food and fodder production (again, following Swiss regulations). Our findings indicate that Pb leaching from typical PSCs under most assumptions presents no to minimal impacts on soils themselves as well as through soil usage.

## ***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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[1] Schmidt, F. et al., *J. Haz. Mat.* **2022**, 436, 128995.

[2] Huang, H. et al., *Soil Security*, **2024**, 15, 100150.

# CHARACTERIZATION TECHNIQUE DEVELOPMENT AND FAILURE ANALYSIS OF PEROVSKITE SOLAR CELLS

**Chuanxiao Xiao**<sup>1</sup>

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In-depth characterization of materials and device properties is crucial for enhancing photovoltaic conversion efficiency and improving reliability. In this presentation, I will share our recent advancements in the characterization of state-of-the-art perovskite solar cells, focusing on the following key areas:

- 1) **Silicon-Perovskite Tandem Cells:** I will begin by discussing our contributions to the development of champion silicon-perovskite tandem cells. Using Kelvin probe force microscopy, we gained unique insights into the effects of carrier transport layer treatments and the distribution of internal electric fields within the tandem structure.
- 2) **New Techniques in Characterization:** I will present preliminary results from ongoing efforts in my group to develop advanced characterization techniques. Specifically, we applied scanning capacitance microscopy to perovskite materials by incorporating a high-quality alumina thin film, which allowed us to map carrier distribution and investigate variations in carrier concentration and type. Additionally, I will introduce a 3D tomography current mapping method to evaluate how surface and bulk passivation treatments influence carrier transport properties in perovskite thin films. Furthermore, I will discuss steady-state current-voltage analysis, highlighting the comparison of modified asymptotic Pmax scans and maximum power point tracking of high-performance perovskite solar cells.
- 3) **Failure Analysis of Perovskite Solar Cells:** Finally, I will address the failure mechanisms in perovskite solar cells and modules, including potential-induced degradation, Ultraviolet-induced degradation, and phase segregation, providing insights into the challenges and opportunities for improving long-term stability.

# CONNECTING ATOMIC STRUCTURE TO PERFORMANCE OF PEROVSKITE SOLAR CELLS

**Weilun Li,<sup>1</sup> Qimu Yuan,<sup>2</sup> Mengmeng Hao,<sup>3,4</sup> Lianzhou Wang,<sup>3,4</sup> Michael Johnston,<sup>2</sup> Joanne Etheridge<sup>1,5,6</sup>**

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<sup>5</sup>*Monash Centre for Electron Microscopy, <sup>5</sup>Department of Material Science and Engineering, Monash University, Australia*

<sup>2</sup>*Department of Physics, University of Oxford, United Kingdom*

<sup>3</sup>*Nanomaterials Centre, Australian Institute for Bioengineering and Nanotechnology*

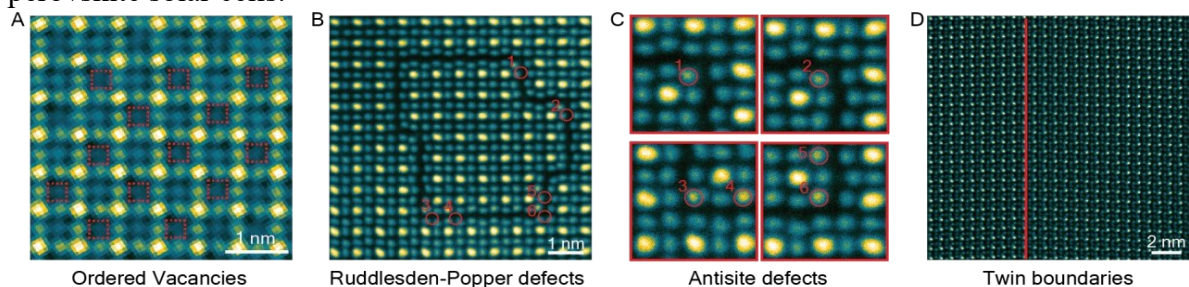
<sup>4</sup>*School of Chemical Engineering, The University of Queensland, St Lucia, Queensland, Australia.*

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Metal halide perovskites, renowned for their exceptional light-harvesting capabilities, have emerged as promising candidates for next-generation high-efficiency, low-cost solar cells. Advancements in photovoltaics materials rely on understanding the intricate relationships between material properties and structure. While extensive research has been conducted on perovskite solar cells, most characterisation techniques operate at mesoscopic to macroscopic scales, using large-area probes. These methods, which solve features from a few nm to mm, cannot fully capture the remarkable performance of perovskite solar cells, such as defect tolerance, ferroic properties, and unsolved challenges like ion migration and hysteresis.

In contrast, transmission electron microscopy (TEM) offers unmatched atomic-scale resolution, however, applying TEM to halide perovskites has been severely restricted due to their extreme sensitivity to beam damage, preventing reliable direct characterisation.

In this work, we develop and apply low-dose electron microscopy techniques to elucidate the atomic structures of critical defects in electron-sensitive metal halide perovskites and examine their effects on material stability and optoelectronic behaviour. We uncover vacancy ordering and ion migration during the degradation in organic-inorganic hybrid  $\text{Cs}_{1-x}\text{FA}_x\text{PbI}_3$ .<sup>[1]</sup> Additionally, we study Ruddlesden-Popper defects<sup>[2]</sup> and twin defects<sup>[3]</sup> in vapour deposited  $\text{CsPbI}_3$  and their correlations with phase stability, optoelectronic properties and ferroic properties (**Figure 1**). These findings offer strategic pathways for defect engineering to advance the performance and durability of perovskite solar cells.



**Figure 1:** Application of low-dose TEM to reveal the atomic structure of defects in halide materials and correlate them to the properties of solar cells. (A) Vacancies. (B) RP planar defects. (C) Antisite defects. (D) twin boundaries.

[1] Li, Weilun, et al., *Nature Communications* **2023**, 14.1, 8523.

[2] Li, Weilun, et al., *Advanced Materials*, under review.

[3] Li, Weilun, manuscript to be submitted.

# THE RED, WHITE & BLUE: IDENTIFYING THE DOMINANT RECOMBINATION LOSS MECHANISM IN PEROVSKITE SOLAR CELLS

**Sander Heester**,<sup>1</sup> Michele Sessolo,<sup>2</sup> Lidón Gil-Escrig,<sup>2</sup> Henk J. Bolink,<sup>2</sup> L. Jan Anton Koster<sup>1</sup>

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Photovoltaics play a key role in the renewable energy transition, with perovskite solar cells standing out as one of the most promising with high power conversion efficiencies, desirable characteristics and great versatility. The efficiency of these cells is mainly limited by non-radiative recombination, whether at one of the interfaces between the perovskite layer and transport layers or within the bulk of the perovskite itself. However, it is difficult to probe which of these dominates the losses during operation, complicating further improvements. Here we introduce an experimental method for identification of the limiting aspect of perovskite solar cells under operating conditions in terms of recombination losses. We illuminate a bifacial cell from both sides separately with either red, blue or white light, each absorbed differently in the cell depending on the position in the device. Using the fill factor from the device characteristics for each case, taking into account the direction of illumination, we are able to accurately identify which part of the cell is limiting the performance. This method and principle are not limited to bifacial cells, but are equally applicable using two monofacial cells, deposited in *pin* and *nip* configuration respectively. We show that this holds for many typical perovskite solar cells using drift-diffusion simulations. Finally, we issue a protocol to determine the dominant recombination channel under operating conditions in perovskite solar cells.

# 3D CHIRAL HYBRID PEROVSKITE DERIVATIVES: STRUCTURAL AND FUNCTIONAL INSIGHTS

**Marco Moroni,<sup>1</sup> Luca Gregori,<sup>2,3</sup> Clarissa Coccia,<sup>1</sup> Doretta Capsoni,<sup>1</sup> Andrea Olivati,<sup>4</sup> Antonella Treglia,<sup>4</sup> Giulia Folpini,<sup>4</sup> Maddalena Patrini,<sup>5</sup> Chiara Milanese,<sup>1</sup> Annamaria Petrozza,<sup>4</sup> Edoardo Mosconi,<sup>3</sup> Filippo De Angelis,<sup>2,3</sup> Lorenzo Malavasi<sup>1</sup>**

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<sup>3</sup>*Computational Laboratory for Hybrid/Organic Photovoltaics (CLHYO), Istituto CNR di Scienze e Tecnologie Chimiche "Giulio Natta" (CNR-SCITEC), Italy*

<sup>4</sup>*Center for Nano Science and Technology@PoliMi, Istituto Italiano di Tecnologia 20134 Milan, Italy*

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In the past few years, chiral hybrid organic-inorganic perovskites (HOIPs) have emerged as promising materials for applications in optoelectronics, spintronics, photodetection, energy harvesting and beyond, enabling the absorption and subsequent emission of polarized light with enhanced tunability across the electromagnetic spectrum.<sup>[1,2]</sup> So far the research has largely focused on 2D and quasi-2D HOIPs, along with a few 1D and 0D ones, demonstrating remarkable chiroptoelectronic and spin-polarization properties. However, expanding the corner-sharing interconnection of the inorganic motif in the three dimensions is challenging due to steric constraints, as the bulky chiral cations prevent the accordance with the Goldschmidt tolerance factor, but highly demanded for isotropic charge transport since the organic layers usually act as dielectrics in low-dimensional systems.<sup>[3]</sup>

In our work, we have engineered novel chiral HOIPs derivatives featuring a 3D corner-sharing octahedral architecture closely resembling that of prototypical perovskites. This structural motif is attained by incorporating the relatively small ditopic cation *R/S*-3-aminoquinuclidine (*R/S*-3AQ) leading to the (*R/S*-3AQ)Pb<sub>2</sub>Br<sub>6</sub> materials, exhibiting a direct bandgap and an isotropic electronic band structure in agreement with a three-dimensionally delocalized excitation, in sharp contrast with the Ruddlesden-Popper counterpart (*R/S*-3AQ)<sub>2</sub>PbBr<sub>4</sub>·2Br presenting typical 2D features. The measured chiral anisotropy factor is in good agreement with values predicted from first-principles calculations for such a chiral inorganic framework, and a pronounced Rashba-type spin splitting is observed in the conduction band, expected for a non-centrosymmetric semiconductor and arising from the synergy between spin-orbit coupling and structural chirality. A lower exciton binding energy was found out in the 3D composition, indicating a more stable excitonic population and being beneficial for an enhanced charge transport. Conductivity measurements are currently ongoing to further assess the impact of these electronic properties on the material's potential performance in optoelectronic applications. The demonstrated 3D chiral HOIP derivatives, featuring a wide chemical tunability, represents a promising platform for developing next-generation nonlinear functional materials.

**Acknowledgements:** *this work has been supported by Fondazione Cariplo, grant n° 2023-1246.*

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# PHOTODRIVEN IODINE EXPULSION AND ITS IMPACTS ON MICROSCALE HETEROGENEITY

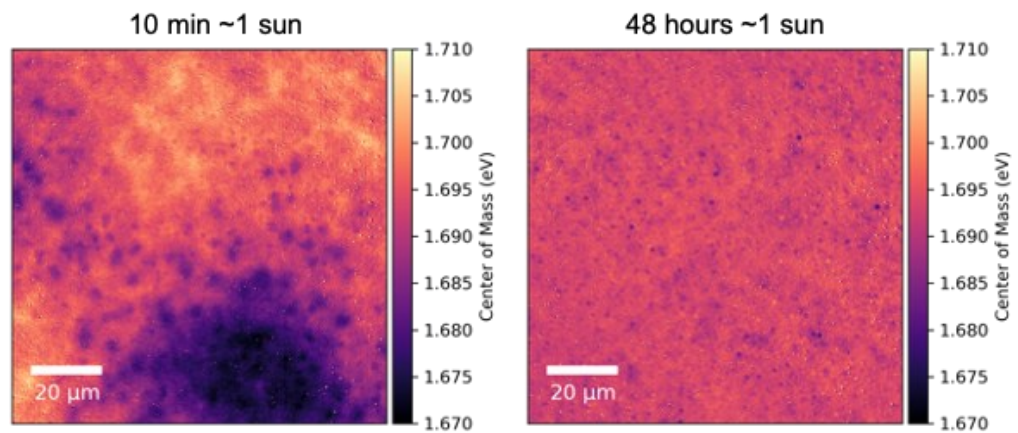
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Selective halogen oxidation has been linked to a variety of compositional and operational instabilities in lead halide perovskite materials. These effects range from largely reversible changes in films and devices (i.e. current-voltage hysteresis and carrier-induced halide segregation) to permanent degradation (i.e. electrode corrosion). What is common amongst these effects is that they stem from a dynamic and mobile ionic defect population, and a deep understanding of the evolution of this population is needed to maximize both the immediate performance and long-term stability of perovskite devices. In this work, we present new insights into the photodriven halogen oxidation process. We show that extended light soaking not only impacts the bulk structure, chemistry, and optoelectronic performance of  $\text{MAPb}(\text{I}_x\text{Br}_{1-x})_3$  perovskite films but also the chemistry and optoelectronic performance at the microscale. Using multimodal microscopy, we document a selective iodine expulsion process that results in substantial morphological and local-compositional changes in perovskite films. With this technique we monitor change in absorption, photoluminescence, and quasi-fermi level splitting at the micron scale for a range of  $\text{MAPb}(\text{I}_x\text{Br}_{1-x})_3$  films under one-sun light soaking conditions. We apply this technique to track reversible changes (that evolve in a period of seconds) and permanent changes (assessed after a period of days) in the film. In the case of  $\text{MAPbI}_2\text{Br}$ , this halogen expulsion and redistribution appears to result in perovskite film with increased bandgap and performance homogeneity, and overall improved optoelectronic performance and stability. Taken together, this work advances our understanding of the complex photostabilities present in lead halide perovskites and elevates the importance of understanding and controlling microstructure to achieve long term performance stability in this class of materials.



**Figure 1:** Map of center of mass for photoluminescence spectra of a  $\text{MAPbI}_2\text{Br}$  perovskite film after 10 minutes (left) and 48 hours (right) of  $\sim 1$  sun light exposure

# COMPOSITIONAL DESIGN APPROACH FOR pe-LED PRODUCTION BASED ON 3D LEAD-FREE HALIDE DOUBLE PEROVSKITES

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The perovskite structure holds immense potential for intelligent synthesis, enabling the creation of new materials grounded in the fundamental science of crystal chemistry. The tuneable crystal structure and variable chemical composition of perovskites position them as promising candidates for fuel cells, memory devices, and photovoltaic applications. Experimental results show that in this case, the halide double perovskites (HDPs) can transform the bandgap from indirect to direct states and alter the photoluminescence quantum yield (PL QY), which characterizes their photoluminescence properties. More importantly, HDPs can emit efficient white luminescence as self-trapped excitons (STEs), making them suitable as inexpensive white phosphors. The STEs can transfer excitons to dopants like  $\text{Sb}^{3+}$  or  $\text{RE}^{3+}$ , further tuning the emission from visible (Vis) to the near-infrared (NIR) region.<sup>[1-2]</sup>

In our case, we investigated various compositions of HDPs:  $\text{Cs}_2\text{NaInCl}_6$ ,  $\text{Cs}_2\text{Na}_{0.6}\text{Ag}_{0.4}\text{InCl}_6$ , and  $\text{Cs}_2\text{AgInCl}_6$  doped with  $\text{Sb}^{3+}$ ,  $\text{Er}^{3+}$ ,  $\text{Ho}^{3+}$ , and  $\text{Yb}^{3+}$ . The samples were obtained by using solid-state, hydrothermal, and precipitation techniques. Additionally, HDPs with the general formula  $\text{Cs}_2\text{NaRECl}_6$  (RE – La, Ce, Pr, Nd, Eu, Tb, Ho, Er, Tm, Yb) were synthesized. The X-ray diffraction and Raman spectroscopy were used to analyse the crystal structures and vibrational characteristics of the samples. The compositions of the samples were checked using the energy-dispersive X-ray spectroscopy (EDS) method, and some X-ray photoelectron spectra (XPS) spectra were measured. The luminescent properties in the range of 250-1600 nm were investigated for the first time, revealing significant potential for advanced applications. Upconversion was also fixed in the investigated samples, which makes them suitable candidates for the transformation of the sunlight from the NIR region to the Vis region.

Some prototypes of the LED, based on the UV chip (320 nm) and synthesized HDPs powder samples as the luminophore material, were prepared. The emission spectra were measured under 4.4-5.0 V bias voltage, and the prepared LED emitted blue, green and white light (depending on the HDP composition). It was possible to obtain efficient, stable multimodal emission in  $\text{Sb}^{3+}/\text{RE}^{3+}$ -codoped HDP samples using down-conversion to cover the Vis-NIR spectral range. The LED prototypes were stable and showed similar characteristics after six months.

**Acknowledgements:** *This research is part of the project No. 2022/47/P/ST5/01816 within the POLONEZ BIS programme co-funded by the National Science Centre and the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No. 945339.*

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# COMPLETE OPERANDO STUDY TRACKING PEROVSKITE SOLAR CELLS DEGRADATION

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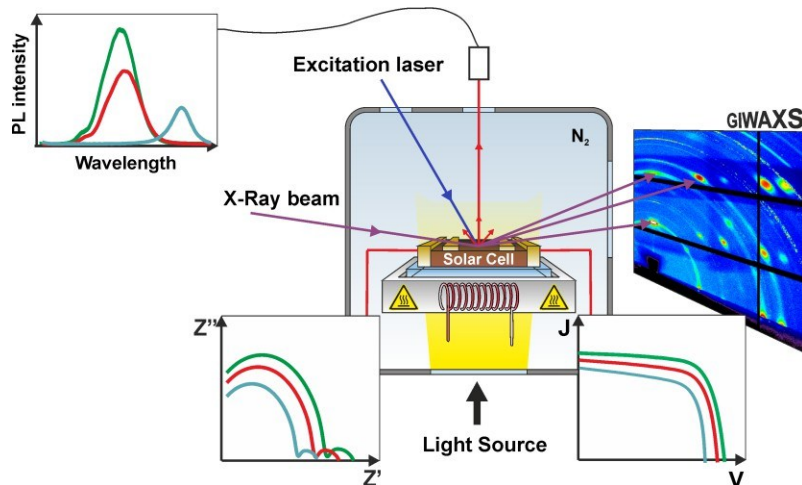
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Over the past fifteen years, perovskite solar cells have experienced a spectacular increase in power conversion efficiency (PCE), with the laboratory-based prototypes now matching the top-performing silicon cells.<sup>[1]</sup> However, the poor long-term stability of perovskite solar cells (SCs) hinders their widespread commercialization.

Our work introduces a comprehensive 24/7 operando degradation monitoring of the vapor-deposited perovskite SCs. Employing targeted diagnostic techniques simultaneously, such as photoluminescence (PL), grazing-incidence wide-angle X-ray scattering (GIWAXS), volt-ampere characteristics (J-V curves), and electrochemical impedance spectroscopy (EIS), we have analyzed the concurrent evolution of the devices' efficiency, optoelectronic properties, and crystallographic structure. The long-term study under conditions simulating an outdoor environment – specifically, one sun illumination intensity, solar cell temperature of 85 °C, and reproducible atmosphere – reveals the perovskite SCs' degradation mechanisms.

To the best of our knowledge, such a complex operando characterization of perovskite SCs is currently lacking and might be of great importance for the future improvement of their efficiency and stability.



**Figure 1:** Schematic illustration of the experiment monitoring the perovskite solar cell degradation in operando.

**Acknowledgements:** We acknowledge the support from the following grants – IMPULZ (IM-2023-82), APVV-21-0297, SK-CZ-RD-21-0043, 2023/727/PVKSC, and OSCARS AI-SCOPE.

