HL 45: Perovskite and Photovoltaics II (joint session HL/KFM)

Time: Thursday 9:30–13:00 Location: H13

HL 45.1 Thu 9:30 H13

Optical Simulations of Nanophotonic Back Contacts for Light Management in Ultrathin CIGSe Solar Cells — •Daniel Jiménez Tejero[1], Merve Demir[1], Bodo Fuhrmann[2], Roland Scheer[1], Ralf Wehrspohn[1], and Alexander Sprafke[1,2] — [1]Martin-Luther-Universität Halle-Wittenberg, Institut für Physik, Von-Danckelmann-Platz 3, 06120 Halle (Saale) — [2]MLU, Interdisziplinäres Zentrum für Materialwissenschaften, Nanotechnikum Weinberg, Heinrich-Damerow-Str. 4, 06120 Halle (Saale)

The development of ultrathin-film Cu(In,Ga)Se_2 (CIGSe) solar cells aims to reduce material usage and expand applications such as bifacial or tandem solar cells. However, CIGSe absorber layers with thicknesses below 1 μm exhibit diminished light absorption, particularly for wavelengths near the bandgap, leading to decreased power conversion efficiency. This can be counteracted by utilising functional back contacts that effectively increase the optical path length within the absorber layer through scattering, reflection, and nanophotonic mechanisms.

This work employs nano-optical simulations to investigate the potential of SiO_2 nanostructures on a flat gold back contact for enhancing the performance of CIGSe solar cells. By solving the Maxwell equations using the finite element method, the quantum efficiency and photocurrent under ideal charge carrier collection conditions are computed, enabling a comparison of various nanostructure geometries viable for fabrication. We find photocurrents higher than those of conventional CIGSe solar cells with an absorber thickness of 4 μm, indicating the potential of our light management approach.

HL 45.2 Thu 9:45 H13

Stabilizing Perovskite Solar Cells by Organic Salts Under One Full Sun and Maximum Power Point Tracking — •Zekarias Teklu Gebremichael[1,2], Niklas Manikowsky[2,3], Chikezie Williams Ugokwe[1,2], Bashudev Bhandari[2,3], Ulrich S. Schubert[1,2], and Harald Hoppe[1,2] — [1]Laboratory of Organic and Macromolecular Chemistry (IOMC Jena), Friedrich-Schiller- University Jena, Jena, Germany — [2]Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich-Schiller-University Jena, Jena, Germany — [3]Faculty of Physics and Astronomy, Friedrich-Schiller- University Jena, Jena, Germany

The use of organic halide salts to passivate metal halide perovskite (MHP) surfaces have been studied extensively. Passivating the surface defects of the MHP is of critical importance for realizing high-efficiency and stability of perovskite solar cells (PSCs). Here we discuss the success of a multifunctional organic salt used as passivation material for grain boundary defects and as molecular sealing layer in terms of stabilization. To assess the stability of PSCs, maximum power point tracking is seemingly the most realistic condition for the ageing test. Here, PSCs made from the four cation RbCsMAFA based perovskite absorber layer were aged under full light with maximum power point tracking and in addition they were tested periodically by IV-characterization, in order to yield all photovoltaic parameters for improved understanding of the ageing process.

HL 45.3 Thu 10:00 H13

Hyperuniform discordered structures for Light Management in Ultrathin CIGSe Solar Cells — •Katharina Trockel[1], Merve Demir[1], Frank Syrowatka[2], Ralf Wehrspohn[1], Roland Scheer[1], and Alexander Sprafke[1,2] — [1]Martin Luther University Halle-Wittenberg, Institute of Physics, 06120 Halle, Germany — [2]Martin Luther University Halle-Wittenberg, Interdisciplinary Center of Materials Science, 06120 Halle, Germany

Ultrathinfilm Cu(In,Ga)Se2 (CIGSe) solar cells are highly attractive due to their reduced material consumption and low manufacturing costs. While conventional CIGSe solar cells can achieve efficiencies of up to 21 %, increasing the efficiency of ultrathin solar cells remains a key research objective to enhance their competitiveness. A promising approach involves extending the optical path length in the absorber layer by integrating textured structures at the back or front contact of the solar cell. Most studies focus on periodic textures.

