HL 4: Perovskite and Photovoltaics: Synthesis and Performance

Time: Monday 9:30–12:00 Location: POT/0251

Invited Talk HL 4.1 Mon 9:30 POT/0251

X-ray nanodiffraction studies of lead-halide perovskite supercrystals — Jonas Hiller[1], Robert Thalwitzer[1], Ata Bozkurt[1], Matheus Ferreira[2], Richard Hodak[1], Fabian Strauss[1], Elke Nadler[1], Gerard Hinsley[3], Bihan Wang[3], Kuan Hoon Ngoi[3], Witold Rudzinski[4], Ekaterina Kneschaurek[1], Wojciech Roseker[3], Michael Sprung[3], Dmitry Lapkin[1], Dmitry Baranov[2], Frank Schreiber[1], Ivan Vartanyants[3], Marcus Scheele[1], and •Ivan Zaluzhnyy[1] — [1]University of Tübingen — [2]Lund University — [3]Deutsches Elektronen-Synchrotron DESY — [4]University of Krakow

We synthesize mechanically robust supercrystals built from cubic lead halide perovskite nanocrystals by a two-layer phase diffusion self-assembly with acetonitrile as the antisolvent. This method yields highly faceted thick supercrystals, which are robust enough to be picked up and relocated by microgrippers. We employed X-ray nanodiffraction together with high-resolution scanning electron microscopy and atomic force microscopy to reveal the structure of $CsPbBr_3$, $CsPbBr_2Cl$, and $CsPbCl_3$ supercrystals and explain their unusual mechanical robustness. We show that the removal of organic ligands from perovskite nanocrystals results in a size gradient of the nanocrystals within the supercrystals.

Hiller et al., ACS Nano **19** (2025) 26117

HL 4.2 Mon 10:00 POT/0251

Impact of Antisolvents on Halide Perovskite Nanocrystal Synthesis — •Tim Julius Hashagen, Leo Luber, and Alexander Skyrme Urban — Nanospectroscopy Group, Nano-Institute Munich, Department of Physics, Ludwig-Maximilians-Universität München, Königinstraße 10, 80539 Munich, Germany

Lead halide perovskite nanocrystals (NCs) offer highly tunable optical properties and high photoluminescence efficiencies, making them promising for optoelectronic and photocatalytic applications. Their synthesis, however, is extremely sensitive to the choice of antisolvent, which governs nucleation and growth kinetics and thereby the structural and optical quality of the resulting NCs. [1] In this work, we systematically investigate how structural and chemical variations among antisolvents affect the formation of CsPbBr2 NCs. By tuning precursor compositions and antisolvent identities, we identify clear trends in crystallization behavior and photoluminescence characteristics. These experimental results are combined with a Gaussian Process regression model that encodes antisolvent geometry to predict NC emission wavelengths.[2] The model performs accurately for well-represented antisolvent classes but still faces challenges when extrapolating to sparsely sampled or previously unseen antisolvents. Our combined experimental and data-driven approach highlights the decisive role of antisolvent molecular structure in NC synthesis and demonstrates a pathway toward predictive control over perovskite nanocrystal properties.

[1]K. Frank et al., Nat. Commun. 2024, 15, 8952.

[2]N. A. Henke et al., Adv. Mater. 2025, e09472.

HL 4.3 Mon 10:15 POT/0251

Tuning Lead Halide Perovskite Nanocrystal Properties via Controllable Synthesis and Machine-Learning Insights — •Maximilian Dörfler, Leo Luber, and Alexander Urban — Nanospectroscopy Group, Nano-Institute Munich, Department of Physics, Ludwig-Maximilians-Universität München, Königinstraße 10, 80539 Munich, Germany

