HL 45: Perovskite and Photovoltaics: Spectroscopy

Time: Thursday 15:00–17:15 Location: POT/0006

HL 45.1 Thu 15:00 POT/0006

The influence of air and light exposure on alkali-metal doped Cu(In,Ga)Se_2 absorber materials measured with in-situ TRPL and XPS — •P. Stötzner, S. Sobisch, A. Stauffenberg, H. Kempa, R. Scheer, and S. Förster — Martin-Luther-Universität Halle-Wittenberg, Germany

Copper indium gallium diselenide (Cu(In,Ga)Se_2/CIGSe) is a promising thin-film solar cell absorber. Alkali-metal doping, especially in combination with heavy alkali metals, enhances solar cell efficiencies. However, air and light exposure (ALE) of the absorber reduces the solar cell efficiency. This is a result of the diffusion of sodium and oxygen toward the absorber surface, which is accompanied by a degradation of the charge-carrier lifetime of doped CIGSe absorbers [1,2].
Here, we study the ALE effect for CIGSe doped with K and cominations of Na and K as well as Na and Rb. Our studies combine X-ray photoelectron spectroscopy (XPS) and in-situ time-resolved photoluminescence (TRPL) conducted in one ultrahigh vacuum system, addressing changes in the chemical composition and charge-carrier lifetime. The setup is completed by a high-pressure gas cell enabling for controlled exposure to specific environments.
We find that the charge-carrier lifetime of non-doped absorbers is unaffected by ALE and all alkali-metal doped absorbers degrade due to ALE. XPS shows that the most heaviest alkali metal present and oxygen are accumulated at the surface. While this effect is reversable over time, the degradation of the charge-carrier lifetime is permanent.
[1] DOI: 10.1063/1.4992116 [2] DOI: 10.1002/pip.3041

HL 45.2 Thu 15:15 POT/0006

Thermal Broadening Statistics of Photoluminescence in Tunable Lead Halide Perovskite Nanocrystals — •Luca B. Reim, Leo Luber, and Alexander S. Urban — Nanospectroscopy Group, Nano-Institute Munich, Department of Physics, Ludwig-Maximilians-Universität München, Königinstraße 10, 80539 Munich

Halide perovskite nanocrystals (NCs) exhibit excellent optoelectronic properties, including high quantum yields and composition-dependent, narrow photoluminescence (PL) that critically depend on control over NC size and uniformity. Understanding the mechanisms governing PL linewidths is therefore essential for evaluating material quality and device performance.

We synthesized size-tunable $CsPbBr_3$ nanocubes under ambient conditions using machine-learning-optimized reaction protocols.[1] The NCs were drop-cast onto substrates and investigated via temperature-dependent PL spectroscopy in a closed-cycle cryostat from 9-300 K. To quantitatively analyze the spectral evolution, we applied a novel fitting approach that enables the extraction of size dispersion, temperature-dependent exciton populations, and signatures of the local energetic environment. The latter is strongly influenced by nanocrystal quality and ligand coverage and provides a sensitive probe of inhomogeneous broadening mechanisms.

These results offer detailed insight into the fundamental limits of emission linewidths in perovskite NCs and support the targeted optimization of materials for optoelectronic applications such as LEDs.

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

HL 45.3 Thu 15:30 POT/0006

Investigation on the efficiency limiting processes of 3C-SiC photoelectrodes using intensity modulated techniques. — •Marius Wasem[1,2], Mario F. Zscherp[1,2], Silas A. Jentsch[1,2], Jörg Schörmann[1,2], Sangam Chatterjee[1,2], and Matthias T. Elm[1,2] — [1]Center for Materials Research, Heinrich-Buff-Ring 16, 35392 Giessen — [2]Institute of Experimental Physics I, Heinrich-Buff-Ring 16, 35392 Giessen

Cubic silicon carbide (3C-SiC) is a compelling photoelectrode for photoelectrochemical water splitting due to its near-ideal band gap energy and excellent chemical stability. Here, we present the characterization of the photoelectrochemical response of epitaxially grown n- and p-type 3C-SiC using different electrochemical methods. A pH neutral phosphate buffer solution was used as electrolyte. The suitable operating conditions, such as potential range and light intensity, were determined using chopped light voltammetry. Insights of the charge carrier dynamics were gained by combining electrochemical impedance spectroscopy (EIS), intensity-modulated photocurrent spectroscopy (IMPS) and intensity-modulated photovoltage spectroscopy (IMVS). While EIS is a common and widely used method, the latter two methods are rarely discussed in the photoelectrochemical community. Here we show how a combination of all three methods enables the differentiation and quantification of key processes (recombination processes, surface effects, charge carrier lifetime) to validate the efficiency of 3C-SiC photoelectrodes.