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# RATIONAL DESIGN OF PHOSPHINE OXIDE FOR EFFICIENT PEROVSKITE LIGHT-EMITTING DIODES

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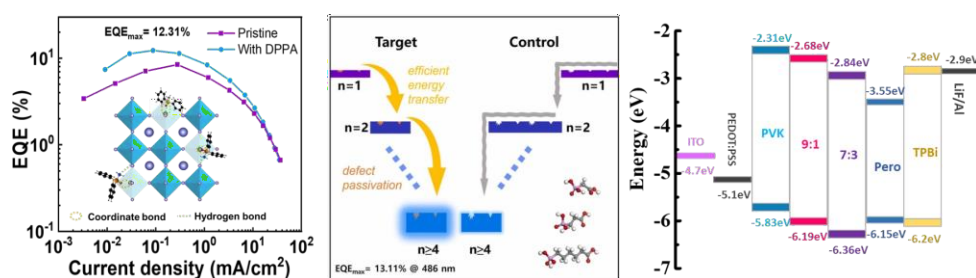
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Metal halide perovskites have shown great potential for next-generation display technologies due to their high colour purity and photoluminescence quantum yields. Although generally considered defect-tolerant compared to conventional semiconductors, accumulating evidence indicates that defects still critically impact the performance and stability of perovskite light-emitting diodes (LEDs).<sup>1</sup> Additionally, the influence of carrier injection and charge transport layers plays a vital role in determining device efficiency. In this work, we systematically investigate the multifunctional roles of phosphine oxide molecules in enhancing perovskite LED performance. Based on the principles of defect passivation, we introduce diphenylphosphinamide and phosphonic acid as additives to effectively passivate surface defects, regulate phase distribution, and promote efficient energy transfer in quasi-2D perovskite films. These treatments lead to significantly improved optoelectronic properties and device efficiencies.<sup>2,3</sup> Furthermore, we design tris(4-trifluoromethylphenyl)phosphine oxide to tailor the energy level alignment and improve hole mobility within the widely used poly(9-vinylcarbazole) (PVK) hole transport layer, achieving further performance enhancements, particularly in blue perovskite LEDs.<sup>4</sup> Our results demonstrate that phosphine oxide can serve dual functions: as effective passivation agents for perovskite films and as modifiers for charge transport layers. This dual strategy provides a versatile platform for simultaneously optimizing both the emissive layer and carrier transport interfaces in perovskite LEDs. These findings offer valuable insights for advancing high-performance, stable perovskite-based optoelectronic devices.



[1] *Joule* **2023**, *7*, 272–308.

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# LARGE SCALE DEPOSITION OF UNIFORM PEROVSKITE FILMS IN AMBIENT ATMOSPHERE BY COMBINING SLOT-DIE COATING AND VACUUM FLASH QUENCHING

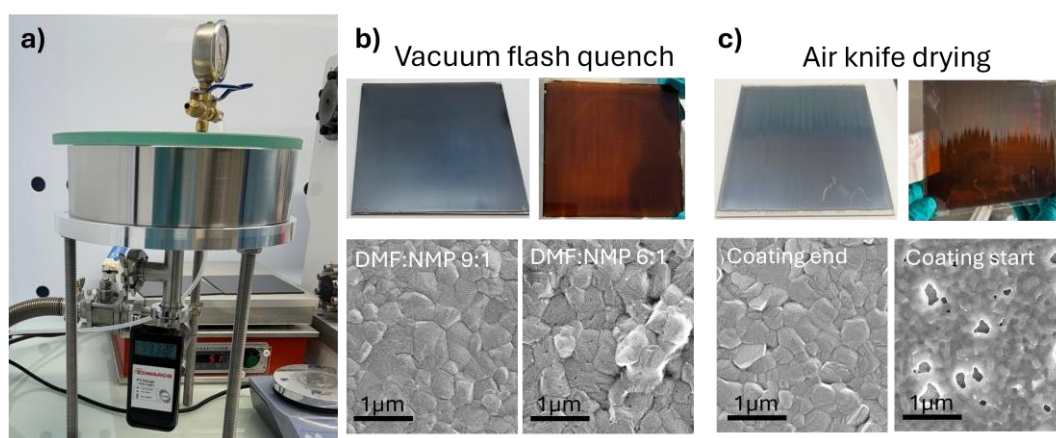
**Iwan Zimmermann**,<sup>1</sup> Emmanuel Tetsi,<sup>1</sup> Mohammed Salim,<sup>1</sup> Van Son Nguyen,<sup>1</sup> Rene Mendez,<sup>1</sup> Jean Rousset<sup>1,2</sup>

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Deposition of uniform and pinhole-free perovskite layers at the industrial scale remains a challenge towards commercializing perovskite solar cells. Slot-die-coating has demonstrated to be a viable technique for deposition of wet films on large surfaces.<sup>[1]</sup> Homogeneous drying of these wet films is crucial for the formation of highly crystalline and dense perovskite layers. In this study we compare conventional air-knife drying (AKD) and vacuum flash quenching<sup>[2]</sup> (VFQ) on 15 x 15 cm<sup>2</sup> substrates. We present the design of an in-house built vacuum chamber allowing to pump to around 10 Pa in 10 seconds (Figure 1a). We observe that AKD for large samples is challenging as the slow-moving air stream affects the drying towards the end of the sample leading to thickness gradients and a non-uniform crystallization with incomplete surface coverage (Figure 1c). On the other hand, VFQ allows for a quick and controlled solvent removal resulting in highly uniform perovskite films (Figure 1b). Furthermore, we demonstrate that the solvent composition is crucial in controlling the perovskite morphology. Different DMF:NMP ratios of 7:3, 6:1 and 9:1 are investigated. We find that lowering the NMP content to 10 vol% improves the perovskite morphology compared to 7:3 and 6:1 DMF:NMP ratios.



**Figure 1:** a) image of the vacuum flash setup, pictures (front and backside) and SEM images of the perovskite films fabricated using: b) vacuum flash quenching: improved deposition with DMF:NMP ratio of 9:1, c) air-knife drying: non-uniform crystallization along the substrate.

Finally, the optimized perovskite is employed in NIP opaque small cells and mini-modules (64cm<sup>2</sup>) with efficiencies up to 18%. Furthermore, this perovskite layer is employed in semi-transparent PIN mini-modules for 4T tandem applications.

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# APPLICATIONS OF PEROVSKITE LEDs IN MULTIFUNCTIONAL DISPLAY AND LIGHT COMMUNICATION SYSTEM

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<sup>1</sup>Clarendon Laboratory, Department of Physics, University of Oxford, Parks Road, Oxford, OX1 3PU, United Kingdom.

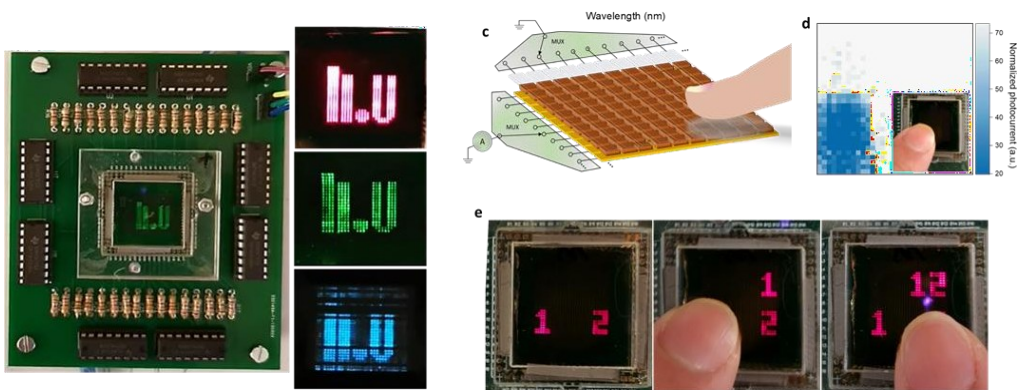
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<sup>3</sup>National Laboratory of Solid State Microstructures, School of Physics, Nanjing University, Nanjing, 210093, China  
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Metal halide perovskites possess unique optical and electronic properties, including high light absorption, high mobility, tuneable bandgaps and high defect tolerance, making them very promising for achieving high performance optoelectronic devices. Here we demonstrate examples of using perovskites as emitters for applications in multifunctional displays and visible light communications (VLCs).

Firstly, we develop multifunctional displays using highly photo-responsive metal halide perovskite LEDs (PeLEDs) as pixels. Here, we develop multifunctional displays using highly photo-responsive metal halide perovskite LEDs (PeLEDs) as pixels following our previous publication.<sup>[1]</sup> With efficient defects passivation in perovskite layers, the red emissive PeLEDs shows an external quantum efficiency (EQE) of 10% when working at LED model and a power conversion efficiency (PCE) of 5.34% at photovoltaic model. Due to the strong photo response of the PeLED pixels, the display can be simultaneously used as touch screen, fingerprint sensor, ambient light sensor, and image sensor without integrating any additional sensors. In addition, decent light-to-electricity conversion efficiency of the pixels also enables the display to act as a photovoltaic device which can charge the equipment.<sup>[2]</sup> The multiple-functions of our PeLED pixels can not only simplify the display module structure and realize ultra-thin and light-weight display, but also significantly enhance the user experience by these advanced new applications, and this is a feature hardly possible for conventional LED technologies.<sup>[3]</sup>

Additionally, we further demonstrate a perovskite-based VLCs system with PeLEDs and PePVs. These demonstrations show that perovskite optoelectronics will have special advantages in the future for high performance and low-cost telecommunication devices.



**Figure 1:** Display and touch control demonstrations of our PeLED display.

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# EXPLORING CHARGE COLLECTION EFFICIENCY LOSSES OF PEROVSKITE SOLAR CELLS USING HYSTERESIS AND IMPEDANCE MEASUREMENTS

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The stability of perovskite solar cells (PSCs) remains a critical challenge, as they degrade under real-world conditions, leading to significant performance losses. Understanding the physical mechanisms behind this reduction of efficiency is essential for mitigation. Our study observes a notable decrease in short-circuit current density (JSC) due to degradation. Contributing factors include the migration of positively charged halide vacancies,<sup>[1]</sup> ionic redistribution, charge accumulation at interfaces leading to field screening,<sup>[2]</sup> and intrinsic material instability.<sup>[3]</sup> These processes impact charge collection and recombination, introduce hysteresis in the J–V curve and alter the impedance response,<sup>[4]</sup> resulting in a double-inductor feature at low frequencies. Negative capacitance in the impedance response is commonly linked to the inverted J–V curve hysteresis.<sup>[5]</sup> We show how PSC degradation leads to significant current reduction in the J–V characteristics, connects to a prominent inverted J–V hysteresis with the hallmark of a curve inclination around 0 V, and causes a double-inductor feature in the impedance responses. A theoretical model numerically identifies the reasons for this type of current hysteresis in degraded halide PSCs, providing new insights into significant current reduction upon degradation via Impedance Spectroscopy. Future efforts to address degradation could focus on defect passivation, interface stabilization with robust materials, optimizing device architecture to reduce ionic migration, and encapsulation techniques to protect against environmental stress. These strategies have the potential to greatly enhance the stability and performance of PSCs over time.

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# WRITING WITH LIGHT: OPTICAL EXCITATION-INDUCED MEMORY IN MIXED HALIDE PEROVSKITES

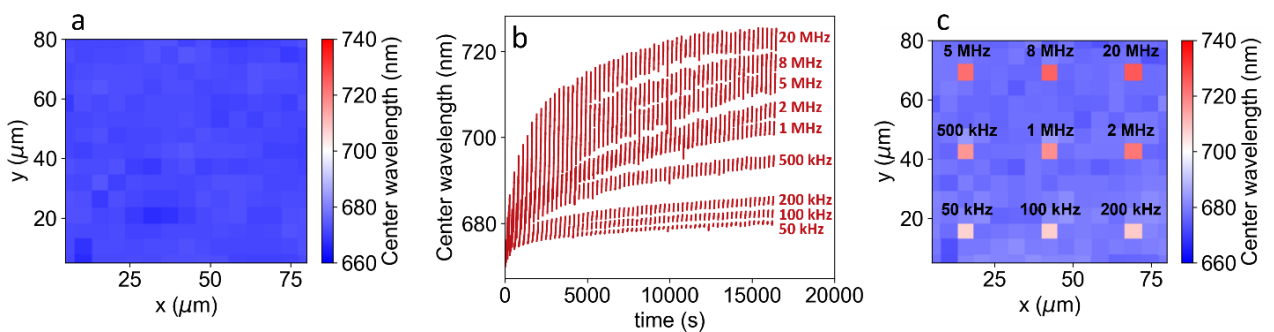
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Mixed Metal halide perovskites ( $AB(X_xY_{x-3})_3$ ) are widely recognized as one of the most promising materials for next generation solar cells, light-emitting diodes, and photodetectors. They display great light harvesting properties, tunability, ease of fabrication, low costs, and defect tolerance. However, their lack of stability under external stimuli, such as light illumination, has so far prevented large scale utilization in devices. One demonstration of this instability is the reversible halide segregation observed in mixed-halide perovskites. Upon illumination, these materials transition from a homogeneously mixed state to a multi-bandgap configuration, with iodide-rich and bromide-rich domains forming over seconds. In this study we show that, rather than being merely a drawback, this photoinduced instability can be leveraged for functional device applications. Specifically, we demonstrate the potential of mixed halide perovskites to be used as optical information storage devices. By tracking the photoluminescence (PL) over time under femtosecond pulsed laser excitation, we show that input dependent optical excitation induces controlled and reversible segregation, leading to distinct PL wavelength shifts that encode excitation parameters. First, we track the PL of  $MAPb(Br_{0.8}I_{0.2})_3$  and  $Cs_{0.07}(FA_{0.83}MA_{0.17})_{0.93}Pb(Br_{0.5}I_{0.5})_3$  over time for different excitation conditions. We show that by varying the laser pulse repetition rate between 10 kHz and 40 MHz for a range of average excitation intensities between 0.5  $\mu W$  and 300  $\mu W$ , we are able to reach pre-determined states of halide segregation in the perovskite. Second, we show that after writing information into the perovskite, it displays long retention time, allowing for the information to be read out with a time delay. Finally, by heating the sample, we demonstrate that the halide segregation can be reversed quickly, essentially erasing the written information. Our findings highlight the potential of perovskites for high-density, rewritable optical memory and neuromorphic computing, utilizing their intrinsic dynamic responses for next-generation photonic technologies.



**Figure 1:** Controlled halide segregation to predetermined wavelength states. The PL center wavelength before initiating the writing (a), the halide segregation dependent on laser repetition rate (b), and the PL center wavelength after writing (c).

# UNRAVELING ION TRANSPORT AND ELECTRONIC STATES IN PEROVSKITE THIN FILMS USING MOVING GRATING TECHNIQUES

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<sup>1</sup>University of Valencia, Spain

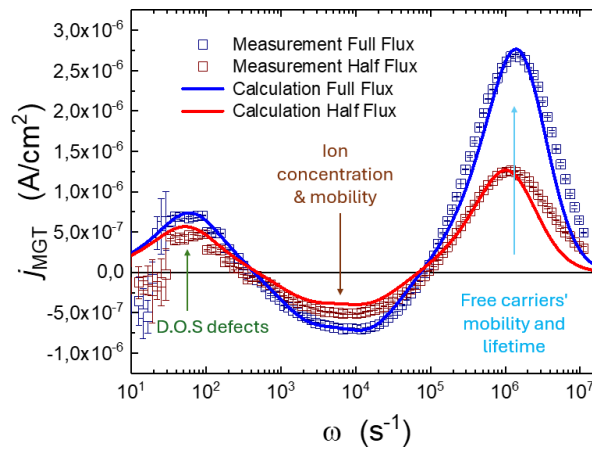
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Ion migration is a defining characteristic of metal halide perovskites (MHPs) and a major contributor to the instability of perovskite solar cells. Understanding this phenomenon requires accurate characterization of ion concentration, mobility, and activation energy. In this work, we demonstrate how the Moving Grating Technique (MGT)<sup>[1]</sup> can provide not only the drift mobility and recombination lifetime of free carriers but also insights into ion transport and the density of states (D.O.S.) in perovskite thin films.

Previous studies<sup>[2]</sup> have shown that MGT measurements exhibit a high-frequency peak associated with photocarriers, as well as a low-frequency peak attributed to ion motion.<sup>[3]</sup> Here, we report the observation of a third peak at even lower frequencies (see Figure 1). By solving the transport equations—accounting for the D.O.S., ion contributions, and multiple recombination pathways—we attribute this additional peak to defects within the D.O.S.

Our findings highlight MGT as a versatile and powerful tool for probing critical transport properties in perovskite films, offering valuable insights into carrier dynamics, ion migration, and defect-related phenomena.



**Figure 1:** MGT curve measured for a triple cation formamidinium based (FA<sub>0.8</sub>Cs<sub>0.2</sub>Pb(I<sub>0.9</sub>Br<sub>0.1</sub>)<sub>3</sub>) wide band gap perovskite thin film. Three clearly visible peaks are seen. From lower to higher frequency these are related to D.O.S. defect states, Ion's mobilities and concentration and free carrier dynamics.

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# ANTI-STOKES OPTICAL COOLING IN CSPBBR<sub>3</sub>/CS<sub>4</sub>PBBR<sub>6</sub> DOT-IN-CRYSTAL PEROVSKITES: EXPLORING THE POTENTIAL AND FUNDAMENTAL LIMITS

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Halide perovskites possess a unique combination of high photoluminescence (PL) efficiency and strong electron–phonon interactions,<sup>[1,2]</sup> which are rarely found together in conventional semiconductors. Among the intriguing applications enabled by these properties is optical cooling via anti-Stokes photoluminescence (ASPL). In ASPL, PL photons have higher energy than excitation light. If the external PL quantum efficiency is 100%, the material loses its internal energy through photoabsorption and subsequent ASPL, resulting in optical cooling. While rare-earth-doped crystals have demonstrated AS cooling down to cryogenic temperatures, their weak optical absorption limits the cooling performance. In contrast, halide perovskite semiconductors offer both strong light absorption and efficient ASPL, making them promising candidates for optical cooling materials. However, it is still difficult to achieve and maintain the near-unity PL quantum efficiency required for AS cooling.

In this study, we focus on a novel perovskite nanostructure composed of CsPbBr<sub>3</sub> quantum dots (QDs) embedded in a Cs<sub>4</sub>PbBr<sub>6</sub> host crystal (CsPbBr<sub>3</sub>/Cs<sub>4</sub>PbBr<sub>6</sub>). This “dot-in-crystal” structure exhibits near-unity PL quantum efficiency and improved photostability.<sup>[3,4]</sup> To evaluate the cooling potential of this system, we performed time-resolved PL spectroscopy. In particular, we investigated the role of Auger recombination, an intrinsic nonradiative process in QDs under intense excitation. From the excitation-intensity-dependent PL dynamics, we quantified the Auger recombination rate and determined the optimal excitation conditions for maximizing cooling gain. Based on these results, we estimate the upper limit of cooling power to be approximately 2 fW per QD.

Finally, we experimentally demonstrated optical cooling by applying continuous-wave laser excitation to highly luminescent CsPbBr<sub>3</sub>/Cs<sub>4</sub>PbBr<sub>6</sub> microparticles in a vacuum environment.<sup>[4]</sup> Temperature changes were evaluated using a newly developed PL thermometry technique with an accuracy of ~1 K. Under optimized conditions, we observed a temperature reduction of approximately 9 K, providing the first clear evidence of optical cooling in halide perovskite QDs. These findings highlight the unique advantages of halide perovskites for optical cooling and clarify fundamental limitations stemming from Auger recombination. Our work offers a viable route toward light-driven solid-state cooling and opens new possibilities for thermally managed optoelectronic devices based on perovskite materials.

Part of this work was supported by the Asahi Glass Foundation, JSPS KAKENHI (Grant No. JP25K01649), and JST-CREST (Grant No. JPMJCR21B4).

[1] Y. Yamada et al., *Phys. Rev. Lett.* **2021**, 126, 237401.