In this work, we investigate hyperuniform disordered (HuD) structures for light management in ultrathin CIGSe solar cells. The HuD structures are fabricated using polymethyl methacrylate (PMMA) particles deposited onto the back contact of the solar cells. These particles are covered with an indium tin oxide (ITO) layer and subsequently removed via a calcination process. The resulting ITO layer functions as a textured back contact, improving both light scattering and electrical performance.

First experimental results on the implementation of CIGSe solar cells with integrated HuD structures will be presented.

HL 45.4 Thu 10:15 H13

A Theoretical study of charge transport properties in perovskite analogues for high performance solar cells. — •Prerna Prerna[1,2] and Harald Oberhofer[1,2] — [1]University of Bayreuth — [2]Bavarian Center for Battery Technology, Bayreuth, Germany

Perovskite materials have emerged as promising candidates in solar cell technology, offering exceptional efficiency and affordability. Their remarkable performance, surpassing that of conventional inorganic materials, has placed them at the forefront of next-generation solar cell research, attracting significant attention from both academic and industry.

To harness their potential, we are investigating their charge transport properties using first-principles calculations (DFT) within the band transport regime. Our focus includes the calculation of carrier mobility, scattering rates and relaxation time through a detailed analysis of effective mass, deformation potential, and elastic properties. Our studies also incorporate the effects of structural deformations, aiming to align theoretical predictions with experimental results, providing deeper insights into the transport mechanisms in perovskites.

Furthermore, we are exploring the anisotropic nature of perovskites to understand directional dependencies in their electronic and mechanical properties. This anisotropy analysis is crucial for optimizing their performance and tailoring their application in advanced solar technologies. Together, these studies offer a comprehensive approach to enhancing the functionality of perovskites for cutting-edge solar energy solutions.

HL 45.5 Thu 10:30 H13

THz-Driven Phonon Fingerprints of Hidden Symmetry Breaking in 2D Layered Hybrid Perovskites — •Joanna M. Urban[1], Michael S. Spencer[1], Maximilian Frenzel[1], Gaëlle Trippé- Allard[2], Marie Cherasse[1,3], Charlotte Berrezueta Palacios[4], Olga Minakova[1], Luca Perfetti[3], Stephanie Reich[4], Martin Wolf[1], Emmanuelle Deleporte[2], and Sebastian F. Maehrlein[1,5,6] — [1]FHI Berlin — [2]LuMIn, Université Paris-Saclay, ENS Paris-Saclay, CentraleSupélec, CNRS — [3]LSI, CEA/DRF/IRAMIS, CNRS, École Polytechnique, Institut Polytechnique de Paris — [4]FU Berlin — [5]HZDR — [6]TU Dresden

Metal halide perovskites (MHPs) are emerging as promising candidates for spintronic applications. In MHPs which lack inversion symmetry, strong spin-orbit coupling induces the Rashba-Dresselhaus effect, allowing spin current control. Here we use intense THz fields to coherently drive lattice dynamics in Ruddlesden-Popper 2D layered perovskites. We identify simultaneous IR and Raman activity of specific inorganic cage modes, suggesting the presence of inversion symmetry breaking despite the globally centrosymmetric crystal structure. By exploring the driving pathways of coherent phonons bearing the signatures of broken inversion symmetry, we lay the groundwork for simultaneous ultrafast control of optoelectronic and spintronic properties in 2D MHPs.