Halide perovskite nanocrystals (NCs) combine high photoluminescence efficiency with tunable emission, but achieving narrow linewidths requires tightly controlled, highly monodisperse synthesis. In this work, we perform in situ observations of CsPbBr3 NC formation under ambient conditions and systematically evaluate how synthesis parameters shape their optical response. By analyzing the evolving photoluminescence spectra, we assess how reaction time, dilution, and precursor-to-antisolvent ratios jointly influence crystal growth and resultant morphology. The in situ approach allows us to track nanocrystal growth pathways and provides the opportunity for real-time steering of the synthesis. Particular emphasis is placed on understanding the conditions under which the NCs adopt 2D versus 3D morphologies. In future work, we will employ machine-learning tools - specifically Bayesian optimization - to efficiently navigate the sparsely sampled synthesis parameter space. This data-driven strategy aims to identify regions that yield high quantum efficiencies and narrow linewidths, enabling rapid discovery of conditions that favor predominantly monodisperse nanocrystals or nanoplatelets with minimal experimental iteration.

HL 4.4 Mon 10:30 POT/0251

Scalable Perovskite-Silicon Tandem Photovoltaics by Hybrid 2-Step Inkjet Printing — •Theresa Kuechle[1], Raphael Pesch[1,2], Jinzhao Li[1,2], and Ulrich W. Paetzold[1,2] — [1]Light Technology Institute, KIT, Germany — [2]Institute of Microstructure Technology, KIT, Germany

In recent years, the power conversion efficiency (PCE) of perovskite-silicon tandem photovoltaics has improved significantly on a lab scale. For photovoltaics industry, fully scalable processes are required 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 dots per inch in the second step. Through inkjet printing parameter optimization, we achieve wide-band gap single-junction perovskite solar cells with close to 20 % PCE. Additionally, we successfully fabricate large-textured (3 to 5 μm pyramid size) tandem solar cells with an active area of 1 cm^2, achieving a single-JV-scan PCE of 27.4 %. 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.

HL 4.5 Mon 10:45 POT/0251

A Materials Perspective on Sequential Inorganic Scaffold Deposition for Hybrid-Processed Perovskite Thin Films — •Ronja Pappenberger[1,2], Julian Petry[1,2], Alexander Welle[3,4], Tonghan Zhao[1], Alexander Diercks[2], Raphael Pesch[1,2], Paul Fassl[1,2], and Ulrich W. Paetzold[1,2] — [1]Institute of Microstructure Technology, KIT, Germany — [2]Light Technology Institute, KIT, Germany — [3]Institute of Functional Interfaces, KIT, Germany — [4]Karlsruhe Nano Micro Facility, KIT, Germany

As perovskite solar cells (PSCs) advance toward industrial-scale production, fabrication processes must combine high-throughput with simple integration. In this regard, the hybrid two-step deposition route has emerged as a promising method, allowing for conformal coatings on micron-scale textures, a critical feature for perovskite/silicon tandem photovoltaics. This work presents a fully sequential route, wherein the inorganic materials CsCl and PbI_2 are deposited separately, simplifying industrial implementation compared to co-deposition. Microstructural analysis shows that sequential deposition promotes vertical PbI_2 growth with a secondary tilted orientation, unlike the horizontal orientation from co-deposition. Elemental distribution reveals high diffusivity for Cs, formamidinium, and I, yielding a homogeneous distribution in the perovskite absorber, while Pb and Cl remain largely scaffold-bound. PSCs with a 1.69 eV bandgap achieve efficiencies of 19.3% (co-deposition) and 18.7% (sequential), highlighting fully sequential hybrid deposition as a promising route toward industrial PSC production.

15 min. break

HL 4.6 Mon 11:15 POT/0251

How stable are mixed-metal chalcohalides? — •Pascal Henkel[1], Jarno Laakso[1], Jingrui Li[2], and Patrick Rinke[1,3] — [1]Department of Applied Physics, Aalto University, Espoo, Finland — [2]Xi'an Jiaotong University, Xi'an, China — [3]Technical University of Munich, Garching, Germany

Perovskite-inspired quaternary mixed-metal chalcohalides (MMCHs, $M(II)_2M(III)Ch_2X_3$) are an emerging materials class for photovoltaics,[1,2] capable of delivering high conversion efficiencies.[3] Yet, their thermodynamic stability remains largely unexplored.