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# CHEMICAL VAPOR DEPOSITED HIGHLY CRYSTALLINE CsPbBr<sub>3</sub> FILMS FOR ENHANCED BROAD-RANGE PHOTODETECTION WITH ULTRA LOW DARK CURRENT

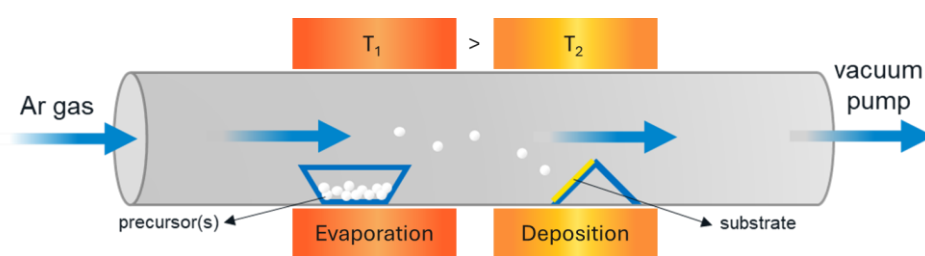
**Roel Vanden Brande**,<sup>1</sup> **Sudipta Seth**,<sup>1</sup> **Elke Debroye**<sup>1</sup>

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CsPbBr<sub>3</sub> has attracted significant attention as potential material for high-performance optoelectronic applications, including X-ray detection, owing to its superior charge transport properties, long carrier diffusion lengths, broad light absorption, and tuneable bandgap.<sup>[1]</sup> In particular, CsPbBr<sub>3</sub> has demonstrated strong promise as an active material in low-cost, high-sensitivity direct X-ray detectors, surpassing current market standards limited by poor X-ray absorption or expensive processing methods.<sup>[2]</sup>

In this presentation, I will focus on the fabrication of CsPbBr<sub>3</sub> thin films using a custom home-built chemical vapor deposition (CVD) system (Figure 1). Unlike conventional spin-coating techniques, this solvent-free vapor-phase approach significantly reduces crystal surface defects and enhances film uniformity. I will elaborate on the impact of different CVD settings and substrate. Structural and optical characterization reveals that these films exhibit unprecedented quality compared to wet synthesis methods. X-ray diffraction (XRD) confirms phase-pure CsPbBr<sub>3</sub> formation, both directly from precursor powders or pre-synthesized crystals, demonstrating the reproducibility and versatility of the CVD technique. Scanning electron microscopy reveals large grain sizes (~20 μm), while time-resolved photoluminescence spectroscopy demonstrates extended luminescence lifetimes of up to 45 ns.

To evaluate their practical applicability, proof-of-concept photo- and X-ray detectors based on these films have been developed. Under 100 mW light irradiation, the CsPbBr<sub>3</sub>-based device exhibits a signal-to-noise ratio (SNR) of  $5 \times 10^4$  under a bias voltage of 5 V. The ultralow dark current of sub-pA is proof of the improved quality of the thin films. Notably, devices maintained performance and stability over several days of continuous operation (bias voltage of 5 V). These findings position CVD-grown CsPbBr<sub>3</sub> as a highly promising platform for next-generation, stable (high-energy) radiation detection technologies.



**Figure 1.** Schematic representation of the CVD technique.

[1] Clinckemalie L., "Phase-Engineering Compact and Flexible CsPbBr<sub>3</sub> Microcrystal Films for Robust X-Ray Detection" *J. Mater. Chem. C* **2024**, 12(2), 655-663.

[2] Clinckemalie L., "Challenges and opportunities for CsPbBr<sub>3</sub> Perovskites in Low- and High- Energy Radiation Detection" *ACS Energy Letters* **2021**, 6(4), 1290-1314.

# ENERGETICS AND DEFECT LANDSCAPE OF SOFT-SPUTTERED SnO<sub>x</sub>: IMPLICATIONS FOR PEROVSKITE SOLAR CELLS AND LOW-LEAKAGE PHOTODETECTORS

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<sup>1</sup>imec, imo-imomec, Belgium

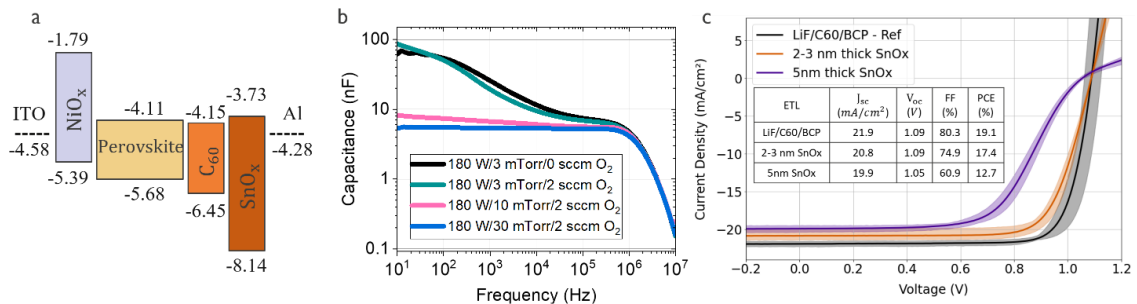
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SnO<sub>2</sub> is a promising electron transport layer (ETL) for inverted p–i–n perovskite solar cells,<sup>[1]</sup> but the scalability of commonly used atomic layer deposition is limited by precursor cost and low throughput. We explore sputtering as a scalable alternative, studying the impact of sputtering power, pressure and O<sub>2</sub>/Ar ratio in the plasma on SnO<sub>x</sub> optoelectronic properties and demonstrate its application in solar cells and photodetectors.

X-ray photoelectron spectroscopy (XPS) and ultraviolet photoelectron spectroscopy (UPS) measurements reveal improved conduction band alignment (**Fig.1a**) between SnO<sub>x</sub>, C<sub>60</sub>, and the perovskite at higher sputtering pressures, while the film remains sub-stoichiometric (O/Sn<sup>4+</sup> ≈ 1.74). Although this points to oxygen deficiency and under-coordinated Sn species (defects), the capacitance-voltage profiling (**Fig.1b**) reveals that depositing at higher pressure (and consequently higher power) suppresses trap state formation. Devices using ultra-thin (2–3 nm) SnO<sub>x</sub> in a C<sub>60</sub>/SnO<sub>x</sub> bilayer ETL show a decent performance (**Fig.1c**) compared to LiF/C<sub>60</sub>/BCP references. In contrast, thicker SnO<sub>x</sub> layers (>4–5 nm) result in S-shaped current-voltage (JV) curves, likely due to charge buildup and transport limitations from low electron mobility (~10<sup>-9</sup> cm<sup>2</sup>/V·s) of as-deposited SnO<sub>x</sub>. Thin layers reduce the transport path, mitigating these effects. Notably, the same sub-stoichiometric SnO<sub>x</sub> exhibit strongly suppressed leakage current (10<sup>-8</sup> A/cm<sup>2</sup> at -0.5V)—favourable for photodetector applications requiring low dark current. We hypothesize that higher pressure reduces energetic damage to the substrate, while increased power help in densification of the films. Current efforts focus on substrate heating and post-annealing to enhance mobility. These findings underscore key process–property–performance relationships in SnO<sub>x</sub> and its dual-use potential in perovskite solar cells and photodetectors.



**Figure 1** (a) Energy level alignment of sputtered SnO<sub>x</sub> with other layers, (b) Capacitance vs frequency plots for different SnO<sub>x</sub> (Power /Pressure /O<sub>2</sub> flow rate), (c) JV curves comparison with reference ETL.

**Acknowledgements:** This work has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement No. 101147311 of the LAPERITIVO project

[1] Gao, D. et al., *Science* **2024**, 386, 187–192.

# GRAPHENE OXIDE DOPING BOOSTS EFFICIENCY OF PEROVSKITE SOLAR CELLS WITH CARBON ELECTRODE TOWARDS 24%

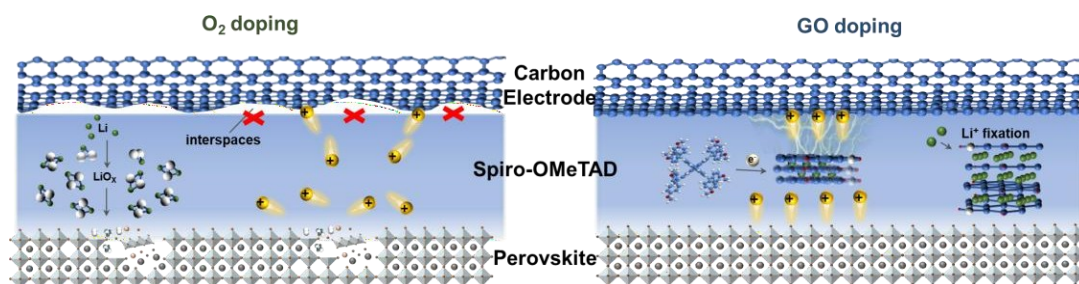
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Carbon-based perovskite solar cells (C-PSCs) processed at low temperature are gaining attention due to their enhanced stability and cost-effectiveness. However, these benefits are typically offset by inferior device performance stemming primarily from inadequate charge transfer between the hole transport layer (HTL) and the carbon electrode. Herein, we introduce a novel approach utilizing graphene oxide functionalized with carboxyl groups (GO-COOH) to efficiently dope the Spiro-OMeTAD, simultaneously facilitating interfacial charge transfer and immobilizing the  $\text{Li}^+$  ions, thereby improving device performance and stability. Mechanistic study elucidates the valence electron transfer between GO-COOH and Spiro-OMeTAD, as well as the delocalized electron of GO-COOH enables the p-doping without oxygen exposure and establishes a strong  $\pi$ - $\pi$  conjugated HTL/carbon interface. The formation of Li-C bonds allows the fixation of mobile  $\text{Li}^+$  ions for enhanced device stability. The resulting C-PSCs achieve a record power conversion efficiency (PCE) of up to 23.7% (certified: 23.08%) with exceptional operational stability. This work remarks a significant breakthrough in improving the performance of C-PSCs processed at fully low temperature to catch up with PSCs with metal electrodes.



**Figure 1:** A schematic showing that conventional  $\text{O}_2$  doping is time-consuming and leads to perovskite degradation, while GO-COOH doping achieves rapid oxidation and  $\text{Li}^+$  fixation as well as conjugated interfacial contact.

**Acknowledgements:** The authors thank Shaik M. Zakeeruddin and Michael Grätzel for their help with the initial phase of preparation of this manuscript. The work was supported by the National Natural Science Foundation of China (22109019, 52272193).

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**Day 3 - Wednesday, September 17th 2025**

08:45 09:00

**CONFERENCE DESK**

**Town Hall**

**Session Chair**

**Pablo Boix, ITQ (UPV-CSIC), Spain**

**Session Title**

**Session 1 – Invited Lectures**

09:00 09:25

16° INVITED LECTURE - **Alex Kwan Yue Jen**, City University of Hong Kong, Hong Kong  
*Molecular engineering of organic and hybrid materials for highly efficient and stable perovskite solar cells*

09:25 09:50

17° INVITED LECTURE - **Silvia Colella**, CNR-NANOTEC, Italy  
*Interface engineering of perovskite solar cells*

09:50 10:15

18° INVITED LECTURE - **Shuxia Tao**, Eindhoven University of Technology, The Netherlands  
*Materials theory of halide perovskites*

10:15 10:40

19° INVITED LECTURE - **Yuanyuan Zhou**, HKUST, Hong Kong  
*Perovskite microstructural disorder*

10:40 11:20

**COFFEE BREAK AM**

**Town Hall**

**Session Chair**

**Daniele Meggiolaro, CNR-SCITEC, Italy**

**Session Title**

**Session 2 – Invited Lectures – VALHALLA**

11:20 11:45

20° INVITED LECTURE - **Daniele Cortecchia**, University of Bologna, Italy  
*Lasing in 2D perovskites: the critical role of composition and structure*

11:45 12:10

21° INVITED LECTURE - **Annamaria Petrozza**, Istituto Italiano di Tecnologia, Italy  
*Tin-Halide Perovskite Semiconductors for Near-Infrared Light-Emitting Sources*

12:10 12:35

22° INVITED LECTURE - **Henk Bolink**, UVEG, Spain  
*Vapor Phase Deposited Perovskite Solar Cells*

12:41 14:00

**LIGHT BUFFET LUNCH**

# MOLECULAR ENGINEERING OF ORGANIC AND HYBRID MATERIALS FOR HIGHLY EFFICIENT AND STABLE PEROVSKITE SOLAR CELLS

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A novel strategy has been developed to reduce the photovoltage loss of wide-bandgap (WBG) perovskite solar cells by constructing a localized 2D/3D perovskite heterojunction at the buried interface through intricate Lewis acid-base interaction between hole-selective self-assembled monolayer (SAM) and organic ammonium ligands. This not only significantly reduced defect density but also facilitated charge extraction and perovskite crystallization without compromising bulk optoelectrical properties of 3D perovskite. These led to a record  $V_{oc}$  of 1.382 V for 1.79 eV-PSC, which exceeds 90% of its Shockley-Queisser limited value. The device retained 95% of its initial PCE (20.3%) after maximum power point tracking for over 700 h. By integrating this WBG PSC with an organic rear subcell, a perovskite-organic tandem cell was fabricated to achieve a record-high PCE of 27.11% (certified 26.3%).

Regarding the development of regular bandgap PSCs, several novel interface and additive engineering approaches have been implemented, like polyoxometalates (POMs) and Ti-containing clusters to enable PSCs to achieve very high PCE ( $> 27\%$ ) and excellent stability. Moreover, new multifunctional redox additives have also been developed for their incorporation in Pb/Sn binary perovskite devices to overcome the crystallization and oxidation issues that strongly hinder the development of highly efficient and stable narrow bandgap PSCs. Their integration with a WBG perovskite subcell to form 2-T tandem devices has achieved a record-high PCE of 30.1% with good operational stability.

1. “Redox Mediator Stabilized Wide Bandgap Perovskites for Monolithic Perovskite-Organic Tandem Solar Cells”, S. Wu, Y. Yan, J. Yin, K. Jiang, F. Li, Z. Zeng, S. Tsang, and A. K.-Y. Jen, *Nature Energy* **2024**, *9*, 411.
2. “Advances in inverted perovskite solar cells”, X. Zhang, S. Wu, H. Zhang, A. K.-Y. Jen, Y. Zhan & J. Chu, *Nature Photonics*, **2024**, *18*, 1243.
3. “Molecularly tailorable metal oxide clusters ensured robust interfacial connection in inverted perovskite solar cells”, F. Li, C. Zhao, Y. Li, Z. Zhang, X. Huang, Y. Zhang, J. Fang, T. Bian, Z. Zeng, A. K.-Y. Jen, *Sci. Adv.*, **2024**, *10*, eadq1150.
4. “Hydrogen Bond-Bridged Intermediate for Perovskite Solar Cells with Enhanced Efficiency and Stability”, F. Li, X. Deng, Z. Shi, S. Wu, Z. Zeng, D. Wang, Y. Li, F. Qi, Z. Zhang, Z. Yang, S.-H. Jang, F. R. Lin, S.-W. Tsang, X. K. Chen, and A. K.-Y. Jen, *Nature Photonics*, **2023**, *17*, 478.
5. “Advances and Challenges in Understanding the Microscopic Structure–Property–Performance Relationship in Perovskite Solar Cells”, Y. Zhou, L. Herz, A. K.-Y. Jen, and M. Saliba, *Nature Energy*, **2022**, *7*, 794.

# INTERFACE ENGINEERING OF PEROVSKITE SOLAR CELLS

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The control of interfaces in perovskite solar cells is a central lever for improving charge extraction, reducing recombination losses, and enabling high device performance.

We report on two unconventional strategies for modifying the surface of various perovskite compositions. The first exploits molecular passivation by using compounds capable of generating light-induced zwitterionic states, such as polychlorinated Thiele hydrocarbons (TTH).[1] These stable singlet diradicaloids, when employed as interfacial modifiers in CsPbI<sub>3</sub> devices, simultaneously ensure efficient Pb passivation through chlorine substituents, favorable energy level alignment, and a photoinduced dipole effect. Altogether, these features reduce interfacial resistance and enable a marked enhancement of the open-circuit voltage in inverted solar cells. The second strategy relies on plasma-based processes, which provide solvent-free, scalable, and versatile means of tailoring the perovskite surface.[2] Different gas plasmas, including Ar, N<sub>2</sub>, and sulfur-containing atmospheres, were explored on both Pb-based and Pb-free perovskites. Among the most notable effects, Ar plasma was found to reduce defect density in MAPbI<sub>3</sub>,[3] while N<sub>2</sub> plasma effectively suppressed the oxidation of Sn<sup>2+</sup> in FASnI<sub>3</sub>,[4-5] thereby improving both device stability and performance. Interface engineering through molecular modifiers and plasma treatments can be tailored to different perovskite compositions, however it remains highly specific to each material system and thus a key determinant of the future development of perovskite solar cells.

## ***References:***

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- [5] S. Covella *et al.*, *manuscript in preparation*.

# MATERIALS THEORY OF HALIDE PEROVSKITES

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Halide perovskites are a versatile class of materials with tunable photonic, electronic, and spin-related properties, making them promising for applications from solar energy to quantum technologies. Their soft, ionically conductive lattice and chemical flexibility enable tailored functionalities and seamless device integration. Our group applies first-principles simulations and machine learning to uncover the structure–property relationships that influence performance and stability.

A key focus is the chemistry and physics of defects, which play a central role in long-term stability. We model defect formation and migration pathways, and propose strategies such as compositional tuning and surface passivation. In parallel, we explore chirality in hybrid perovskites, examining how chiral ligands induce spin-selective effects like chiral induced spin selectivity (CISS) and enhance chiroptical responses, paving the way for spintronic and chiral optoelectronic devices.

# PEROVSKITE MICROSTRUCTURAL DISORDER

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[yyzhou@ust.hk](mailto:yyzhou@ust.hk)*

Hybrid perovskites are a class of emerging semiconductors that have shown great promise for low-cost, printable solar cells and optoelectronics. Regardless of the numerous, swift developments of perovskite devices in the recent decade, the field still lacks a quantitative materials-science understanding of these fascinating solids. In this context, while the long-range or short-range microstructural disorder is known to affect the overall performance of perovskite solar cells and optoelectronics, it remains terra incognita worthy of in-depth, systematic exploration. In my talk, I will elaborate on two key types of microstructural disorder, interfacial nano-groove, and intra-crystal disorder, which show nontrivial effects on carrier injection, chemical stability, and device reliability of perovskite. We then translated our fundamental understanding of such microstructure disorder into the device practice, innovating material microstructures to enable stable and efficient perovskite solar cells. This research is a prototype for paving the way toward theory-driven, predictable processing/synthesis for more commercially viable solar cells and optoelectronics.

## LASING IN 2D PEROVSKITES: THE CRITICAL ROLE OF COMPOSITION AND STRUCTURE

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Low-dimensional metal halide perovskites are attracting great interest for photovoltaics and photonics. In particular, 2D tin perovskites have been shown to have good optical gain properties which make them promising for applications as coherent light sources.<sup>[1]</sup> On the other hand, the ability of lead-based 2D perovskites to sustain lasing remains highly controversial, and stable operation at room temperature in 2D perovskite films is still challenging.<sup>[2]</sup>

Here we show that both Sn and Pb-based 2D perovskites thin films can achieve amplified stimulated emission (ASE) and compare their properties as function of temperature and optical pumping conditions. We further investigate the effects of the materials' structural characteristics by studying perovskite structures employing different aromatic and alkylammonium templating cations. By employing <sup>1</sup>H, <sup>13</sup>C, <sup>15</sup>N, <sup>119</sup>Sn and <sup>207</sup>Pb solid state NMR spectroscopy, we were able to discern the local structural environments of the 2D perovskite of interest through their characteristic spectral fingerprints. Spin-lattice relaxation measurements reveal that the local supramolecular spatial arrangements, the molecular motions and structural rigidity are key factors shaping the energetic landscape of the material and its luminescence properties.

Our work provides a deeper understanding of the structure-properties relationship of this class of soft semiconductors to assist the rational engineering of materials with improved optical properties for lasing applications.

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# TIN-HALIDE PEROVSKITE SEMICONDUCTORS FOR NEAR- INFRARED LIGHT-EMITTING SOURCES

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Light-emitting diodes (LED) with different emission spectra are widely used in our daily life for a variety of applications. However, due to fundamental restrictions of light-emitting materials, the development of near-infrared LEDs (NIR-LEDs) is still modest. Recently, solution-processed tin-halide perovskites (THPs) have emerged as one of the most promising light-emitting materials for NIR-LED applications. Here, first, how the defects chemistry of THPs affects the light emission efficiency of the semiconductor will be presented. Then, efforts in materials engineering to design and master the electronic properties of THP films will be discussed. In particular, a facile yet highly effective strategy will be presented to master the defects activity in THPs by developing self-encapsulated tin-halide perovskite films. The resulting film exhibits a significantly reduced trap density and mitigated p-doping density such that it is exploited to boost radiative charge recombination to reach a photoluminescence quantum yield approaching 50%. Leveraging these advancements, NIR-LEDs demonstrate a peak external quantum efficiency of 12.4%, accompanied by a substantial improvement in operational lifetime.