HL 45.6 Thu 10:45 H13

Analysis of real-space transport channels in halide perovskites — •Frederik Vonhoff[1], Maximilian J. Schilcher[1], David R. Reichman[2], and David A. Egger[1] — [1]Physics Department, TUM School of Natural Sciences, Technical University of Munich, James-Franck-Straße 1, 85748 Garching, Germany — [2]Department of Chemistry, Columbia University, New York, NY 10027, USA

The charge carrier transport is a crucial factor for the performance of halide perovskites as solar energy conversion material. However, standard semiconductor transport theories fail to model the transport properties of halide perovskites because of their unusual transport behavior triggered by the anharmonic nuclear dynamics and its dynamic disorder [1]. For an accurate prediction of electron and hole mobilities of MAPbI$_3$ and MAPbBr$_3$, we capture the anharmonicity with molecular dynamics trajectories as a backbone for a time-dependent real-space hopping model [2,3] parametrized with hybrid density functional theory. With our transport model, we trace back the transport behavior of MAPbI$_3$ and MAPbBr$_3$ to their band structures via the projected density of states and the dynamics in the orbital occupation configurations. The real-space nature of our model allows us to determine the microscopic transport mechanisms which are driven by three transport channels.

[1] M. J. Schilcher et al, ACS Energy Lett. 6, 2162 (2021)
[2] M. Z. Mayers et al, Nano Lett. 18, 8041 (2018)
[3] M. J. Schilcher et al, Phys. Rev. Mater. 7, L081601 (2023)

15 min. break

HL 45.7 Thu 11:15 H13

Unravelling how solvated PbI$_2$ Crystallites precede the Crystallization of Lead Halide Perovskites by UV/VIS In-Situ measurements — •Maximilian Spies[1], Simon Biberger[1], Fabian Eller[2], Eva M. Herzig[2], and Anna Köhler[1] — [1]Soft Matter Optoelectronics, University of Bayreuth, Bayreuth, Germany — [2]Dynamics and Structure Formation, University of Bayreuth, Bayreuth, Germany

The fabrication of reproducible, high-quality lead iodide perovskite films via solution-based methods requires a comprehensive understanding of crystallization dynamics. The formation of perovskite films is primarily dictated by the composition of the precursor solution and its processing conditions. In this study, we present an in-situ absorption study, i.e. during spin-coating, of the critical pre-nucleation stage to unravel the formation mechanisms of lead iodide perovskite films. We tracked the evolution of iodoplumbate complexes within the precursor solution and identified a distinctive absorption feature at 3.15 eV, emerging prior to film formation. We attribute this feature to the development of a crystalline PbI$_2$-DMF solvated (PDS) phase. In particular, we propose that PDS crystallites serve as precursors to the crystalline perovskite phase, acting as nucleation sites within the precursor solution. Notably, the amount of this PDS phase correlates closely with the concentration of the solution layer during spin coating, suggesting that increasing concentration promotes PDS formation. These findings provide valuable insights into the early stages of perovskite crystallization.

HL 45.8 Thu 11:30 H13

Effect of a 2D/3D Heterostructure on Contact Formation of the Double Perovskite Cs$_2$AgBiBr$_6$ with Hole Transport Layers Revealed by In-Situ KPFM Growth Studies — •Tim P. Schneider and Derck Schlettwein — Justus-Liebig-Universität Gießen, Institut für Angewandte Physik, Heinrich-Buff-Ring 16, D-35392 Gießen

The application of a 2D perovskite interlayer caused by surface modification with organic amines between the absorber and contact layers is widely known to significantly improve the performance of perovskite solar cells. This has already been approved as well for the lead-free double perovskite absorber Cs$_2$AgBiBr$_6$. To better understand the interaction of the contact layer with the 2D/3D heterostructure, in this work, film growth of Copper Phthalocyanine (CuPc), used as a model hole conductor, onto Cs$_2$AgBiBr$_6$ modified by different 2D phases was investigated and compared to bare Cs$_2$AgBiBr$_6$. Employing solar cell geometry, the morphology and work function were inspected intermittently to the evaporation of CuPc by Kelvin Probe Force Microscopy at different average film thickness. The energy alignment was revealed to be more confined on the 2D/3D heterostructures and the growth of CuPc was improved: a more homogenous growth led to formation of closed films even at early stages of deposition. These changes in growth and energy alignment are accompanied by preferential formation of different crystal phases in the CuPc.