HL 45.4 Thu 15:45 POT/0006

Nano-sensing of AC-Fields with Perovskite Quantum Dots and Electro-Switching of Luminescence — •Emanuel Eckl[1], Fabian Brütting[1], Moritz B. Heindl[1], Maryna Bodnarchuk[2], Mariia Svyrydenko[2], Maksym Kovalenko[2], and Georg Herink[1] — [1]University of Bayreuth, Bayreuth, Germany — [2]ETH Zürich, Zürich, Switzerland

Perovskite quantum dots (PQDs) currently attract significant research interest, particularly owing to their broad tunability of optoelectronic properties with applications in energy conversion, solid-state lighting and sensing technologies.

In this study, we investigate the potential of PQDs as nano-sensors for transient electric fields up to multi-Terahertz (THz) frequencies [1]. Combining electro-absorption, lifetime and photoluminescence measurements of inorganic and hybrid lead-halide PQDs, we demonstrate a massive electro-switching effect observed via luminescence. The emission modulation is directly correlated with reduced photoluminescence lifetimes and can be attributed to a switching of radiative quantum efficiency. Furthermore, we present evidence for a memory effect that exhibits significantly delayed responses in comparison to the well-understood quasi-instantaneous Quantum-Confined Stark Effect that is also observable in these PQDs. In particular, the Stark effect is utilized for the purpose of validating and comparing our measurements to those of conventional inorganic CdSe QDs, previously employed in ultrafast imaging of THz near-fields.

[1] M.B. Heindl, et al., Light Sci Appl 11, 5 (2022).

15 min. break

HL 45.5 Thu 16:15 POT/0006

Resolving Ultrafast Conductivity Dynamics in 2D-Perovskites via correlative THz-NIR Spectroscopy — •Lion Krüger[1], Fabian Brütting[1], Michael Baumann[2], Moritz B. Heindl[1], Maximilian Spies[3], Anna Köhler[3], Alexander JC Kühne[2], and Georg Herink[1] — [1]Experimental Physics VIII, University of Bayreuth, Germany — [2]Institute of Organic and Macromolecular Chemistry, Ulm University, Germany — [3]Experimental Physics II, University of Bayreuth, Germany

Quasi-2D Metal-Halide Perovskites offer flexible tuning of optoelectronic properties via composition and quantum confinement.

In this contribution we present measurements of the ultrafast carrier dynamics and mobilities of 3D- and quasi-2D-methylammonium lead iodide (MAPI) using optical-pump terahertz-probe spectroscopy (OPTP). The comparison with corresponding optical transient absorption measurements allows for the extraction of an ultrafast feature on a picosecond timescale that is correlated with the delayed hot-carrier cooling, known from 3D hybrid perovskites. Here this "hot phonon bottleneck" manifests as a 2D-specific, intensity-dependent signature in the THz-conductivity and is attributed to transient exciton formation [1].

[1] Lion Krüger, Fabian Brütting, Michael Baumann, Moritz B. Heindl, Maximilian Spies, Anna Köhler, Alexander JC Kühne, Georg Herink. "Confinement-induced Ultrafast Conductivity in 2D Perovskites resolved by correlative Terahertz-NIR Spectroscopy". 2025. In review.