# VAPOR PHASE DEPOSITED PEROVSKITE SOLAR CELLS.

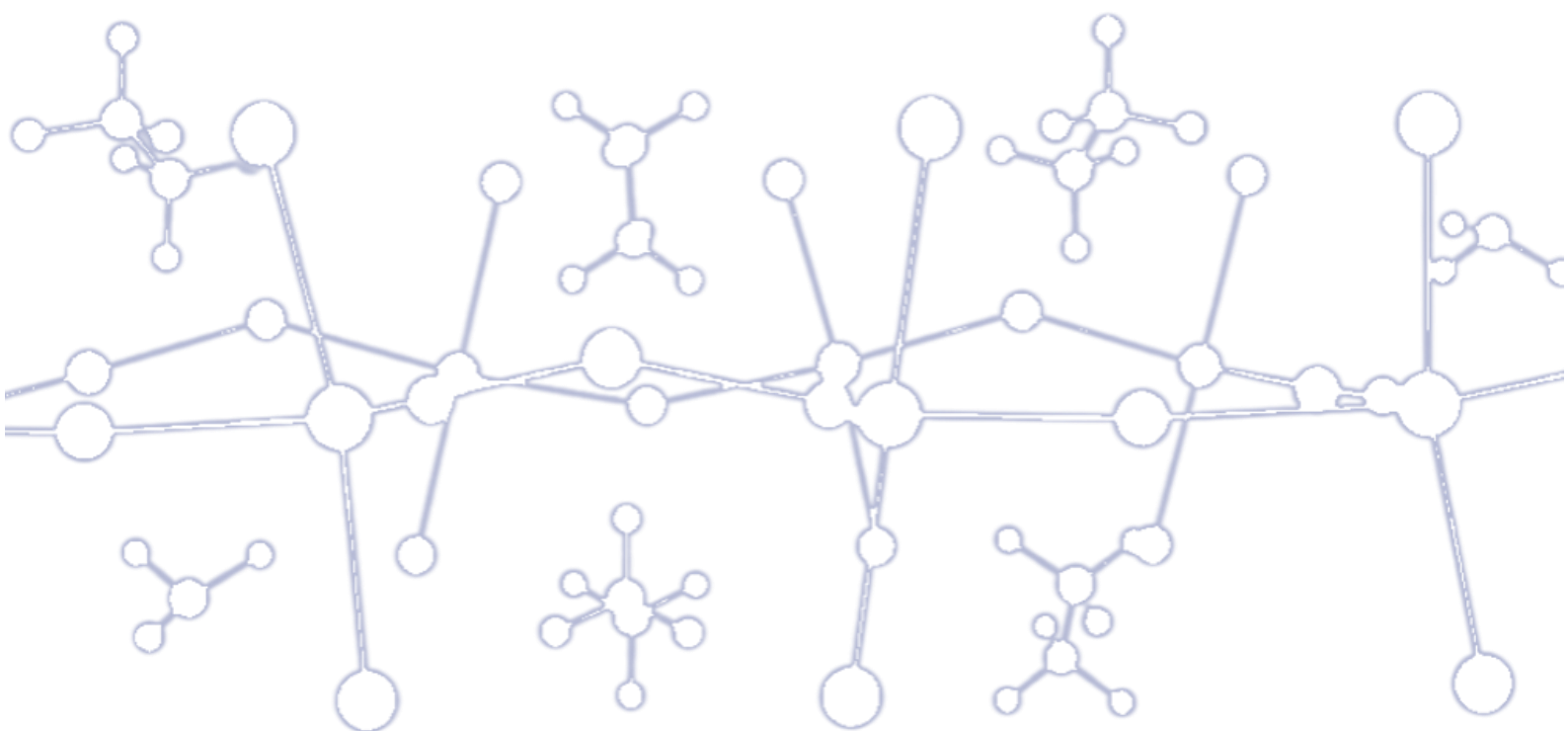
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I will report on the progress on vapor phase deposited perovskites, including novel low vacuum based deposition methods such as close-space and vapor transport sublimation. The integration of these perovskite in single and tandem type solar cells will be discussed. Also the performance evolution of these films and devices under accelerated and outdoor stress conditions will be presented.

	<b>Town Hall</b>	<b>Trumpet</b>
<b>Session Chair</b>	<b>Henk J. Bolink, UVEG, ES</b>	<b>Silvia Colella, CNR-NANOTEC, Italy</b>
<b>Session Title</b>	<b>Session 1A – VALHALLA</b>	<b>Session 1B – Stability</b>
14:00 14:12	<b>Introduction to VALHALLA Project by Prof. Henk J. Bolink</b>	<b>Cynthia Farha</b> , Institut Photovoltaïque d'Île-de-France, France <i>Evaluating 10×10 CM<sup>2</sup> perovskite module durability: performance under iec damp heat conditions</i>
14:12 14:24	<b>Tadas Malinauskas</b> , Kaunas University of Technology, Lithuania <i>Electron and hole selective self-assembling monolayers for perovskite solar cells</i>	<b>Hadi Mohammadzadeh</b> , Fraunhofer ISE, Germany <i>Pioneering metal-free perovskite solar cells: enhancing carbon electrode performance through post-lamination treatments</i>
14:24 14:36	<b>Daniele Meggiolaro</b> , CNR-SCITEC, Italy <i>Lattice and photo-stability of metal halide perovskites: a computational perspective</i>	<b>Muhammed Salim Kunnummal Mangott</b> , Institut Photovoltaïque d'Île-de-France, France <i>Scalable fabrication of efficient FAPbI<sub>3</sub> perovskite solar modules using green solvent-based inks</i>
14:36 14:48	<b>Isabella Poli</b> , Istituto Italiano di Tecnologia, Italy <i>DMSO-Free mixed tin-lead perovskite solar cells with enhanced stability</i>	<b>Jongin Huh</b> , SKKU, South Korea <i>Fully eco-friendly solvent strategies for scalable, high-performance perovskite solar cells</i>
14:48 15:00	<b>Vladimir Held</b> , University of Valencia - Instituto de Ciencia Molecular, Spain <i>Insights from the in situ photoluminescence: growth, defect formation, and passivation during perovskite vacuum co-deposition</i>	<b>Zijing Dong</b> , National University of Singapore, Singapore <i>Thermostable perovskite solar cells enabling operational lifetime over 25 years</i>
15:00 15:10	<b>COMFORT BREAK</b>	



# EVALUATING 10×10 CM<sup>2</sup> PEROVSKITE MODULE DURABILITY: PERFORMANCE UNDER IEC DAMP HEAT CONDITIONS

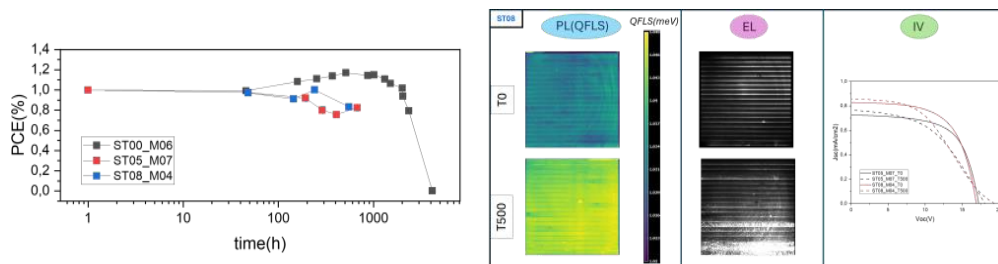
**Cynthia Farha,<sup>1</sup> Yves Abou Khalil,<sup>1</sup> Thomas Guillemot,<sup>1</sup> Jean Rousset,<sup>1,2</sup> Marion Provost,<sup>1</sup> Iwan Zimmermann,<sup>1</sup> Karim Medjoubi<sup>1</sup>**

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This study investigates the long-term stability of 10×10 cm<sup>2</sup> perovskite photovoltaic modules subjected to accelerated aging under damp heat (85 °C/85% RH), following IEC 61215 protocols.<sup>[1]</sup> The aim was to limit power degradation to below 5% after 1000 hours of exposure.<sup>[2]</sup> Six modules, fabricated across three production batches, were tested for up to 4150 hours in a climate chamber. Module performance was monitored through J–V characterization, optical imaging, photoluminescence (PL) and electroluminescence (EL). As illustrated in Figure 1, some modules remained stable or even improved during the early stages of aging, while others showed significant degradation, with power conversion efficiency losses up to 30%. A key difference between batches was the perovskite drying method: vacuum drying was used for batch ST08, whereas air knife drying was applied in ST00 and ST05. Notably, the vacuum-dried module exhibited an S-shaped I–V curve after only 500 hours. PL-QFLS mapping shows an increase up to 3% correlated to the VOC enhancement observed in I–V characteristics. Bandgap mapping revealed no changes in the perovskite composition over time, thereby ruling out moisture ingress as a contributing factor in the degradation mechanism. Using EL imaging, heterogeneous degradation was observed, suggesting the occurrence of electrode degradation. This mechanism is the primary contributor, notably influencing the fill factor and charge extraction pathways, and it may be responsible for the S-shaped distortion observed in the I–V curves. PL at both OC and SC will be presented for different perovskite stacks showing the charge extractions efficiency evolution through DH. This work confirms the potential for perovskite modules to remain stable under harsh conditions but also underscores the critical influence of drying method on perovskite thermal stability. In addition, using advanced characterization techniques, is essential to better understand the degradation mechanisms and proposing pathway for enhancing the stability of the perovskite PV technologies.



**Figure 1:** Performance Evolution and Degradation Analysis of Perovskite Modules Under Damp Heat Aging

[1] M. V. Khenkin et al., “Consensus statement for stability assessment and reporting for perovskite photovoltaics based on ISOS procedures” *Nat. Energy* **2020**, 5(1), 35–49, doi: 10.1038/s41560-019- 0529-5.

[2] M. Köntges, S. Kurtz, C. Packard, U. Jahn, K. A. Berger and K. Kato, “Performance and reliability of photovoltaic systems: subtask 3.2: Review of failures of photovoltaic modules: IEA PVPS task 13: external final report IEA-PVPS” **2014**, Sankt Ursen: International Energy Agency, Photovoltaic Power Systems Programme, doi: 10.2314/GBV:856979287.

# ELECTRON AND HOLE SELECTIVE SELF-ASSEMBLING MONOLAYERS FOR PEROVSKITE SOLAR CELLS

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Introduction of the materials forming hole selective self-assembled monolayer (SAM) made a significant contribution towards development of p-i-n architecture perovskite solar cells (PSCs). Applying small but important structural changes resulted in a steady increase in p-i-n PSC performance. Combined with conformal coverage, minimal parasitic absorption, and low material consumption, SAM HTMs became an important research subject for optoelectronic applications, such as hybrid and organic photovoltaics, perovskite/silicon tandems or organic light-emitting diodes. These materials effectively combine two functionalities: a hole-selective unit and a phosphonic acid group that facilitates monolayer formation. While this general strategy has been also used with electron-selective chromophores, progress in this area has been hindered by the limited availability of suitable chromophores and their challenging properties, such as low solubility.

Recent advancements with non-fullerene acceptors have demonstrated potential of alternative chromophores, inspiring new approaches in development of electron-selective monolayers (eSAMs).

To improve performance of both hole and electron selective materials, we are focusing on the molecular design of the compounds. This includes optimizing the central core as well as modification of functional groups attached to it. In the current work we demonstrate new electron selective and hole selective materials suitable for n-i-p and p-i-n architectures as well as for various perovskite compositions.

**Acknowledgements:** *The PEPPERONI Project No. 101084251 is acknowledged. This project is co-funded by 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 the European Climate, Infrastructure and Environment Executive Agency (CINEA). Neither the European Union nor the granting authority can be held responsible for them.*

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- [1] Hao Chen et al., *Science* **2024**, 384, 189–193.
  - [2] <https://www.freethink.com/energy/tandem-solar-cell>.
  - [3] M. Jošt et al., *ACS Energy Lett.* **2022**, 7, 1298–1307.
  - [4] K. O. Brinkmann et al., *Nature* **2022**, 604, 280–286.

# PIONEERING METAL-FREE PEROVSKITE SOLAR CELLS: ENHANCING CARBON ELECTRODE PERFORMANCE THROUGH POST-LAMINATION TREATMENTS

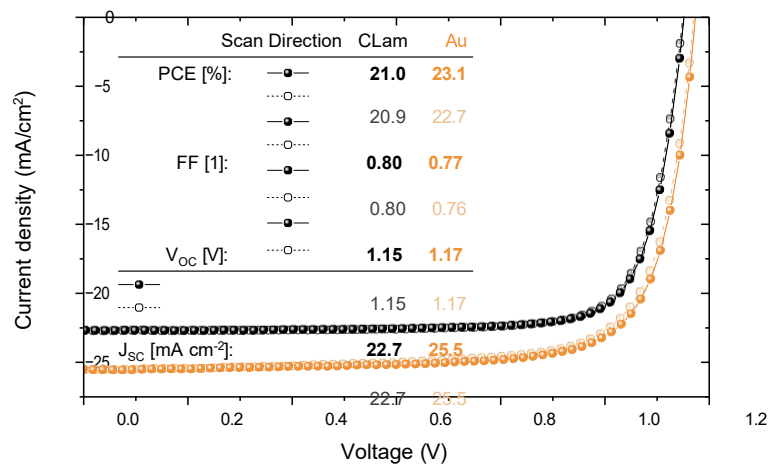
**Hadi Mohammadzadeh,<sup>1,2</sup> Clemens Baretzky,<sup>1,2</sup> Mohammad Kamrul Hasan Jony,<sup>1</sup>  
Georgios Loukeris,<sup>1,2</sup> Markus Kohlstädt,<sup>1,2</sup> Uli Würfel<sup>1,2</sup>**

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<sup>2</sup>Materials Research Center (FMF), University of Freiburg, Germany  
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Perovskite solar cells (PSCs) have emerged as a breakthrough technology, achieving efficiencies comparable to silicon photovoltaics.<sup>[1]</sup> However, their reliance on metal top electrodes, such as gold (Au), introduces challenges related to cost and long-term stability. Carbon-based electrodes offer a promising alternative to overcome these challenges. Nevertheless, conventional deposition techniques, such as blade coating, often face solvent incompatibility with underlying charge transport layers, limiting efficiency and reproducibility.<sup>[2-3]</sup>

In this study, we explore a lamination-based approach where pre-dried carbon films are applied to perovskite half-cells. This technique mitigates solvent-related issues, leading to increased open-circuit voltage and photoluminescence intensity. However, laminated carbon (CLam) electrodes exhibit a larger series resistance, negatively impacting the fill factor and power conversion efficiency (PCE). To address this, we introduce a post-lamination solvent treatment and demonstrate that *o*-xylene significantly reduces the series resistance, achieving a PCE of 21%, as one of the highest efficiencies reported for carbon-based perovskite solar cell (CPSCs) with almost zero hysteresis. In comparison, devices with Au electrodes reached a PCE of 23.1%.

While the lamination process itself may not yet be ideal for direct industrial implementation, this study provides a crucial step toward developing scalable, stable, and metal-free PSCs. The insights gained from this work contribute to the broader goal of achieving cost-effective and sustainable photovoltaics, highlighting the potential of post-processing treatments to overcome limitations in laminated carbon electrodes. This advancement brings the field closer to commercially viable CPSCs, reinforcing their role in the future of renewable energy.



**Figure 1:** JV curves of perovskite solar cell with Au and CLam electrodes.

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- [1] NREL Best Research-Cell Efficiency Chart. <https://www.nrel.gov/pv/cell-efficiency.html> (27 March 2025)  
[2] M. Hadadian, et al., *Energy Environ. Sci.* **2020**, *13*, 1377-1407.  
[3] D. Bogachuk, et al., *Adv. Energy Mater.* **2022**, *12*(10), 2103128.

# LATTICE AND PHOTO-STABILITY OF METAL HALIDE PEROVSKITES: A COMPUTATIONAL PERSPECTIVE

**Daniele Meggiolaro**<sup>1</sup>

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Metal halide perovskites are outstanding materials for photovoltaics due to their excellent optoelectronic properties and the tunable band gaps.<sup>[1]</sup> Despite the very high efficiencies provided in solar cells, 26% for lead-based perovskites, one of the most critical issues to be addressed is the limited long-term stability of these materials. The elaboration of successful strategies aimed at improving the stability requires a deep understanding of the degradation mechanisms for the different chemical compositions.

In this presentation, based on DFT simulations, we provide a theoretical perspective about the degradation mechanisms of metal-halide perovskites vs the chemical composition (Pb vs Sn, I vs Br), by focussing on the defect-activated lattice instabilities and the photo-degradation of the materials. Potential strategies to increase long-term stability will also be discussed.

I<sub>2</sub> expulsion is a critical photo-degradation path in lead-iodide perovskites. The computational analysis of the defect chemistry highlights that the photo-degradation process is activated by the photo-oxidation of iodide and it is strongly correlated with the thermodynamic stability of the lattice, with FA- being less photo-stable than MA- than Cs-perovskites.<sup>[2]</sup> Alloying the halide site with Br improves lattice stability but it does not deactivate iodide photo-oxidation and the derived perovskites demix under light stress. Strategies based on the use of passivating molecules to reduce defect density and limit I<sub>2</sub> nucleation at the surface will be analyzed, as well as the impact of the molecule dipoles on the electronic levels at the interface.<sup>[3]</sup>

On the other hand, in Sn-based low band gap perovskites, tin oxidation is the main process limiting the stability of the material. Beside direct oxidation by oxygen which can be prevented by encapsulation, tin oxidation is triggered by hole trapping at the surface as a response to the high p-doping in the bulk.<sup>[4]</sup> Defect analysis highlights that the organic cation does not sensibly impact the stability of the acceptor defects responsible for the p-doping, which is mainly modulated by the metal. Computationally designed strategies based on trivalent ion doping and the use of Sn(IV) chelating agents upon synthesis to reduce p-doping will be discussed.<sup>[5]</sup>

**Acknowledgements:** *Funded by 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 CINEA. Neither the European Union nor the granting authority can be held responsible for them. VALHALLA project has received funding from Horizon Europe Research and Innovation Action programme under Grant Agreement n° 101082176.*

[1] Green et al., “The Emergence of Perovskite Solar Cells” *Nat. Photon.* **2014**, 8 (7), 506–514.

[2] Zhou et al., “How Photogenerated I<sub>2</sub> Induces I-Rich Phase Formation in Lead Mixed Halide Perovskites.” *Advanced Materials* **2024**, 36 (1), 2305567.

[3] Gregori et al., “Quantifying the Effect of Interfacial Dipoles on the Energy Level Alignment of Metal-Halide Perovskites.” *ACS Energy Lett.* **2024**, 9 (11), 5329–5333.

[4] Gregori et al., “Combining Trivalent Ion-Doping with Halide Alloying to Increase the Efficiency of Tin Perovskites.” *Small* **2024**, 2403413.

# SCALABLE FABRICATION OF EFFICIENT FAPbI<sub>3</sub> PEROVSKITE SOLAR MODULES USING GREEN SOLVENT-BASED INKS

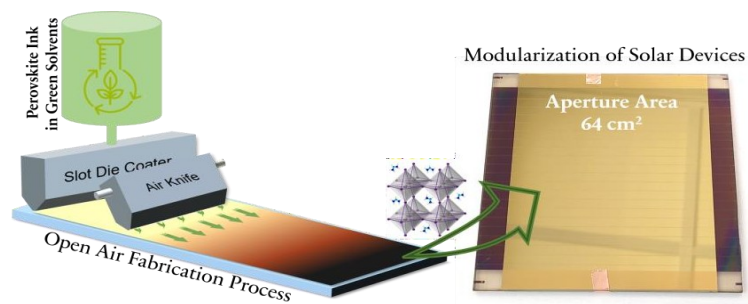
**Kunnummal Mangott Muhammed Salim,<sup>1</sup> Amelie Petitjean,<sup>1</sup> Rene Mendez,<sup>1</sup> Iwan Zimmermann,<sup>2</sup> Nao Harada,<sup>1</sup> Alexandra Levtchenko,<sup>1</sup> Jean Rousset<sup>1,2</sup>**

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High-performance perovskite solar cells (PSCs) are traditionally fabricated using toxic solvents and inert atmosphere-based spin-coating, which hinder scalable, eco-friendly manufacturing.<sup>[1]</sup> To address these limitations, we developed a green, low-toxicity, volatile solvent-based ink for formamidinium lead iodide (FAPbI<sub>3</sub>), a promising low-bandgap perovskite material.<sup>[2,3]</sup> This formulation enables slot-die coating under ambient conditions, a method compatible with large-scale production.<sup>[4]</sup> We investigated the influence of additives on the structural and optoelectronic properties of FAPbI<sub>3</sub> thin films. Characterization through hyperspectral photoluminescence mapping (e.g., QFLS, bandgap, Urbach energy) and electrical techniques (KPFM, SPV, EL) demonstrated reduced non-radiative recombination and improved reproducibility across films and complete devices. These enhancements directly result from the green solvent processing route, which facilitates more uniform film formation and improved defect passivation. Using this optimized ink, we achieved PSCs with >19% power conversion efficiency on small areas (0.09 cm<sup>2</sup>) and >16% for series-interconnected minimodules (64 cm<sup>2</sup> aperture area). Our results demonstrate the feasibility of scalable, environmentally responsible perovskite fabrication using green solvents. Furthermore, the developed semi-transparent minimodule architecture presents a promising platform for 4-terminal tandem integration with silicon photovoltaics, pushing forward the commercial viability of next-generation solar technologies.