HL 45.9 Thu 11:45 H13

The influence of oxygen and water on MAPbI$_3$ absorber materials measured with in-situ TRPL and PES — •P. Stötzner[1], M. Müller[1], T. Schulz[1], P. Pistor[2], R. Scheer[1], and S. Förster[1] — [1]Martin-Luther-Universität Halle-Wittenberg, Germany — [2]Universidad Pablo de Olavide Sevilla, Spain

Methylammonium lead halide perovskites (MAPbI$_3$) are promising thin-film solar cell absorber materials, but their response to environmental conditions like moisture and oxygen is not well understood. Here, we present a combined photoelectron spectroscopy (PES) and in-situ time-resolved photoluminescence (TRPL) study conducted in one ultrahigh vacuum system, which allows for studying changes in the chemical composition, the electronic structure and charge carrier lifetime. The setup is completed by a high-pressure gas cell enabling for controlled exposure to specific environments.

For MAPbI$_3$, we observe a significant reduction of the charge carrier lifetime compared to ex-situ TRPL measurements. To bridge between the different measurement environments, we conducted additional TRPL measurements in a closed cell having the as-grown sample in nitrogen atmosphere, which is pumped to high vacuum. These results show a decreased lifetime in vacuum but an increased lifetime linked to air contact. Consequently, we exposed MAPbI$_3$ samples to water vapor to mimic air contact, resulting in increased lifetime but also in a decomposition of MAPbI$_3$. Pure oxygen exposure did not affect the lifetime. Surprisingly, the simultaneous exposure to both gases did not show the detrimental effect of water.

HL 45.10 Thu 12:00 H13

On the Nature of Light Induced Defects in MAPI Thin Films: Long Pulses in TrPL — •Maxim Simmonds and Eva Unger — Kekuléstraße 5, 12489 Berlin, Germany

Metal-halide perovskite (MHP) semiconductors are highly relevant candidates for the fabrication of next generation solar cells but suffer from instability under continuous irradiation. This has been shown with a non-constant steady state PL during illumination. In order to better understand the evolution of recombination mechanisms at play, we usetime resolved photoluminescence (trPL) and differential lifetime plots.

Therefore, in this presentation, we will focus on methylammonium-lead-iodide (MAPI) thin films and the (ir)reversible introduction of traps triggered by quasi-continuous illumination. For this, we develop a method that uses long pulses of light in combination with trPL counting schemes, calling it long pulsed trPL (LP-trPL). From the method, we observe the inclusion of long lived and non-deep trapping sites due to continuous illumination. The data also suggests a highly asymmetric mechanism of trap formation, where trap annihilation is much slower than observed formation. We conclude that previously described mechanisms of iodine outgassing is compatible with the observed shallow nature of traps introduced as well as the asymmetric process of formation/annihilation.

HL 45.11 Thu 12:15 H13

Phase evolution of sequential evaporated (FA/Cs)SnI$_3$ halide perovskite thin films via in situ X-ray diffraction — •Pu-Chou Lin[1], Josha Damm[1], Roland Scheer[1], and Paul Pistor[2] — [1]Institute of Physics, Photovoltaics Group, Martin-Luther-University, 06120 Halle, Germany — [2]Departamento de Sistemas Físicas, Universidad Pablo de Olavide, 41013 Sevilla, Spain