HL 45.6 Thu 16:30 POT/0006

Intra- and Interlayer Excitonic Finestructure of $(PEA)_2PbI_4$ — •Patrick Grenzer[1], Fabian Lie[2], Klaus H. Eckstein[1], Linn Leppert[2], and Tobias Hertel[1] — [1]Institute of Physical and Theoretical Chemistry, Julius-Maximilians-University Würzburg, Germany — [2]MESA+ Institute for Nanotechnology, University of Twente, Enschede, The Netherlands

Layered halide perovskites exhibit strongly bound excitons shaped

by reduced dimensionality, dielectric confinement, and significant spinorbit coupling. Despite extensive work, the origin of the multiple resonances in absorption and PL of $(PEA)_2PbI_4$ remains subject to debate. We investigate the excitonic fine structure in high-quality, mechanically exfoliated single crystals by combining temperature- and polarization-resolved photoluminescence with first-principles GW+BSE calculations. The polarization dependence unambiguously assigns the observed features to distinct excitonic states and resolves the contributions from exchange interactions, crystal symmetry, and interlayer coupling. We further identify and spectroscopically separate intra- and interlayer excitons and their respective transition dipole moments. The results provide a consistent microscopic picture of the exciton manifold in $(PEA)_2PbI_4$ and clarify the origins of the multi-line structure characteristic of this material class.

HL 45.7 Thu 16:45 POT/0006

Dynamic Screening Effects on Auger Recombination in Metal-Halide Perovskites from First Principles — •Utkarsh Singh — Theoretical Physics Division, IFM, Linköping University, Sweden

Auger recombination is the dominant nonradiative loss in perovskite LEDs and nanolasers at carrier densities $> 10^{17}\,\mathrm{cm}^{-3}$.[1,2] Conventional first-principles treatments[3] use static dielectric screening $W(\mathbf{q}, 0)$ and neglect its frequency dependence in polar iodide perovskites.

I present a framework that incorporates the frequency-dependent screened interaction $W_{00}(\mathbf{q}, \omega)$, computed from low-scaling GW, into direct and phonon-assisted Auger amplitudes.[4] For γ-$CsPbI_3$ and γ-$CsSnI_3$, dynamic screening enhances the dielectric response at optical energies and reduces the room-temperature Auger coefficient by 50–60% compared with the static approximation.[5] The critical crossover density is shifted by a factor of 2, with implications for efficiency roll-off and lasing thresholds in optoelectronic devices.

These results establish dynamic screening as a quantitative determinant of Auger losses in polar semiconductors and provide a transferable framework for device modeling.

[1] J. Qin *et al.*, *Trends Chem.* **3** (2021). [2] Y. Sun *et al.*, *Appl. Phys. Rev.* **11** (2024). [3] E. Kioupakis *et al.*, *Phys. Rev. B* **92** (2015). [4] F. Yuan *et al.*, *Nat. Photonics* **18** (2024). [5] U. Singh & S. I. Simak, in preparation (2025).

HL 45.8 Thu 17:00 POT/0006

Influence of static disorder on the low temperature photoexcitation dynamics in triple cation lead halide perovskites — •Alexander Schauerte[1], Anton Krüger[1], Isabel Allegro[2], Dominik Muth[1], Ian Howard[2], Uli Lemmer[2], and Marina Gerhard[1] — [1]Department of Physics and Marburg Centre for Quantum Materials and Sustainable Technologies, Hans-Meerwein-Str. 4, Philipps-Universität Marburg, 35032 Marburg, Germany — [2]Light Technology Institute, Karlsruhe Institute of Technology, Kaiserstraße 12, 76131 Karlsruhe, Germany

We study the recombination dynamics of phase stable triple cation lead halide perovskites $Cs_{0.1}(MA_{0.17}FA_{0.83})_{0.9}Pb_{1-x}(I_{0.84}Br_{0.16})_{3-2x}$ with intentionally induced deficiencies of Pb over a broad temperature range using time-resolved photoluminescence (PL) spectroscopy. In the temperature range below 70 K, we find pronounced sub-nanosecond PL dynamics which are accompanied by an increase of the carrier diffusivity by more than one order of magnitude. The findings are attributed to the polaronic Mott transition, beyond which polaron radii overlap, leading to efficient transport and bimolecular recombination. Moreover, the observed energy dependent PL dynamics at low temperatures indicate the presence of a phonon bottleneck, which inhibits efficient cooling of the excited population. We find that a higher degree of static disorder slows down bimolecular recombination, while the phonon bottleneck effect is more pronounced, potentially because slower recombination does not effectively reduce the hot carrier population.