**Figure:** Schematic representation of the open-air based slot-die coating process from green solvent-based perovskite ink and the modularization of perovskite solar devices.

[1] S. Sidhik, *Science* **2024**, 384(6701), 1227-1235

[2] S. K. Podapangi, *RSC Adv.* **2023**, 13(27), 18165–18206.

[3] S. Masi, *ACS Energy Letters* **2020**, 5(6), 1974-1985

[4] R. Patidar, *Materials Today Communications* **2020**, 22, 100808.

# DMSO-FREE MIXED TIN-LEAD PEROVSKITE SOLAR CELLS WITH ENHANCED STABILITY

**Isabella Poli**,<sup>1</sup> **Tristan Quinson**,<sup>2</sup> **Mirko Prato**,<sup>3</sup> **Hui Li**,<sup>2</sup> **Angelica Chiodoni**,<sup>1</sup> **Annamaria Petrozza**<sup>2</sup>

<sup>1</sup>Center for Sustainable Future Technologies, Istituto Italiano di Tecnologia, Via Livorno 60, Torino, 10144 Italy

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Mixed tin-lead halide perovskites are promising candidates for low-bandgap solar cells in tandem architectures. However, their practical application is hindered by poor stability, often aggravated by solvent residues and uncontrolled oxidation of Sn<sup>2+</sup>. Furthermore, the conventional solvent to process these materials, dimethyl sulfoxide (DMSO), can be reduced in the presence of iodide ions, generating in turn iodine-based oxidant species that can further degrade Sn(II) perovskite material.<sup>[1-2]</sup>

In this work, we present a DMSO-free fabrication route for mixed tin-lead perovskite solar cells that enables operation under maximum power point tracking (MPPT) for over 1000 hours with minimal efficiency loss. Our approach employs MACl as an additive. A combination of XPS and EDX analyses reveal that Cl<sup>-</sup> accumulates at the film surface, likely forming a tin oxychloride layer via interaction with surface Sn and O species. This layer acts as a passivation barrier, suppressing oxygen adsorption, preventing Sn<sup>2+</sup> oxidation upon ambient air exposure, and mitigating photoinduced I<sub>2</sub> expulsion – a known degradation pathway in halide perovskites that leads to device instability under operation. These findings highlight the critical role of interface chemistry and processing conditions in achieving long-term stability in low-bandgap perovskite solar cells.

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[1] Saidaminov et al., *ACS Energy Lett.* **2020**, 5, 4.

[2] Pascual et al., *Chem. Eur. J.* **2022**, 28, 12.

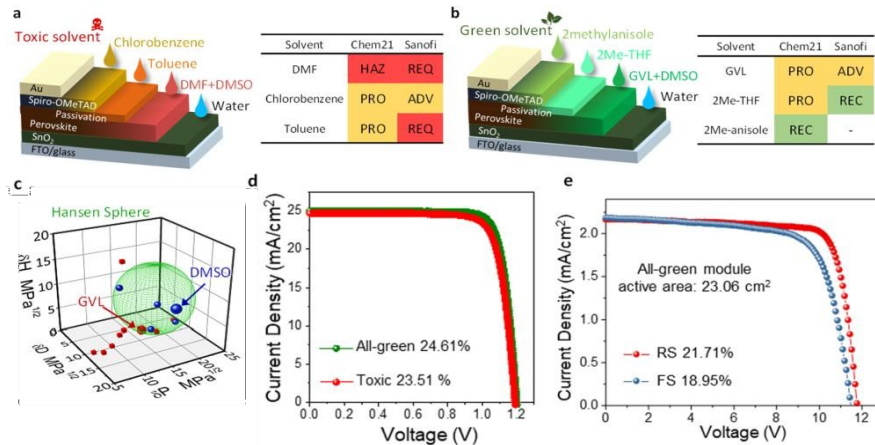
# FULLY ECO-FRIENDLY SOLVENT STRATEGIES FOR SCALABLE, HIGH-PERFORMANCE PEROVSKITE SOLAR CELLS

**Jongin Huh,<sup>1</sup> Hee Jung Kim,<sup>1</sup> You Hyon Seo,<sup>2</sup> Jae Myeong Lee,<sup>1</sup> Gill Sang Han,<sup>2</sup> Hyun Suk Jung<sup>1</sup>**

<sup>1</sup>SungKyunKwan University, Republic of Korea

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**Figure 1:** Schematics of PSCs using different solvent processes: **a**, toxic solvents and **b**, all-green solvents. **c**, Hansen sphere for the perovskite precursor where each axis represents dispersion ( $\delta D$ ), polar ( $\delta P$ ), and hydrogen-bonding ( $\delta H$ ) forces. **d**, Device performances of PSCs fabricated with toxic and all-green solvents. **e**, PCMs fabricated by all green solvents.

The commercialization of perovskite solar cells (PSCs) remains limited by the environmental and health risks associated with toxic solvents used during fabrication<sup>[1]</sup>. In this study, we present a fully green solvent system composed of  $\gamma$ -valerolactone (GVL) and dimethyl sulfoxide (DMSO) for the formation of perovskite active layers. Solvent selection was guided by Hansen solubility parameters and further supported by solvation energy calculations. GVL facilitates the dissolution of formamidinium, while DMSO enhances the solubility of lead halides, jointly enabling the formation of uniform, crystalline perovskite films with low trap-state densities. This green solvent system was extended to the processing of surface passivation and hole-transport layers, with 2-methyltetrahydrofuran employed to enhance charge carrier extraction. Devices fabricated using this all-green approach achieved a power conversion efficiency (PCE) of 24.61%, comparable to benchmark devices processed with conventional toxic solvents. Notably, the scalability of the system was demonstrated by achieving a PCE of 21.71% over a 23.06 cm<sup>2</sup> active area. Life cycle assessment (LCA) indicates a substantial reduction in both environmental burden and human health impact, supporting the viability of this solvent system for sustainable, large-scale PSC manufacturing. This work provides a scalable and eco-conscious pathway toward high-efficiency perovskite photovoltaics.

[1] Kim, H. J. et al., "Green Solvent Strategies toward Sustainable Perovskite Solar Cell Fabrication." *Solar RLL* 2024, 8(5).

# INSIGHTS FROM THE IN SITU PHOTOLUMINESCENCE: GROWTH, DEFECT FORMATION, AND PASSIVATION DURING PEROVSKITE VACUUM CO-DEPOSITION

**Vladimir Held,<sup>1</sup> Matthieu Pascal,<sup>2</sup> Lidon Gil-Escrig,<sup>1</sup> Yunseong Choi,<sup>1</sup> Nathan Rodkey<sup>1</sup> and Henrik J. Bolink<sup>1</sup>**

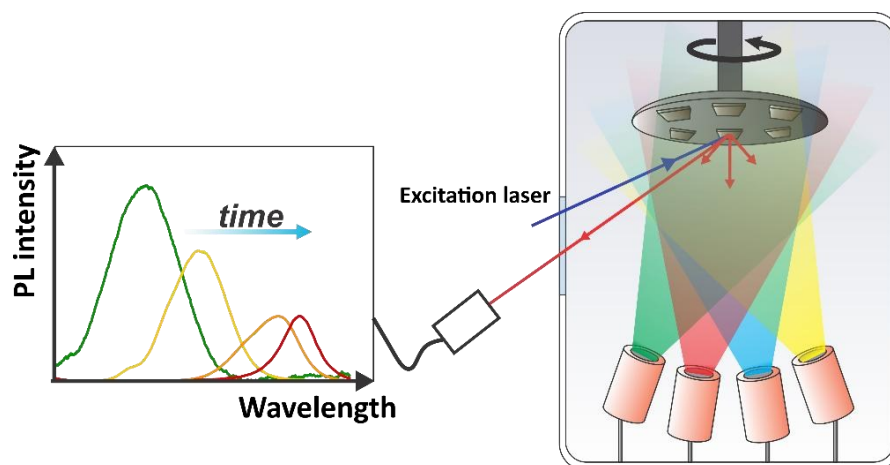
<sup>1</sup>*Institute of Molecular Sciences, University of Valencia, Paterna, Spain*

<sup>2</sup>*Institute of Materials, Ecole Polytechnique Fédérale de Lausanne (EPFL), Lausanne, Switzerland*

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Despite the high efficiencies achieved in perovskite-based applications, further advancements are limited by considerable defect densities throughout the perovskite thin films, including the bulk, grain boundaries, and interfaces. Various passivation strategies have been applied to alleviate defect densities and suppress charge recombination. Although the concepts of defect formation and passivation are widely investigated and implemented in solution-based methods, their development in vapor-deposited perovskite devices is less explored. Vapor deposition of perovskites offers benefits such as enhanced film uniformity, improved control over stoichiometry and morphology, and the potential for large-area high-throughput processing.

In this work, we deposit the perovskite by thermal co-sublimation of its precursor salts and monitor the properties of the perovskite film by in situ photoluminescence spectroscopy. With this method, we can obtain information on growth dynamics, optoelectronic properties, and defect formation in real time. This approach provides direct information on the non-radiative defect density evolution.<sup>[1,2]</sup> Moreover, it offers direct insights into the interface and bulk passivation strategies employed. We believe that this real-time study offers a promising pathway toward effective defect mitigation and enhanced device fabrication optimization.



**Figure 1:** Schematics of experimental setup

[1] V. Held, *ACS Appl. Mater. Interfaces* **2024**, *16*(27), 35723–35731.

[2] V. Held, *J. Phys. Chem. Lett.* **2022**, *13*(51), 11905–11912.

# THERMOSTABLE PEROVSKITE SOLAR CELLS ENABLING OPERATIONAL LIFETIME OVER 25 YEARS

**Zijing Dong,<sup>1,2</sup> Xiao Guo,<sup>1,2</sup> Yi Hou<sup>1,2</sup>**

<sup>1</sup>*Department of Chemical and Biomolecular Engineering, National University of Singapore, Singapore* <sup>2</sup>*Solar Energy Research Institute of Singapore, National University of Singapore, Singapore*

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Despite perovskite solar cells (PSCs) have demonstrated a promising power conversion efficiency, their long-term operational stability is still widely recognized as the key bottleneck to next-step development and commercialization<sup>[1]</sup>. Specifically, mixed-cation perovskites, which pushes the record efficiency up to more than 26%, suffer from intrinsic instability, especially under thermal stress<sup>[2]</sup>. However, for outdoor operation, solar cells must face with extreme and harsh conditions during their service lifetime, which has important implications for real-world energy yields. Up to now, most reported lifetimes are within thousands of hours, significantly lagging behind silicon photovoltaics with a 25 years' lifetime<sup>[3]</sup>.

Regarding this stability concern, in this work we employ a novel deposition method to achieve state-of-the-art efficiency and excellent long-term stability under thermal and illumination stress, fundamentally overcoming the intrinsic instability challenge for mixed-cation perovskite materials. The as-fabricated PSCs can maintain its power output for over 2,000 hours without any sign of degradation under continuous max power point tracking (MPPT) at room temperature. To further explore the full potential of the stability of our devices, we elevated to an unprecedentedly high temperature of 110°C and found that it can maintain 80% of initial efficiency ( $T_{80}$ ) for more than 520 hours under MPPT. This performance drives us to conduct accelerated aging test to investigate the degradation mode and predict the lifetime of our devices under real-world operations. Here, we monitor indoor operational output of PSCs at different high temperatures ranging from 65 to 110°C. The data from accelerated tests is then fitted with Arrhenius model, returning an estimation of the field lifetime. As a result, the projected operational lifetimes of different temperatures converge at 45,000 hours, which aligns with the extrapolated  $T_{80}$  lifetime derived from room-temperature measurement. Furthermore, considering different local global horizontal irradiation worldwide, the converted lifetime of PSCs can sufficiently ensure 25 years of outdoor exposure in Singapore, Japan and most areas in US. This result is the best-to-date stability performance of mixed-cation PSCs reported so far in literature. More importantly, it's the first time that PSCs is proved to realize such a long lifespan comparable to silicon solar cells, paving the way to future development and commercialization of perovskite-based photovoltaics.

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[1] D.P. McMeekin *et al.*, *Nature Materials* **2023**, 22, 73-83.

[2] H. Zhu *et al.*, *Nature Reviews Materials* **2023**, 8, 569-586.

[3] P. Zhu *et al.*, *Advanced Materials* **2024**, 36, 2307357.

15:00 15:10		COMFORT BREAK	
		Town Hall	Trumpet
Session Chair		Yuanyuan Zhou, HKUST, Hong Kong	Steve Albrecht, Helmholtz-Zentrum Berlin, Germany
Session Title		Session 2A – Tandem PV 1	Session 2B – Interface
15:10	15:22	<b>Lina Wang</b> , City University of Hong Kong, Hong Kong <i>Highly efficient monolithic perovskite/topcon silicon tandem solar cells</i>	<b>Yang Lu</b> , University of Cambridge, United Kingdom <i>Layer-by-layer heteroepitaxial growth of perovskite heterojunctions</i>
15:22	15:34	<b>Han-Ki Kim</b> , SKKU, South Korea <i>Isolated plasma soft deposition of NIR transparent IGTO top and bottom electrodes for semi-transparent perovskite solar cells</i>	<b>Tianwei Duan</b> , The Hong Kong University of Science and Technology, Hong Kong <i>On-Chip Light-Incorporated In Situ Transmission Electron Microscopy for Metal Halide Perovskites</i>
15:34	15:46	<b>Kilian Alcocer</b> , CEA, France <i>Scalable fabrication of large-area black phase CsPbI<sub>3</sub> and inorganic contact layers on 707cm<sup>2</sup> substrates by PLD</i>	<b>Bhavya Rakheja</b> , Uppsala University, Sweden <i>Electron transport layer interfaces in inverted perovskite solar cells</i>
15:46	15:58	<b>Xiao Guo</b> , National University of Singapore, Singapore <i>Suppressing halide phase segregation in wide-bandgap perovskite for perovskite-organic tandem solar cells</i>	<b>Aslihan Babayigit</b> , Hasselt University, Belgium <i>Artifact-induced ion gradients during time-of-flight secondary ion mass spectrometry in multilayered stacks of perovskite solar cells</i>
15:58	16:10	<b>Deniz Turkay</b> , EPFL/PV-LAB, Switzerland <i>Step-by-step evolution of stability: single-junction perovskite to perovskite-Si tandem solar cells</i>	<b>Pengfei Guo</b> , The Hong Kong University of Science and Technology, Hong Kong <i>Synthesis of a lattice-resolved laminate-structured perovskite heterointerface</i>
16:10	16:22	<b>Xuzheng Liu</b> , Karlsruhe Institute of Technology, Germany <i>Enhanced charge carrier transport and extraction for perovskite/silicon tandem solar cells</i>	<b>Gennaro Vincenzo Sannino</b> , University of Naples "Federico II", ENEA, Italy <i>Novel isoindigo derivatives as electron transport materials for perovskite solar cells</i>
16:22	16:52	COFFEE BREAK PM	



# HIGHLY EFFICIENT MONOLITHIC PEROVSKITE/TOPCON SILICON TANDEM SOLAR CELLS

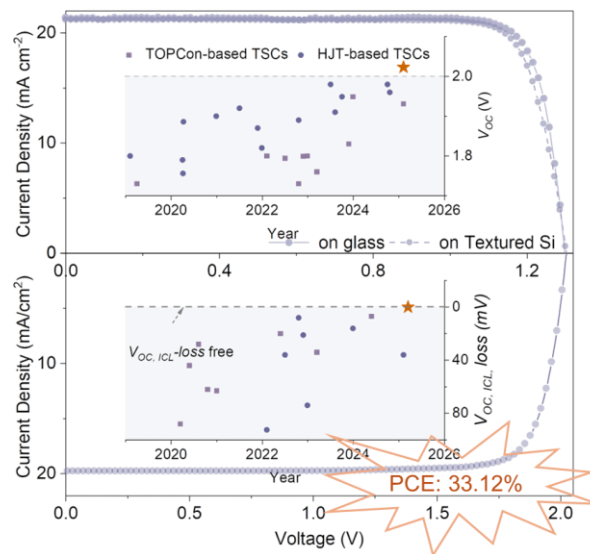
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Tunnel oxide passivating contact (TOPCon) silicon tandem solar cells have gained substantial market traction due to their cost-effectiveness and operational stability.<sup>[1-2]</sup> However, their monolithic perovskite-based architectures exhibit lower power conversion efficiencies (PCEs) compared to heterojunction (HJT) counterparts, primarily due to significant open-circuit voltage ( $V_{OC}$ ) losses at the textured interconnection layer (ICL).<sup>[3-4]</sup> Here, we address this critical bottleneck by engineering an energy-loss-free ICL for perovskite/TOPCon tandem solar cells. The tailored ICL achieves barrier-free energy-level alignment, enabling efficient hole extraction and elevating the  $V_{OC}$  of wide-bandgap perovskite subcells to 1.30 V. This innovation yields a certified PCE of 32.32% (lab-measured: 33.12%) for 1-cm<sup>2</sup> devices—the highest reported for perovskite/TOPCon tandems—alongside a record  $V_{OC}$  of 2.015 V (certified) and near-zero  $V_{OC}$  loss at the ICLs. Our work establishes a creative strategy for suppressing interfacial energy losses in textured tandem photovoltaics, advancing scalable pathways toward ultrahigh-efficiency architectures.



**Figure:** *J-V* curves for single-junction and monolithic tandem devices.

[1] Liu, J., He, Y., Ding, L. et al., “Perovskite/silicon tandem solar cells with bilayer interface passivation” *Nature* **2024**, 635, 596–603.

[2] Zheng, J., Ying, Z., Yang, Z. et al., “Polycrystalline silicon tunnelling recombination layers for high-efficiency perovskite/tunnel oxide passivating contact tandem solar cells” *Nature Energy* **2023**, 8, 1250–1261.

[3] Kan, C., Hang, P., Wang, S. et al., “Efficient and stable perovskite-silicon tandem solar cells with copper thiocyanate-embedded perovskite on textured silicon” *Nature Photonics* **2025**, 19, 63–70.

[4] Wang L., Wang N., Wu X. et al., “Highly Efficient Monolithic Perovskite/TOPCon Silicon Tandem Solar Cells Enabled by “Halide Locking”” *Advanced Materials* **2025**, 37, 2416150.