Tin-based halide perovskites, particularly FASnI$_3$ and CsSnI$_3$, offer promising potential for photovoltaic applications. This study employs in situ X-ray diffraction to investigate these materials' real-time growth mechanisms and thermal stability during sequential vapor deposition and annealing. Our results demonstrate that the deposition sequence significantly impacts the resulting perovskite film quality. For FASnI$_3$, the SnI$_2$-FAI stack yields superior, cavity-free films compared to the FAI-SnI$_2$ stack. This suggests that FAI is the primary diffusing species, with FASnI$_3$ forming at interfaces and completing its formation around 160°C. In contrast, the CsSnI$_3$ system exhibits more complex behavior. The SnI$_2$-CsI sequence leads to the formation of the intermediate phase Cs$_2$SnI$_6$, while the CsI-SnI$_2$ sequence directly forms CsSnI$_3$ with minimal defect formation. This suggests that SnI$_2$ is the dominant diffusing species in the Cs-based system. FASnI$_3$ and CsSnI$_3$ undergo thermal degradation at 200°C and 240°C, respectively, through co-desorption of their constituent elements. These findings provide valuable insights into tin-based perovskites' growth mechanisms and thermal stability, which can guide future efforts to improve their performance and long-term stability.

HL 45.12 Thu 12:30 H13

Determining the key parameters of 3C-SiC photoelectrodes for water splitting application — •Marius Wasem[1,2], Sebastian Benz[1,3], Philip Klement[1,2], Joachim Sann[1,3], Jürgen Janek[1,3], Sangam Chatterjee[1,2], and Matthias T. Elm[1,2,3] — [1]Center for Materials Research, Heinrich-Buff-Ring 16, 35392 Giessen — [2]Institute of Experimental Physics I, Heinrich-Buff-Ring 16, 35392 Giessen — [3]Institute of Physical Chemistry, Heinrich-Buff-Ring 17, 35392 Giessen

We investigated the photoelectrochemical properties of n- and p-doped

3C-SiC thin films on n- or p-doped Si substrates, respectively, in a phosphate buffer solution. Key parameters such as the flat band potential and open-circuit potential were determined using various electrochemical methods. The combination of ultraviolet photoelectron spectroscopy and low energy inverse photoelectron spectroscopy measurements yields the estimation of the positions of the Fermi level, as well as the positions of the valence and conduction bands of the differently doped 3C-SiC thin films. Impedance spectroscopy characterized the interfacial processes in more detail. The flat band potential was derived from the space-charge layer capacitance using Mott-Schottky analysis. The determination of these key parameters enabled the construction of an energy level diagram, which explains the electrochemical behavior of n- and p-type 3C-SiC thin films under both dark conditions and illumination.

HL 45.13 Thu 12:45 H13

Circular Dichroism Engineering via Bismuth Doping and Cation Substitution in 2D Lead-Halide Perovskites — •Jan-Heinrich Littmann[1], Keito Mizukami[1,2], Henrik Spielvogel[1], Philip Klement[1], Satoko Fukumori[2], Hirokazu Tada[2], and Sangam Chatterjee[1] — [1]Institute of Experimental Physics I and Center for Materials Research (ZfM), Justus Liebig University Giessen, Giessen, Germany — [2]Graduate School of Engineering Science, Osaka University, Japan

Hybrid lead halide perovskites have garnered significant attention for their remarkable semiconductor properties. Their building blocks allows for tuneable features such as the crystal structure and the electronic bandgap. Introducing chiral cations into these materials endows them with chiroptical properties, such as circularly polarized luminescence (CPL) and spin-polarized charge transport, promising applications in optoelectronics and spintronics. However, the mechanism of chirality transfer remains poorly understood due to complex structure-property relationships. This study delves into the impact of heterovalent Bi^{3+} doping on the genuine circular dichroism (CD) of 2D lead iodide perovskites incorporating methylbenzylamine (MBA) and (pyridyl)ethylamine (PyEA) cations. Bi^{3+} doping, while preserving the band gap, significantly influences the genuine CD, suggesting a doping-dependent chirality transfer mechanism. Our findings provide valuable insights into the structure-property relationships in chiral perovskites and pave the way for the rational design of advanced chiroptical materials.