We assess the thermodynamic stability of 54 MMCH compounds by modelling their phase diagrams using DFT, *pymatgen* tools from Materials Project[4] and the Alexandria Materials Database.[5] All studied MMCHs lie above the convex hull, independent of their space group ($Cmcm$, $Cmc2_1$, $P2_1/c$). Accounting for computational uncertainty (mostly from the applied exchange-correlation functional) moves a considerable fraction of MMCHs close to or below the hull. The MMCH decomposition paths follow five reactions, with $4\,\mathrm{M(II)_2M(III)Ch_2X_3} \leftrightarrow 2\,\mathrm{M(III)_2Ch_3} + 6\,\mathrm{M(II)X_2} + 2\,\mathrm{M(II)Ch}$ occurring most frequently. Experiments show that compounds close to the convex hull can be synthesized, whereas compounds far from the hull decompose following the predicted reactions. Overall, our results show that MMCHs are synthesizable, but fabrication conditions need further optimisation.

[1] *Chem. Mater.* **35**, 7761-7769 (2023), [2] *Phys. Rev. Materials* **9**, 115405 (2025), [3] *Mater. Horiz.* **8**, 2709 (2021). [4] *Chem. Mater.* **20**, 1798-1807 (2008). [5] https://alexandria.icams.rub.de/.

HL 4.7 Mon 11:30 POT/0251

minimizing ionic losses in DMSO-free tin-based perovskite solar cells — •Paria Forozi Sowmeeh[1], Shengnan Zuo[2], Chiara Frasca[2], Biruk Alebachew Seid[1], Sercan Ozen[1], Wentao Liu[2], Mahmoud Hussein Aldamasy[2], Yuan Zhang[3], Fengshuo Zu[2,3], Norbert Koch[2,3], Martin Stolterfoht[4], Antonio Abate[2], Artem Musiienko[2], and Felix Lang[1] — [1]Institute of Physics and Astronomy University of Potsdam, Potsdam-Golm, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany — [3]Department of Physics, Humboldt University of Berlin, Berlin, Germany — [4]Electronic Engineering Department, The Chinese University of Hong Kong, Hong Kong SAR, China

The presence of mobile ions and the potential toxicity of Pb-based perovskite solar cells remain two major drawbacks for their commercialization despite their exceptional optoelectronic properties. On the other hand, Sn-based perovskites, which are believed to exhibit smaller ion-induced instabilities, have been revealed as eco-friendly perovskite counterparts, though thorough investigations are still missing. Herein, we investigate the nature of mobile ions, quantify the ionic loss within Sn-based perovskite solar cells and compare with those of Pb-based and mixed PbSn devices. We report minimal ionic losses and over 10-fold lower ion densities in DMSO-free processed Sn samples compared to Pb-based perovskites. The Sn-based devices also exhibit the lowest associated ionic losses with sustained device stability upon illumination. This study paves the way for development of innovative, stable thin film solar cells with suppressed ion migration.

HL 4.8 Mon 11:45 POT/0251

Beyond 1D: How Edge Effects Impact Ion Densities and Stability in Perovskite Solar Cells — •Jarla Thiesbrummel[1,2], Francisco Peña-Camargo[2], Bruno Ehrler[3], Dilara Abdel[4], Patricio Farrell[4], and Felix Lang[1] — [1]University of Potsdam, Potsdam, Germany — [2]Helmholtz-Zentrum zu Berlin, Berlin, Germany — [3]AMOLF, Amsterdam, Germany — [4]Weierstrass Institut, Berlin, Germany

Understanding how mobile ions redistribute within metal halide perovskites is essential for interpreting device stability and quantitative ion-density measurements. While most studies focus on ion transport along the device stack, lateral ion motion and edge effects remain relatively unexplored, despite their strong relevance, especially in small-area, lab-scale photovoltaic devices. In this work, we investigate side collection of ions at device edges and its consequences for both apparent ion densities and long-term material stability, using a combination of 2D drift-diffusion simulations and experiments.