# LAYER-BY-LAYER HETEROEPITAXIAL GROWTH OF PEROVSKITE HETEROJUNCTIONS

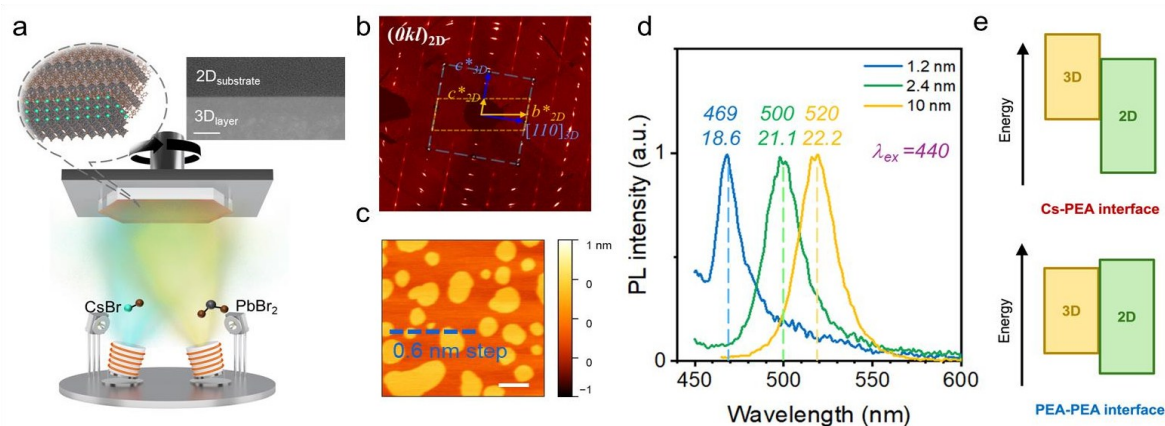
Yang Lu,<sup>1,2</sup> Young-Kwang Jung,<sup>1</sup> Richard H. Friend,<sup>2</sup> Sam D. Stranks<sup>1,2</sup>

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Main text: Halide perovskites exhibit superior optoelectronic properties but lack precise thickness and band offset control in heterojunctions, critical for modular multilayer architectures such as multiple quantum wells.<sup>[1]</sup> Here, we demonstrate vapor-phase layer-by-layer heteroepitaxial growth of perovskite heterostructures, exemplified by CsPbBr<sub>3</sub> deposition on single crystals of PEA<sub>2</sub>PbBr<sub>4</sub> (PEA: 2-phenylethylammonium) (Figure 1a, b). Angstrom-level thickness control (Figure 1b) and sub-angstrom smooth layers (roughness 0.01 nm) enable quantum-confined photoluminescence of CsPbBr<sub>3</sub> from monolayer, bilayer and through to bulk. Furthermore, we confirmed both experimentally and theoretically that the interfacial structure controls the electronic structure from Cs–PEA-terminated interface (type-II heterojunction) to PEA–PEA-terminated (type-I), with band offset shift exceeding 0.5 eV (Figure 1d). The large band offset is a combined effect from surface dipole and interface bonding.<sup>[2-3]</sup> The 2D templated growth also demonstrated greatly reduced defects, with three to seven times enhancement in in-plane transport and three orders of magnitude reduction in contact resistance. The combined precise quantum confinement control and large band offset tunability unlock perovskite heterojunctions as platforms for scalable, low-cost modular quantum- and superlattice-based optoelectronic applications.



**Figure 1:** Layer-by-layer heteroepitaxial growth of perovskite heterojunction. (a) Thermal evaporation of 3D perovskite on top of 2D perovskite. (b) Reciprocal space mapping confirming heteroepitaxy. (c) Surface morphology by atomic force microscopy, showing growth in units of octahedral cage. (d) Quantum-confined PL emission from 2D-like CsPbBr<sub>3</sub> with precisely controlled thickness. (e) Tunable band alignment between 2D and 3D perovskite, with band offset shift exceeding 0.5 eV.

[1] L. R. W. White et al., *ACS Energy Lett.* **2024**, 9(3), 835–842.

[2] A. Mahata et al., *Chem. Mater.* **2020**, 32, 105–113.

[3] Y.-K. Jung et al., *J. Phys. Chem. C* **2017**, 121, 27351–27356.

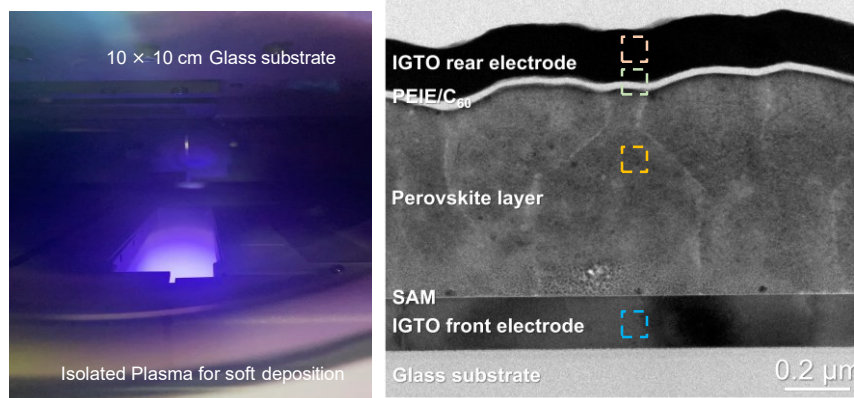
# ISOLATED PLASMA SOFT DEPOSITION of NIR TRANSPARENT IGTO TOP AND BOTTOM ELECTRODES FOR SEMI-TRANSPARENT PEROVSKITE SOLAR CELLS

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Achieving high-efficiency perovskite-silicon (Si) tandem solar cells requires the development of semi-transparent perovskite solar cells (STPSCs) with transparent top and bottom electrodes. In this study, we propose gallium and titanium co-doped  $\text{In}_2\text{O}_3$  (IGTO) as near infrared (NIR) transparent top electrode, fabricated using isolated plasma soft deposition (IPSD) to minimize plasma-induced damage. By employing the specially designed IPSD system, we can prepare the top IGTO electrode without plasma damage caused by bombardment of energetic particles. Despite being processed at room temperature, the IPSD-grown IGTO electrode exhibits high carrier mobility ( $\approx 77 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ ), excellent optical transparency ( $>90\%$  in the visible and NIR regions), low sheet resistance ( $28 \Omega \text{ sq}^{-1}$ ), and a smooth surface (roughness  $\approx 0.4 \text{ nm}$ ). An STPSC incorporating IPSD-grown IGTO electrodes achieved a power conversion efficiency (PCE) of 18.71%, with a near-infrared transmittance of 88.8%. When integrated into a four-terminal (4-T) perovskite/Si tandem configuration, the IGTO-based tandem cell demonstrated an enhanced short-circuit current density compared to conventional indium tin oxide (ITO)-based tandem cells, resulting in a PCE of 26.05%. These findings highlight the potential of IPSD-grown IGTO as a promising alternative to conventional ITO electrodes for high-performance tandem solar cells.



**Figure 1: Isolated plasma for deposition of InGaTiO electrode and cross section TEM image for semi-transparent PSC with InGaTiO bottom and top electrodes**

[1] Han-Ki Kim *et al*, *Advanced Materials* **2025**, 37, 2414800

[2] Han-Ki Kim *et al*, *Nano Energy* **2023**, 11, 108431

# ON-CHIP LIGHT-INCORPORATED IN SITU TRANSMISSION ELECTRON MICROSCOPY FOR METAL HALIDE PEROVSKITES

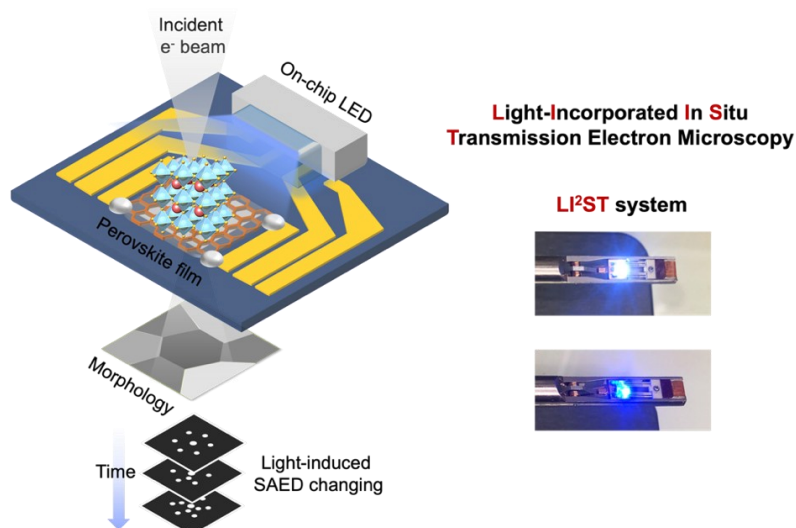
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Light-incorporated in situ transmission electron microscopy (TEM) is vital for visualizing the dynamic structural evolution of light-responsive materials. However, conventional in situ TEM platforms lack integrated light control, limiting their utility in studying light-induced transformations. Here, we introduce an on-chip Light-Incorporated In Situ TEM (LI<sup>2</sup>ST) technique, specifically designed to investigate metal halide perovskites (MHPs) at the nanoscale under light exposure. Built on a custom microelectromechanical systems (MEMS) chip, our platform enables real-time, site-specific monitoring of light-triggered structural changes with adjustable intensity and multi-wavelength illumination. This robust setup supports continuous, localized observation of perovskite grain and grain boundary evolution under light, offering unprecedented insights into light–matter interactions. As a proof-of-concept, we demonstrate the light-induced decomposition of polycrystalline MHP films, revealing that degradation initiates and propagates within intragrain regions, rather than at grain boundaries—a surprising departure from conventional assumptions. Our findings highlight the power of LI<sup>2</sup>ST in capturing complex structural-phase dynamics in situ and in real time. This technique not only advances fundamental understanding of MHP behavior under illumination but also provides a critical tool for optimizing the performance and stability of perovskite-based energy devices.



**Figure 1:** Schematic illustration of on-chip light integrated into situ transmission electron microscopy setups for monitoring morphology and diffraction changes.

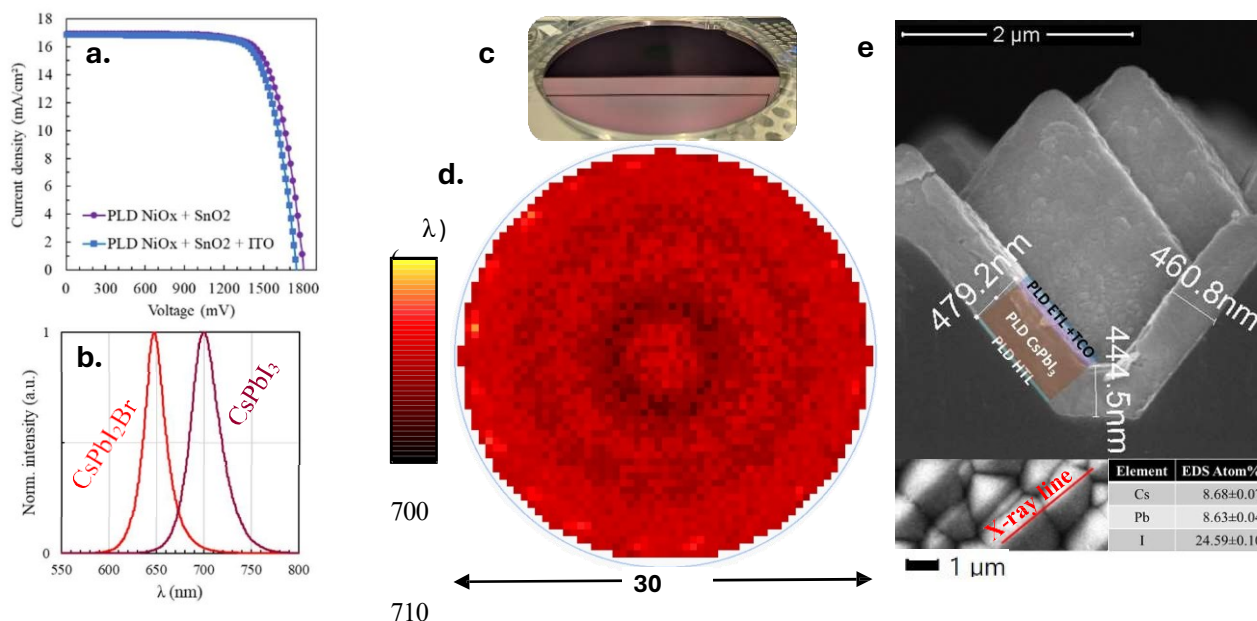
[1] T. Duan, et al., *ACS Energy Lett.* **2023**, 8, 3048–3053.

# SCALABLE FABRICATION OF LARGE-AREA BLACK PHASE CsPbI<sub>3</sub> AND INORGANIC CONTACT LAYERS ON 707 cm<sup>2</sup> SUBSTRATES BY PLD

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Scalable fabrication of efficient and stable large-area perovskite solar cells (PSC) remains a challenge. Here, we propose pulsed laser deposition (PLD)<sup>[1]</sup> as a scalable, solvent-free and room-temperature method to fabricate uniform black phase inorganic perovskites and charge transport layers on 707 cm<sup>2</sup> substrates (> G12 area). We first developed several PLD-grown contact layers (ITO, SnO<sub>2</sub> and NiO<sub>x</sub>), validated together in hybrid perovskite-on-silicon (flat) tandem solar cells that achieved a stable 23% efficiency and 75% fill factor over a 9 cm<sup>2</sup> active area. We now demonstrate the deposition of CsPbI<sub>2</sub>Br and CsPbI<sub>3</sub> on 300 mm wafers, exhibiting PL peaks at  $\lambda=648$  nm ( $\sim 1.91$  eV) and 700 nm ( $\sim 1.77$  eV), with FWHM of 28.9 and 36.5 nm, respectively. The films show excellent uniformity: 0.8% in thickness and 0.2% in PL wavelength. In addition, we deposited in-situ contact layers below and above CsPbI<sub>3</sub>, enabling encapsulation of the black phase. This stack was subsequently transferred onto textured Cz-Si heterojunction bottom cells, showing conformal and stoichiometric CsPbI<sub>3</sub> deposition. Final device integration and performance measurements are currently underway. Looking ahead, we aim to scale-up the growth rate from the current 8 nm/min at 20 Hz to 125 nm/min using an industrial PLD system operating at 300 Hz, further highlighting PLD as a promising route for large-scale PSC manufacturing.



**Figures:** **a.** J-V curves under AM1.5G of 9 cm<sup>2</sup> p-i-n Perovskite/SHJ tandem cells integrating NiO<sub>x</sub>, SnO<sub>2</sub> and ITO by PLD. **b.** PL signal of PLD-grown CsPbI<sub>2</sub>Br and CsPbI<sub>3</sub> excited by a 532 nm laser. **c.** Photograph of black-phase perovskite deposited on a 300 mm wafer. **d.** PL mapping of  $\sim 450$  nm thick CsPbI<sub>3</sub> over 707 cm<sup>2</sup>. **e.** SEM cross-section of PLD-grown CsPbI<sub>3</sub> and contact layers on a textured (Cz-Si) SHJ bottom cell, with EDS analysis.

[1] T. Soto-Montero, M. Morales-Masis, *ACS Energy Lett.* **2024**, *9*, 4199.

# ELECTRON TRANSPORT LAYER INTERFACES IN INVERTED PEROVSKITE SOLAR CELLS

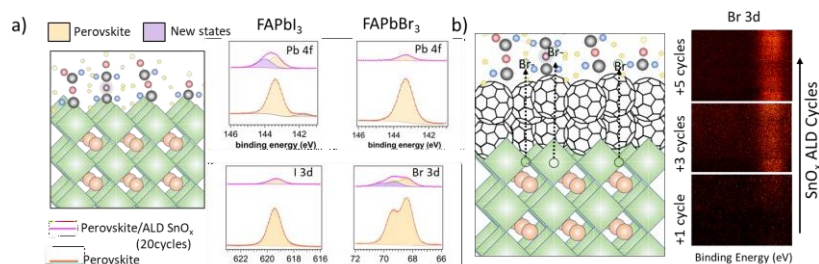
**Bhavya Rakheja,<sup>1</sup> Adam Hultqvist,<sup>1</sup> Natalia M. Martin,<sup>1</sup> Tobias Törndahl<sup>1</sup>**

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Metal halide perovskites (HaPs) have revolutionized the field of photovoltaics, achieving power conversion efficiencies (PCEs) comparable to silicon and III-V semiconductors. In recent times, perovskite solar cells (PSCs) have found their relevance in the inverted (p-i-n) architecture due to its compatibility as a front cell in multi-junction tandems, exceeding 34% PCE.<sup>[1]</sup>

Interfaces between HaPs and transport layers critically influence performance and stability, with non-radiative recombination and irreversible ion migration being the major challenges. In inverted PSCs, electron transport layer (ETL) usually consists of a fullerene (C<sub>60</sub>) and atomic layer deposited (ALD) tin oxide (SnO<sub>x</sub>) bilayer. However, C<sub>60</sub> suffers from poor mechanical and thermal stability, and its interface introduces non-radiative recombination. Direct ALD SnO<sub>x</sub> deposition on HaPs could eliminate C<sub>60</sub>, but often acts as a transport barrier, adversely affecting device performance.

To gain deeper insights into perovskite-ALD SnO<sub>x</sub> interfacial chemistry, we investigated formamidinium based HaPs (FAPbI<sub>3</sub> and FAPbBr<sub>3</sub>) using soft and hard X-ray photoelectron spectroscopy. Our findings reveal that direct ALD SnO<sub>x</sub> deposition leads to FA<sup>+</sup> ion degradation, with PbI<sub>2</sub> formation at the FAPbI<sub>3</sub> interface and Sn-Br bond formation in the case of FAPbBr<sub>3</sub> (presented in Figure 1a). Incorporation of C<sub>60</sub> or alternative interlayers to mitigate these detrimental interfacial reactions is indispensable in achieving high PCEs. To further explore this, we conducted in situ ambient pressure X-ray photoelectron spectroscopy measurements to examine ALD SnO<sub>x</sub> growth on FAPbX<sub>3</sub>/C<sub>60</sub> structures. Our findings demonstrate the presence of halide migration through the C<sub>60</sub> layer into the bulk of SnO<sub>x</sub>. Besides, the halide migration was dictated majorly by the employed HaP composition underneath the C<sub>60</sub> layer, where I only migrates if Br is present in the HaP. We clearly observed an increase in the intensity of Br 3d peak (Figure 1b) as a function of the number of ALD cycles on top of C<sub>60</sub>, with signal majorly intensifying during Sn pulses. Our findings provide insights toward the importance of employing ion blocking layers between HaPs and C<sub>60</sub> to improve the long-term stability of PSCs.



**Figure 1:** X-ray photoelectron spectroscopy studies conducted on a) Perovskite/ALD SnO<sub>x</sub> interface and b) Perovskite/C<sub>60</sub>/ALD SnO<sub>x</sub> interface

[1] M. A. Green, E. D. Dunlop, M. Yoshita, N. Kopidakis, K. Bothe, G. Siefer, D. Hinken, M. Rauer, J. Hohl-Ebinger and X. Hao, *Progress in Photovoltaics: Research and Applications* **2024**, 32 (7), 425–441.

# SUPPRESSING HALIDE PHASE SEGREGATION IN WIDE-BANDGAP PEROVSKITE FOR PEROVSKITE-ORGANIC TANDEM SOLAR CELLS

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Iodide and bromide integration facilitate broad bandgap tunability in wide-bandgap perovskites,<sup>[1]</sup> yet high concentrations of bromide incorporation leads to notorious halide phase segregation phenomenon,<sup>[2]</sup> which will adversely affect the efficiency and stability of solar cell devices.<sup>[3]</sup> Herein,<sup>[4]</sup> 2-amino-4,5-imidazolecarbonitrile (AIDCN), with highly polarized charge distribution, compact molecular configuration and designed functional groups, is incorporated into a 1.86 eV wide-bandgap perovskite to effectively suppress photoinduced iodine escape and halide phase segregation by inducing specific chemical interactions with perovskite. Hyperspectral photoluminescence microscopy reveals that AIDCN mitigates halide phase segregation under continuous laser exposure. Concurrent *in situ* grazing-incidence wide-angle X-ray scattering and X-ray fluorescence measurements further validate suppressed iodine escape, evidenced by a notable slowing down of lattice shrinkage and a well-maintained overall chemical composition of the perovskite under continuous illumination. These findings, for the first time, provide experimental evidences that correlate the initiation of halide phase segregation to the photoinduced iodine escape process. Ultimately, by applying AIDCN, we achieve a power conversion efficiency (PCE) of 18.52% in 1.86 eV wide-bandgap perovskite solar cells with a T<sub>80</sub> lifetime of 271 hours under continuous tracking at the maximum power point. By integrating this perovskite subcell with a PM6:BTP-eC9 organic subcell, the perovskite-organic tandem solar cell attains a maximum PCE of 25.13%, with a Japan Electrical Safety & Environment Technology Laboratories-certified stabilized PCE of 23.40% included in the “best research-cell efficiency chart” by National Renewable Energy Laboratory of US. These results underscore the efficacy of our approach in strategically designing the molecular structure of additives to induce specific chemical interactions, which not only mitigate halide phase segregation and photoinduced iodine escape but also significantly enhance the efficiency and stability of perovskite-based tandem solar cells.

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[2] E. T. Hoke, D. J. Slotcavage, E. R. Dohner, A. R. Bowring, H. I. Karunadasa, M. D. McGehee, *Chem. Sci.* **2015**, *6*, 613-617.

[3] S. Mahesh, J. M. Ball, R. D. Oliver, D. P. McMeekin, P. K. Nayak, M. B. Johnston, H. J. Snaith, *Energy Environ. Sci.* **2020**, *13*, 258-267.

[4] X. Guo, Z. Jia, S. Liu, R. Guo, F. Jiang, Y. Shi, Z. Dong, R. Luo, Y. D. Wang, Z. Shi, J. Li, J. Chen, L. K. Lee, P. Müller-Buschbaum, D. S. Ginger, D. J. Paterson, Y. Hou, *Joule* **2024**, *8*, 2554-2569.

# ARTIFACT-INDUCED ION GRADIENTS DURING TIME-OF-FLIGHT SECONDARY ION MASS SPECTROMETRY IN MULTILAYERED STACKS OF PEROVSKITE SOLAR CELLS

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Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS) has seen a notable surge in use, with >50% of ToF-SIMS studies in the past five years focusing on perovskites (PVK), highlighting its growing relevance in studying these materials.<sup>[1]</sup> Widely known as an exceptionally advanced characterization technique with a fingerprint-like precision in three-dimensional elemental analysis, ToF-SIMS has gained growing interest in PVK solar cells for its ability to probe the effects of (i) post-deposition treatments, (ii) additives, (iii) interfacial passivation and (iv) various degradation protocols (i.e. tracing ion migration) that can be linked to changes in corresponding devices' parameters. Additionally, its ability to probe spatial molecular information at the buried interface that is otherwise hard to reach without requiring additional and detrimental modifications to the pristine sample—common in other techniques like focused-ion beam (FIB) for electron microscopy (EM)—is another key factor in its growing popularity.<sup>[2]</sup> However, previous studies have cautioned that the ToF-SIMS sputtering process can introduce artifacts, such as the 'matrix-effect', leading to misinterpreted ion gradients.<sup>[3,4]</sup> Although best practices to mitigate such artifacts during PVK thin film analysis have been established by these reports, evaluating multilayered PVK devices presents additional complexities. In this work, we have developed an improved ToF-SIMS approach by systematically and rigorously studying the archetypical MAPbI<sub>3</sub> (1.6 eV) and the emerging Sn-based binary metal (FA<sub>75</sub>CS<sub>25</sub>)(Pb<sub>60</sub>Sn<sub>40</sub>)I<sub>3</sub> (1.25 eV). While ion gradients are not observed in films, aligning with prior reports,<sup>[3,4]</sup> they appear when evaluating device stacks. Through peeling experiments that allow us to probe the same PVK thin film with and without a top layer, we demonstrate that these gradients are artifacts not previously discussed. Our approach shows that the top layer, regardless of the PVK composition, can influence the appearance of ambiguous ion traces, leading to false conclusions. Hereby, our rigorous methodology and findings present an important and timely message to the PVK community, providing a detailed manual on how to depth profile PVK-based multilayered devices with ToF-SIMS, including the characterization of increasingly relevant self-assembled monolayers (SAMs).

[1] Web of Science, research paper publication statistics, keywords: 'ToF-SIMS' and 'perovskites', year: 2019-2024, retrieved on 20<sup>th</sup> January 2025.

[2] Rothmann, M. U., Li, W., Zhu, Y., Liu, A., Ku, Z., Bach, U., Etheridge, J. and Cheng, Y. B., *Advanced Materials* **2018**, 30(25), 1800629.

[3] Noël, C., Pescetelli, S., Agresti, A., Franquet, A., Spampinato, V., Felten, A., di Carlo, A., Houssiau, L. and Busby, Y., *Materials* **2019**, 12(5), 726.

[4] Harvey, S. P., Zhang, F., Palmstrom, A., Luther, J. M., Zhu, K. and Berry, J. J., *ACS applied materials & interfaces* **2019**, 11(34), 30911-30918.

# STEP-BY-STEP EVOLUTION OF STABILITY: SINGLE-JUNCTION PEROVSKITE TO PEROVSKITE-SI TANDEM SOLAR CELLS

**Deniz Turkay,<sup>1</sup> Mostafa Othman,<sup>1</sup> Jonas Diekmann,<sup>1</sup> Christophe Ballif,<sup>1,2</sup> Christian M. Wolff<sup>1</sup>**

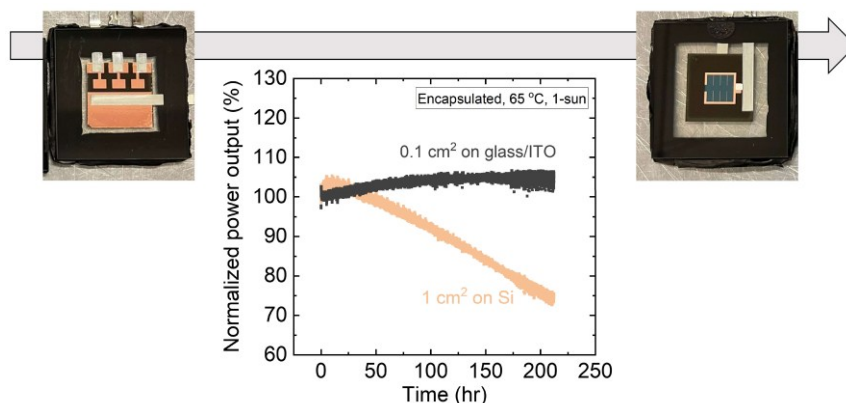
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Metal halide perovskite solar cells have shown a steady improvement in power conversion efficiency (PCE) over the past decade. Yet, for commercialization of the technology, the devices must also exhibit a high degree of stability, i.e., maintain high power output over prolonged operation. In this regard, recent reports on the stability of single-junction perovskite devices show considerable promise. However, reports on the stability of perovskite-Si tandem devices, a prominent candidate for commercialization, remain limited. The tandem devices exhibit numerous architectural differences compared to small-area, single-junction devices typically fabricated on glass substrates. To effectively transfer stability improvements from single-junction devices to tandems, individual effects of these architectural changes should be identified.

Here, starting from a 0.1 cm<sup>2</sup> single-junction perovskite device on a transparent conductive oxide (TCO)-coated glass substrate, we vary the device architecture step by step, ultimately arriving at a 1 cm<sup>2</sup> two-junction perovskite-Si device. At each step, we subject the devices to elevated temperatures and light intensities to assess the stability. As an exemplary case, we investigate an inverted perovskite cell configuration that yields a PCE of about 20% and a T<sub>90</sub>

>1000 hr for 0.1 cm<sup>2</sup> devices when maximum-power-point tracked at 65 °C under continuous 1-sun illumination. The results show that T<sub>90</sub> can decrease considerably, to about 100 hr, for 1 cm<sup>2</sup> perovskite-on-Si devices stressed under the same conditions. In the presentation, critical architectural modifications that contribute to this difference, as well as the effects of area scaling, substrate and electrode configuration, and current-mismatch will be presented. Finally, pathways to enhance the stability of perovskite-Si devices to match that of single-junction perovskite devices will be discussed.



**Figure 1:** Power output normalized to its initial value (i.e., at Time ~ 0 s) for 0.1 and 1 cm<sup>2</sup> perovskite devices on glass/ITO (photograph on the left) and Si (on the right) substrates, respectively. The devices are encapsulated and a shadow mask is used to confine the illumination to the active area.

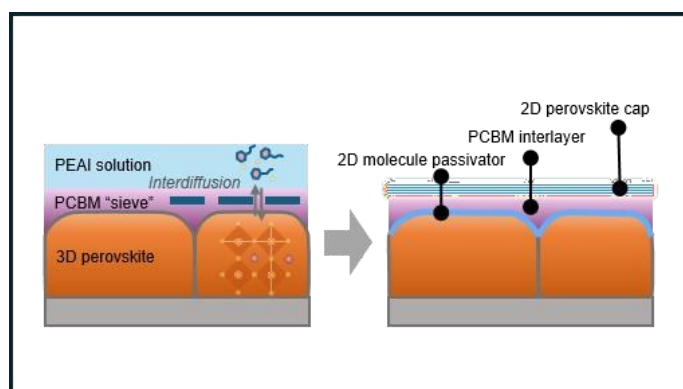
# SYNTHESIS OF A LATTICE-RESOLVED LAMINATE-STRUCTURED PEROVSKITE HETEROINTERFACE

**Pengfei Guo,<sup>1</sup> Zhimin Li,<sup>2</sup> Songhua Cai,<sup>2</sup> Yuanyuan Zhou<sup>1</sup>**

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2D surface passivation has been shown to be useful for achieving state-of-the-art perovskite optoelectronics, and the microstructural and phase heterogeneities of 2D perovskite passivators can influence their roles. However, the synthesis of co-homogenized, stable microstructure and phase in such passivators remains challenging. Herein, we leverage a [6,6]-phenyl-C61-butyric acid methyl ester (PCBM) molecular interlayer to mediate the reaction of 2D passivator and perovskite, leading to a uniform phase-purer 2D perovskite capping layer (Figure 1). This PCBM interlayer further mitigates grain-boundary etching encountered in conventional approaches, creating molecular passivation directly onto the perovskite surface. The inverted PSCs made as such feature a laminate-structured perovskite heterointerface at the electron-extracting side, which contributes to improved charge energetics and film stability, owing to regulated band transition and laminate-layer protection, respectively. Power conversion efficiencies up to 26% are achieved, together with enhanced device stabilities under ISOS-standardized protocols, showing T90 lifetimes over 1,000 h in both the damp-heat test (85 °C, 85% relative humidity) and maximum-power-point tracking under one-sun illumination. Lattice-resolved insights are provided to link the microstructure to device performance, shedding light on the significance of passivator-microstructure uniformity and reliability on the performance of perovskite optoelectronics.



**Figure 1:** Schematic illustration of the laminate-structured perovskite surface formed via the PCBM interlayer

## **Acknowledgements:**

[1] Z. Li, P. Guo, Y. Zhang, W. Wang, S. Cai, Y. Zhou, *Nature Synthesis* **2025**, In Press.

# ENHANCED CHARGE CARRIER TRANSPORT AND EXTRACTION FOR PEROVSKITE/SILICON TANDEM SOLAR CELLS

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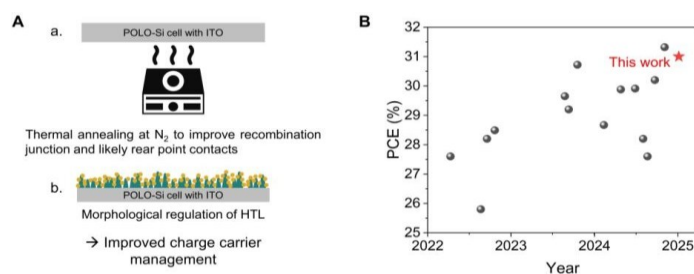
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The integration of perovskite as a top absorber with a silicon bottom cell in a tandem architecture has been demonstrated to further enhance power conversion efficiency (PCE), offering an effective pathway to surpass the Shockley-Queisser limit of single junction solar cells. However, realizing high-performance monolithic tandem devices remains challenging—particularly progress on tandem solar cells based on industrial silicon cells with POLycrystalline silicon on Oxide (POLO) passivating contacts is scarce compared to perovskite/heterojunction-Si tandem cells.

Here, we utilize an advanced silicon bottom cell architecture featuring POLO contacts at both sides. An annealing treatment in nitrogen is employed on the silicon bottom cells to heal sputtering-induced damage at the electron-selective POLO contact within the recombination junction. It simultaneously promotes contact quality at the TCO/n<sup>+</sup> poly-Si interface and also might enhance the Al/p<sup>+</sup> poly-Si rear contacts.

Furthermore, our systematic investigation in term of morphological regulation and material selection reveals that ultrathin sputtered nickel oxide layer (NiOX) combined with self-assemble monolayer (SAM) as hole transport layer (HTL) combination substantially enhances carrier transport dynamic at the buried interface of perovskite film.

Eventually, carrier transport and extraction are significantly improved by these strategies, conducting the monolithic perovskite/Si tandem solar cell with a PCE of 31%. Furthermore, the device without encapsulation retained 93% of its initial efficiency after 240 hours of continuous operation under ISOS-L-1 condition with an estimated T80 of 740 hours.



**Figure 1:** (A) Schematic illustration of the annealing of the silicon bottom cell to enhance the recombination junction and rear contact, and morphological regulation of the hole transport layer to improve charge extraction. These innovations work to achieve efficient charge carrier management. (B) Efficiency trends in perovskite/Si tandem solar cells, suggesting our 31% PCE—placing this work at the leading edge of current tandem photovoltaic technologies.

# NOVEL ISOINDIGO DERIVATIVES AS ELECTRON TRANSPORT MATERIALS FOR PEROVSKITE SOLAR CELLS

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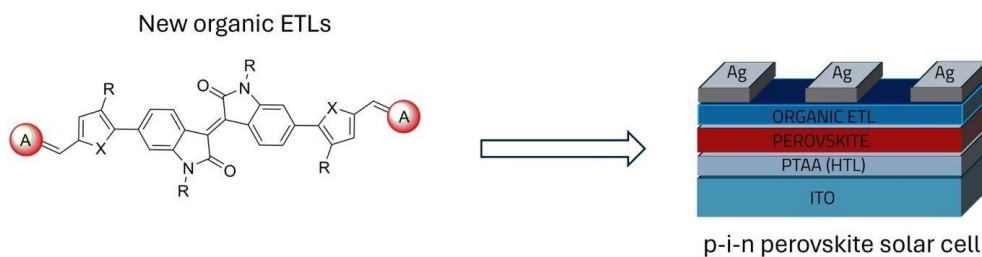
<sup>3</sup>Italian National Agency for New Technologies, Energy and Sustainable Economic Development (ENEA), Portici(NA), Italy

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Recently, there has been extensive research on perovskite solar cells (PSCs) with a p-i-n structure, also known as inverted PSCs, due to their advantages over their n-i-p counterparts, such as low-temperature fabrication, higher stability, and better compatibility for applications in Si-perovskite tandem architectures.

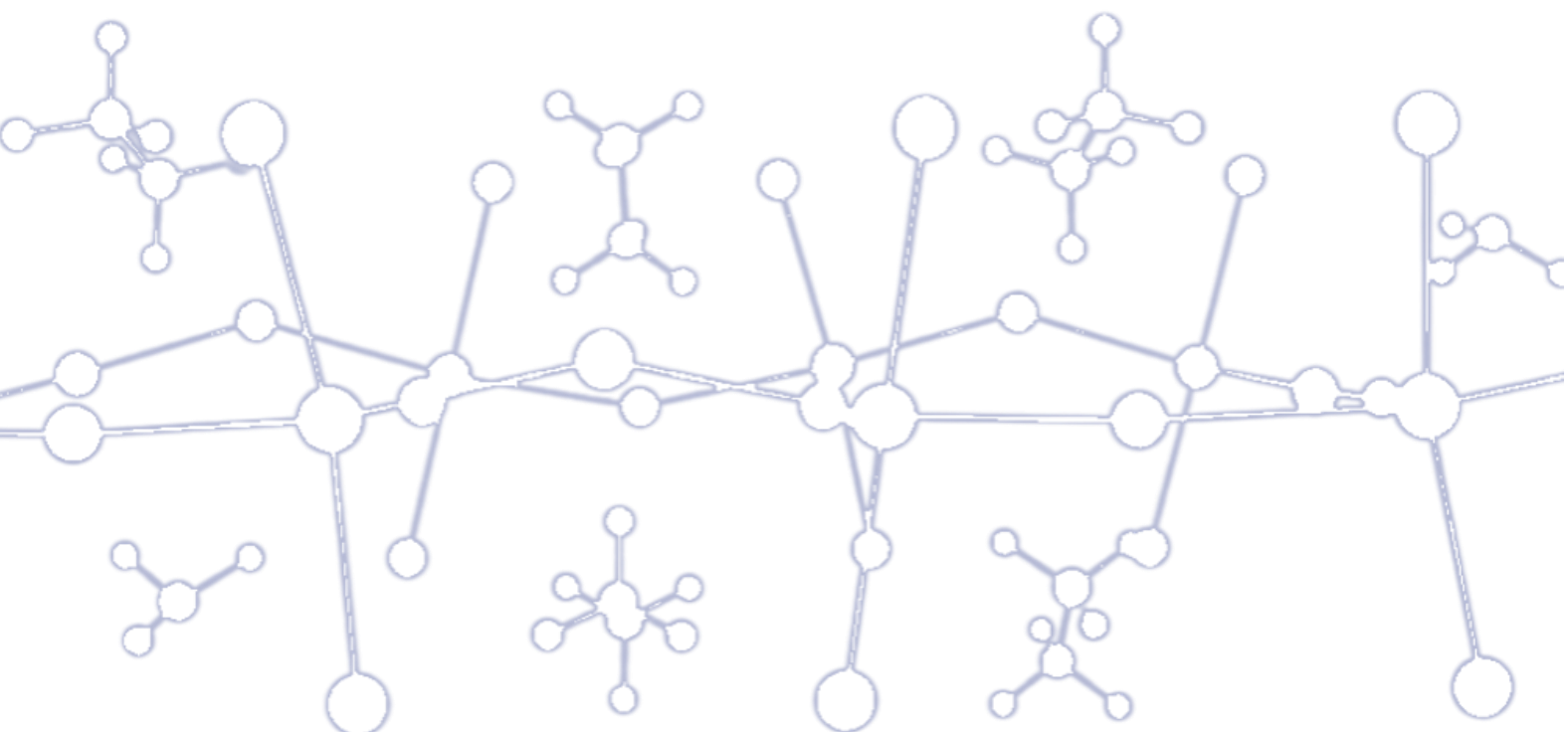
The charge transport layers in such devices must meet several requirements, including proper energy level alignment with the perovskite material, high electron or hole mobility, good stability, and ease of fabrication. In the p-i-n configuration, commonly employed electron transport layers (ETLs) are fullerene C<sub>60</sub> or its derivatives, such as [6,6]-Phenyl-C61-butyric Acid Methyl Ester (PCBM). However, tuning the energy levels of these fullerene-based materials to match different perovskite compositions remains challenging. Moreover, C<sub>60</sub> is typically deposited via thermal evaporation, which increases the overall cost of the device, while solution-processable derivatives like PCBM, although easier to deposit, are expensive and not ideal for large-scale production. Thereby, the development of novel ETLs is essential to overcome these limitations and enable more cost-effective, scalable, and efficient p-i-n PSCs.

In this study, newly synthesized isoindigo derivatives were tested as potential ETLs for PSCs. The prototypal structure is based on an electron acceptor isoindigo core, symmetrically linked to electron donor thiophene moieties and ended with auxiliary acceptor groups. The molecules were thoroughly characterized regarding their structural, optical and electrochemical properties. They were then processed as thin films and tested as ETLs in inverted PSCs with the following stack: ITO/PTAA/CsFAMAPbBr/ETL/Ag. The deposition of the organic semiconductors on the hydrophilic perovskite layer was the most challenging step. To address this, the process was carefully optimized by varying deposition solvents, spin-coating parameters and introducing more polar solubilizing chains into the molecular structure to enhance compatibility with the perovskite layer. The fabricated devices were electrically characterized under solar simulator irradiation, showing promising results with a maximum power conversion efficiency (PCE) exceeding 10%.



**Figure:** Prototypal structure of the organic semiconductors under study and architecture of the PSC

	Town Hall	Trumpet
<b>Session Chair</b>	<b>Filippo De Angelis, University of Perugia, Italy</b>	<b>Shuxia Tao, Eindhoven University of Technology, The Netherlands</b>
<b>Session Title</b>	<b>Session 3A – Tandem PV 2</b>	<b>Session 3B – Performance</b>
16:52 17:04	<b>Johanna Modes</b> , INATECH - University of Freiburg, Fraunhofer ISE, Germany <i>Scalable metal oxide passivation of the perovskite/C60 interface in perovskite-silicon tandem solar cells</i>	<b>Hao Mingwei</b> , The Hong Kong University of Science and Technology, Hong Kong <i>Nanoscopic cross-grain cation homogenization for high-performance perovskite solar cells</i>
17:04 17:16	<b>Kristell Carreric</b> , CEA INES, France <i>Up-scaling perovskite growth using hybrid methods for silicon/perovskite tandem solar cells</i>	<b>Florian Dupont</b> , CEA-Leti, France <i>High-efficiency polycrystalline perovskite thin film color-conversion layers for high-brightness and ultrahigh-resolution MicroLED displays</i>
17:16 17:28	<b>Theresa Kuechle</b> , Karlsruhe Institute of Technology (KIT), Germany <i>Scalable and conformal perovskite-silicon tandem photovoltaics by hybrid 2-step inkjet printing</i>	<b>Weidong Xu</b> , University of Cambridge, United Kingdom <i>Unveiling the role of nanoscale heterogeneities on charge extraction efficiency in inverted perovskite solar cells</i>
17:28 18:00	<b>PSCO CLOSING/AWARDS</b>	



# SCALABLE METAL OXIDE PASSIVATION OF THE PEROVSKITE/C<sub>60</sub> INTERFACE IN PEROVSKITE-SILICON TANDEM SOLAR CELLS

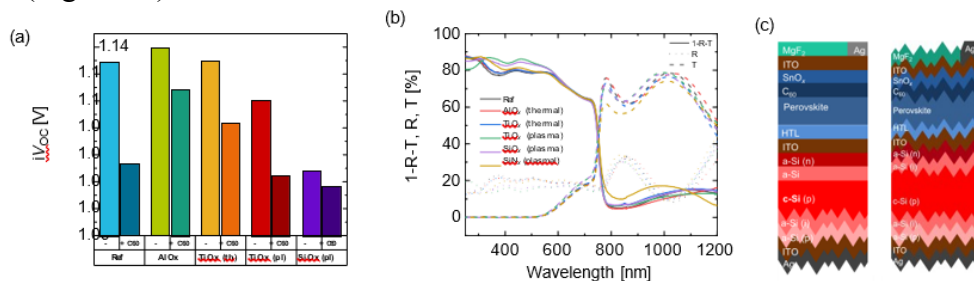
**Johanna Modes,<sup>1,2</sup> Patricia S.C. Schulze,<sup>2</sup> Leon Gutmann,<sup>1,2</sup> Armin Richter,<sup>2</sup> Christoph Messmer,<sup>2</sup> Mohamed A. A. Mahmoud,<sup>1,2</sup> Christian Schwarz,<sup>1,2</sup> Oussama Er-raji,<sup>2</sup> Oliver Fischer,<sup>1,2</sup> Alexander J. Bett,<sup>2</sup> Juliane Borchert<sup>1,2</sup>**

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Perovskite-silicon tandem solar cells are now among the most efficient silicon-based dual-junction solar cell concepts. However, commonly used passivation layers often have a negative impact on long-term stability or rely on laboratory-scale deposition methods.<sup>[1,2]</sup> Therefore, this work focuses on developing scalable, efficient passivation layers that also enhance long-term stability. These passivation layers should also serve as protective coatings to prevent the degradation of the perovskite absorber. Metal oxides are promising candidates due to their excellent chemical stability, favorable band alignment, and high optical transparency. Moreover, they can be deposited using industry-compatible techniques. In this research, atomic layer deposition (ALD) and electron-beam physical vapor deposition (E-beam) are used to deposit various metal oxides and mixed metal oxides to reduce non-radiative losses at the perovskite/C<sub>60</sub> interface. These processes have been optimized to prevent damage to the perovskite layer and to control the deposition of ultrathin layers (1 nm-2 nm). The conductivity of these layers is analyzed in test structures using dark *IV* measurements as well as in perovskite single-junction devices. The lumped device series resistance is determined by comparing *IV* measurements to Suns-*V*<sub>OC</sub> based *pIV* curves.<sup>[3]</sup> To better understand the passivation effects, photoluminescence quantum yield (PLQY), surface photovoltage (SPV) measurements and opto-electrical simulations with a drift diffusion model of the system are carried out.<sup>[4]</sup> Optimized layers are tested for different device architectures (Figure 1c)



**Figure 1:** (a) *iV*<sub>OC</sub> (alternatively referred to as quasi-Fermi level splitting, *QFLS*) determined from absolute photoluminescence measurements at 1 sun for different metal oxide passivation layers at the perovskite/C<sub>60</sub> interface, deposited via plasma enhanced (pl) and thermal (th) ALD. (b) Absorptance (1-R-T), reflectance (R) and transmittance (T) for metal oxide passivation layers from (a), (c) Planar (left) and fully textured (right) tandem device architecture.

**Acknowledgements:** Funded by a scholarship of the state graduate funding Baden-Württemberg, Germany, as well as the BMWK funded project Pero-Si Scale and the Vector Foundation.

[1] K. Artuk, **2025**, preprint, doi.org/10.21203/rs.3.rs-6264086/v1.

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[4] C. Messmer, *Prog Photovoltaics* **2025**, 33, 126.

# NANOSCOPIC CROSS-GRAIN CATION HOMOGENIZATION FOR HIGH-PERFORMANCE PEROVSKITE SOLAR CELLS

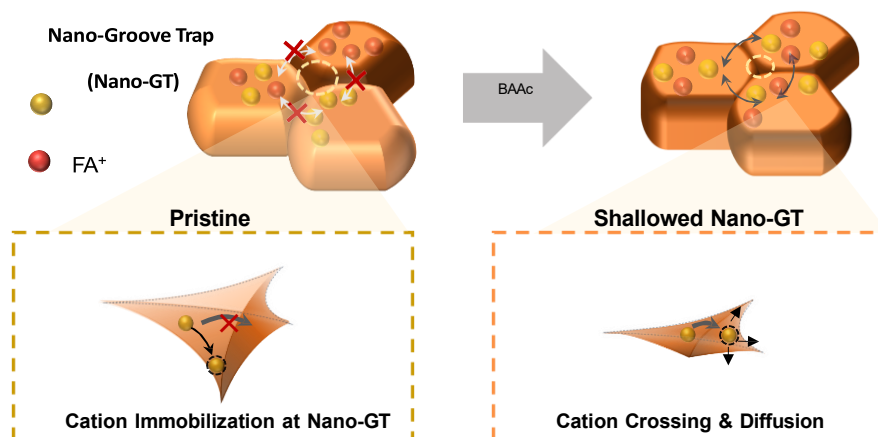
**Mingwei Hao,<sup>1</sup> Yuanyuan Zhou<sup>1,2</sup>**

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Multiscale cation inhomogeneity has been a major hurdle in state-of-the-art formamidinium–caesium (FA–Cs) mixed-cation perovskites for achieving perovskite solar cells with optimal power conversion efficiencies and durability. Although the field has attempted to homogenize the overall distributions of FA–Cs in perovskite films from both plan and cross-sectional views, our understanding of grain-to-grain cation inhomogeneity and ability to tailor it—that is, spatially resolving the FA–Cs compositional difference between individual grains down to the nanoscale—are lacking. Here we report that individual grains, as fundamental building blocks of a perovskite film, exhibit cationic compositions deviating from the prescribed ideal ratio, which severely limits interfacial optoelectronic properties and perovskite layer durability.<sup>[1]</sup> This performance-limiting nanoscopic factor is linked to thermodynamic-driven morphological grooving, leading to a segmented surface landscape. At the grain triple junctions, grooves form nanoscale groove traps that hinder the mixing of solid-state cations across grains and thus retard inter-grain FA–Cs mixing. By rationally modulating the heterointerfacial energies, we reduced the depth of these nanoscale groove traps by a factor of three, significantly improving cation homogeneity. Perovskite solar cells with shallower nanoscale groove traps demonstrate enhanced power conversion efficiencies (25.62%) and improved stability under various standardized international protocols. This work highlights the significance of resolving surface nano- morphologies for homogeneous properties of perovskites.



**Figure 1:** Schematic of how nano-GT depth influences cation homogenization in perovskite thin films.

[1] Hao, M. et al., *Nat. Nanotechnol.* **2025**. <https://doi.org/10.1038/s41565-025-01854-y>

# UP-SCALING PEROVSKITE GROWTH USING HYBRID METHODS FOR SILICON/PEROVSKITE TANDEM SOLAR CELLS

**Kristell Carreric<sup>1</sup>, Polyxeni Tsoulka<sup>1</sup>, Louis Grenet<sup>2</sup>, Elodie Gerente<sup>2</sup>, Solenn Berson<sup>1</sup>**

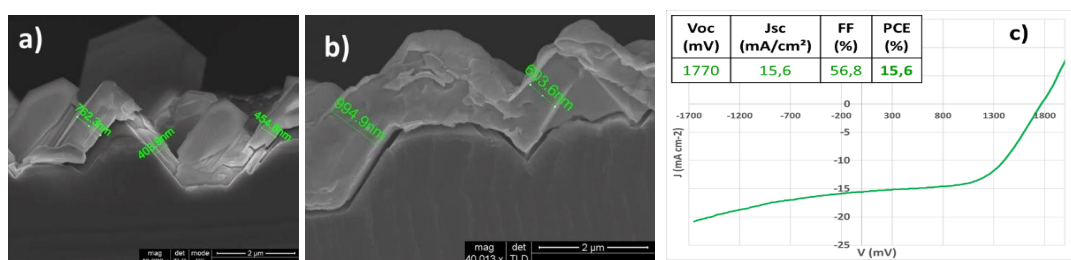
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In the last ten years, tandem solar cells based on perovskite (PK) materials have shown promising results, surpassing the theoretical limits of single junction Silicon (Si) solar cells. Even though Si/PK tandem solar cells appear capable of achieving 39,5 % of power conversion efficiency [1], we need to overcome many challenges in order to upscale the PV devices and pass from the 1 cm<sup>2</sup> laboratory scale to larger areas. With that perspective, vapor deposition of the absorber layer seems promising in order to deposit a conformal and high quality perovskite on top of textured Si wafers. In the literature, the main industrially compatible techniques to grow the PK layer can be divided into two axes: i) PK deposition by full vapor deposition techniques and ii) PK deposition by hybrid processes (mix of a dry and wet processes).

In this work, we focus on a hybrid deposition process where the first inorganic layer is grown by Close Space Sublimation (CSS). This technique allows high deposition rates (deposition time: a few minutes) [2], which would be more viable for the industry than other vapor deposition processes such as the thermal co-evaporation. The organic precursors are then deposited by spin coating in a second step, to convert the initial scaffold into the desired perovskite layer. Using different characterization techniques (X-ray Diffraction, X-Ray Photoelectron Spectroscopy, Scanning Electron Microscope, etc.) we firstly investigate the structural and chemical properties of the inorganic scaffold (see **Figure 1 a**). The goal of this study is to understand how the homogeneity, the porosity and the composition of the first layer affect the growth of the final PK film (see **Figure 1 b**). Simultaneously, we examine the key factors that influence the crystallization mechanism during the second wet step. Hence, we investigate the impact of the concentration of the organic solution, the I/Br ratio, etc. Finally, we associate the material properties of the PK layer to the optoelectronic response of the PV devices. Our preliminary results on a full Si/PK tandem cell exhibited a record efficiency of 15,6% (see **Figure 1 c**).



**Figure 1 :** a) SEM photo of the inorganic scaffold deposited by CSS b) SEM photo of the PK layer after conversion by spin-coating c) J(V) curve and parameters of the best cell made by the hybrid process CSS + spin

**Acknowledgements:** This work benefited from an help of the state generated by the National Agency of Research for France 2030 and referenced as 22-PETA-00005 (PEPR TASE IOTA)

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[2] G. Zhang et al., *ACS Appl. Energy Mater.* **2022**, 5, 5797-5803.

# HIGH-EFFICIENCY POLYCRISTALLINE PEROVSKITE THIN FILM COLOR-CONVERSION LAYERS FOR HIGH-BRIGHTNESS AND ULTRAHIGH-RESOLUTION MICROLED DISPLAYS

**Florian Dupont, Natalia Zambrano Ortega, Stephane Altazin, François Templier**

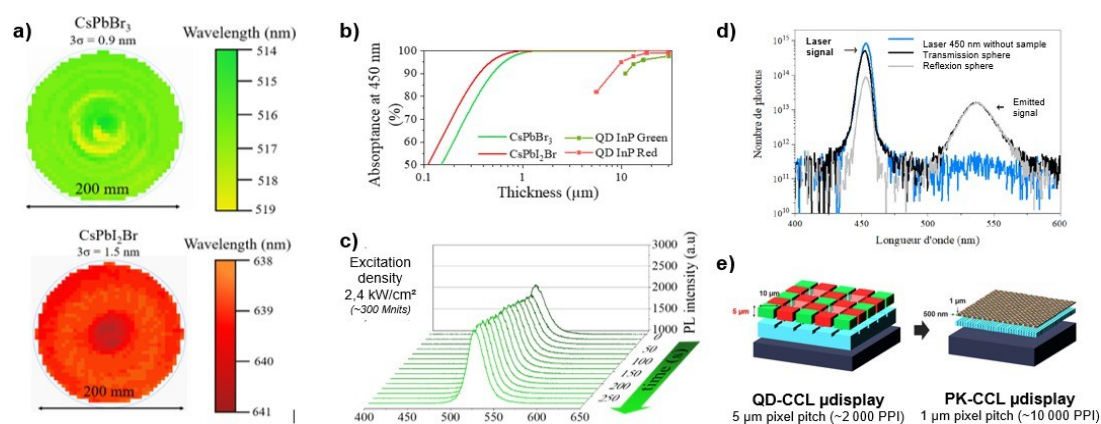
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GaN-based microLEDs are a promising technology to achieve high-brightness and high-contrast microdisplays. However, the fabrication of full-color microLED microdisplays is a technological challenge. Color-conversion layers (CCLs) using quantum dots (QDs) have a stability issue under high brightness, and are difficult to fabricate for pixel pitches below 3  $\mu\text{m}$ .<sup>[1][2]</sup> On the other hand, polycrystalline halide perovskite thin films have a higher absorption coefficient, but this structure has rarely been used as CCLs in the literature.<sup>[3]</sup>

This study reports very thin and high-efficiency inorganic halide perovskite thin films using pulsed laser deposition (PLD) as a new way to fabricate CCLs. CsPbBr<sub>3</sub> and CsPbI<sub>2</sub>Br thin films were fabricated on 200 mm wafers using PLD. Photoluminescence (PL) showed pure green and red light emission emitted uniformly over 200 mm wafers, respectively. The absorption coefficient is superior to QDs and enable the fabrication of sub-500 nm CCLs. The absence of degradation of PL under extremely high illumination (2.4 kW/cm<sup>2</sup>) could indicate a compatible with very high optical flows orders of magnitude superior to QDs. An external photoluminescence yield (PLQY) of 48% was measured, which allows to estimate an internal PLQY of about 89%.

These results indicate that inorganic halide perovskite thin films are promising candidates for CCLs in high-brightness and ultrahigh-resolution microLED displays.



**Figure 1.** a. PL peak position mapping of CsPbBr<sub>3</sub> (up) and CsPbI<sub>2</sub>Br (down), b. Absorptance of perovskite and QD-based CCL depending on the thickness, c. Evolution of the photoluminescence peak of CsPbBr<sub>3</sub> layer under an excitation density of 2.4 kW/cm<sup>2</sup> during 600 seconds, d. Photoluminescence measurement in double integrating sphere leading to the measurement of an external PLQY of 48%, e. Schematic of a microLED display using QD-based CCL with a 5  $\mu\text{m}$  pixel pitch (left) and a perovskite thin film-based CCL with a 1  $\mu\text{m}$  pixel pitch (right)

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# SCALABLE AND CONFORMAL PEROVSKITE-SILICON TANDEM PHOTOVOLTAICS BY HYBRID 2-STEP INKJET PRINTING

**Theresa Kuechle,<sup>1</sup> Raphael Pesch,<sup>1,2</sup> Johannes Schenk,<sup>1</sup> Johannes Sutter,<sup>1,2</sup> Ulrich W. Paetzold<sup>1,2</sup>**

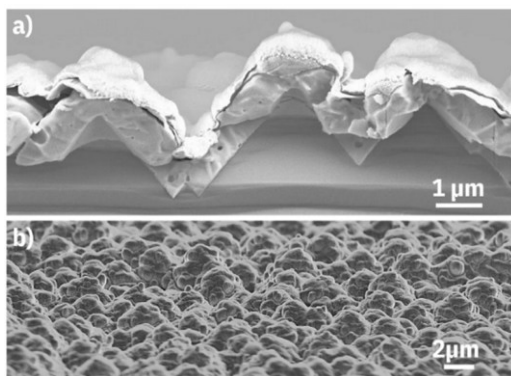
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In recent years, the power conversion efficiency (PCE) of perovskite-silicon tandem photovoltaics has improved significantly on a lab-scale.<sup>[1]</sup> Currently, perovskite thin films are mostly fabricated with non-scalable methods such as spin-coating. For photovoltaics industry, fully scalable processes are beneficial to ensure homogeneous thin-film formation while maintaining conformity to the bottom cell. Here, we show a hybrid two-step process for the perovskite thin film fabrication whereby inorganic components are evaporated, followed by inkjet printing of organic components. Our approach addresses scalability challenges and highlights the suitability of inkjet printing with a green solvent for the fabrication of large textured tandem solar cells. We show that optimizing the stoichiometry is necessary and can be achieved by fine-tuning the droplets per inch in the second step.

Our team has pioneered this process route for perovskite single junction solar cells in 2024.<sup>[2]</sup> Through inkjet printing parameter optimization, we achieve wide-band gap single-junction perovskite solar cells with close to 20 % PCE and stable performance during 60 min of maximum power point tracking. Additionally, we successfully fabricate large-textured (3–5  $\mu\text{m}$  pyramid size) tandem solar cells with an active area of 1  $\text{cm}^2$ , achieving a single-JV-scan PCE approaching 25 %. We succeed in coating areas of more than 30  $\text{cm}^2$  proving the scalability. At the PSCO, we will present our advances in transferring this process to tandem devices and scaling to larger device areas. Figures 1a and 1b show a cross-sectional and tilted surface scanning electron microscopy image of a tandem solar cell fabricated using this approach and illustrate the conformal growth of the perovskite layer on large textures. These results underscore the potential of this hybrid fabrication process to overcome upscaling hurdles and advance the development of highly efficient tandem solar cells for industrial applications.



**Figure 1:** Scanning electron microscopy image of conformally deposited hybrid two-step inkjet-printed perovskite on a textured silicon bottom cell. a) Cross-section, b) inclined top view.

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# UNVEILING THE ROLE OF NANOSCALE HETEROGENEITIES ON CHARGE EXTRACTION EFFICIENCY IN INVERTED PEROVSKITE SOLAR CELLS

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Understanding the dynamic interplay between charge extraction and recombination, and its dependence on material properties such as nanoscale heterogeneities, is crucial for further boosting the efficiency of perovskite solar cells. Here, we investigate the role of guanidinium in altering nanoscale material properties and its impact on optoelectronic properties, device efficiency, stability, and charge carrier dynamics.

Our findings reveal that the improved power conversion efficiency following guanidinium incorporation is primarily due to significant enhancements in short-circuit current density (1.5 mA/cm<sup>2</sup>) and fill factor values (4%), with no notable change in open-circuit voltage.<sup>[1]</sup> Additionally, these devices demonstrate improved operational stability. Spectroscopic and microscopic analyses suggest that these improvements are mainly due to the reduction of nanoscale inhomogeneities (mostly iodine vacancies) after guanidinium incorporation, which hinders ion migration, enhances charge transport properties and light stability in the perovskite materials, consequently improving overall charge extraction efficiency and device stability.<sup>[1-2]</sup>

Our observations provide a comprehensive understanding of the role of nanoscale heterogeneities in device performance and showcase the use of a multimodal measurement toolkit for elucidating the physical chemistry mechanisms behind these inverted perovskite solar cells.

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[1] W. Xu et al., *ACS Energy Lett.* **2025**, DOI: <https://doi.org/10.1021/acseenergylett.5c00469>.

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