

## HL 18: Perovskite and Hybrid Photovoltaics

Time: Tuesday 9:30–12:45

Location: EW 203

HL 18.1 Tue 9:30 EW 203

**Temperature-Dependent Electroabsorption Spectroscopy on Organic-Inorganic Perovskite Solar Cells** — ●FABIAN RUF<sup>1</sup>, ALICE MAGIN<sup>1</sup>, MORITZ SCHULTES<sup>2</sup>, ERIK AHLWEDE<sup>2</sup>, HEINZ KALT<sup>1</sup>, and MICHAEL HETTERICH<sup>3</sup> — <sup>1</sup>Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — <sup>2</sup>Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg (ZSW), 70563 Stuttgart, Germany — <sup>3</sup>Light Technology Institute, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany

Organic-inorganic halide perovskites have demonstrated their potential as promising candidates for efficient, low-cost solar cells with power-conversion efficiencies surpassing established technologies such as amorphous silicon. However, despite the strong progress made, many fundamental material properties are not yet well understood. We investigate the nature of the optical transition in solution-processed perovskite solar cells utilizing temperature-dependent electroabsorption (EA) spectroscopy. The resulting EA spectra are suitable for a precise determination of the energetic position of optical transitions in the band structure. These results can be correlated with generalized Elliott fits of standard absorption spectra to investigate the nature of the observed resonances. Additional lineshape analysis of the spectra supports the conclusion of an excitonic nature of the resonances. Nevertheless, efficient charge-separation is possible in these devices which is reflected by power-conversion efficiencies up to 11.5 % (stabilized).

HL 18.2 Tue 9:45 EW 203

**Active Materials and interfaces for stable perovskite solar cells** — ●ANTONIO ABATE — Helmholtz-Zentrum Berlin für Materialien und Energie GmbH

Halide perovskites are quickly overrunning research activities in new materials for cost-effective and high-efficiency photovoltaic technologies. Since the first demonstration from Kojima and co-workers in 2009, several perovskite-based solar cells have been reported and certified with rapidly improving power conversion efficiency. Recent reports demonstrate that perovskites can compete with the most efficient inorganic materials, while they still allow processing from solution as a potential advantage to deliver a cost-effective solar technology. Compare to the impressive progress in power conversion efficiency, stability studies are rather weak and often controversial. An intrinsic complication comes from the fact that the stability of perovskite solar cells is strongly affected by any small difference in the device architecture, preparation procedure, materials composition and testing procedure. In the present talk, we will focus on the stability of perovskite solar cells in working condition. We will discuss a measuring protocol to extract reliable and reproducible ageing data. We will present new materials and preparation procedures, which improve the device lifetime without giving up on high power conversion efficiency.

HL 18.3 Tue 10:00 EW 203

**Ultrafast dynamics in quadrupole cationmixed halide perovskites** — ●KESTUTIS BUDZINAUSKAS<sup>1</sup>, ELINA PATSIKATHEODOROU<sup>1</sup>, SENOL OEZ<sup>2</sup>, SANJAY MATHUR<sup>2</sup>, and PAUL H.M. VAN LOOSDRECHT<sup>1</sup> — <sup>1</sup>II physikalisches Institut, Zuelpicher 77, Köln — <sup>2</sup>Institut für Anorganische Chemie, Greinstr. 6, Köln

Hybrid perovskites are currently one of the most promising classes of materials for alternative solar cell technologies. Apart from the high power conversion efficiency which can be reached with these materials, one can also easily tune their optoelectronic properties by chemical substitutions. The quadrupole cation mixed halide perovskite  $\text{Gu}_{1.4}\text{Cs}_{4.3}\text{MA}_{13.2}\text{FA}_{72.9}\text{Pb}(\text{I}_{1-x}\text{Br}_x)_3$  is stable at room temperature and allows tuning of the optical absorption spectrum via the Br:I ratio. Nevertheless little is known about the initial steps of the charge generation process. To obtain a better insight in the charge generation and exciton dynamics in this material we performed transient absorption spectroscopy experiments. Our pump-probe experiments show a pronounced pump energy dependence of the response near the optical band-gap. These results are discussed in terms of exciton diffusion and local structural variations

HL 18.4 Tue 10:15 EW 203

**Scalable, uniform coevaporated formamidinium lead triiodide**

**thin-films for photovoltaics** — ●JULIANE BORCHERT, REBECCA L. MILOT, JAY B. PATEL, CHRISTOPHER L. DAVIES, ADAM D. WRIGHT, LAURA MARTÍNEZ MAESTRO, HENRY J. SNAITH, LAURA M. HERZ, and MICHAEL B. JOHNSTON — Clarendon Laboratory, Department of Physics, University of Oxford, Parks Road, OX1 3PU, United Kingdom

A rapid rise in solar cell efficiencies and bandgap tunability over much of the visible spectrum have made perovskite materials the focus of intense research. Initially,  $\text{MAPbI}_3$  was the most commonly investigated material, however recently, a variety of other materials have been developed by substituting the organic cation in the perovskite structure. In particular, perovskites containing formamidinium (FA) and cesium as well as mixed cations have shown promise. With mixed cation perovskites high efficiencies and also stability improvements have been achieved [1]. Coevaporation is an advantageous deposition technique for perovskite thin-films allowing for the deposition of smooth, pinhole free, uniform films over a large area [2]. Currently, only a small number of perovskite materials have been realized using this technique. We present a study showing that coevaporation can be used to deposit  $\text{FAPbI}_3$ . We fabricated solar cells with efficiencies of up to 15%. The material exhibited high charge carrier mobilities and excellent optical properties [3]. This is an important step towards the fabrication of evaporated, stable, mixed cation perovskite thin-films.

[1] S.N. Habisreutinger et al., *APL Mater.* 2016, 4 [2] M. Liu et al., *Nature* 2013, 501 [3] J. Borchert et al., *ACS Energy Lett* 2017, 2

HL 18.5 Tue 10:30 EW 203

**Cation substitution reduces non-radiative bimolecular losses in hybrid lead-halide perovskites** — ●SASCHA FELDMANN, JASMINE P. H. RIVETT, TUDOR H. THOMAS, MICHAEL SALIBA, and FELIX DESCHLER — University of Cambridge, JJ Thomson Avenue, CB3 0HE Cambridge, UK

Tailored monovalent cation substitution in mixed-cation hybrid perovskites enables solar cell efficiencies beyond 20% and enhanced stability. Here, we use transient absorption and photoluminescence spectroscopy to study the effect of cation substitution on the carrier recombination dynamics in  $\text{Rbx}(\text{Csy}(\text{MAzFA}1-z)1-y)1-x\text{Pb}(\text{IO.83Br0.17})_3$  (MA=methylammonium, FA=formamidinium) hybrid perovskite thin-films. We perform a detailed analysis of the recombination dynamics, from which we separate radiative and non-radiative recombination pathways. We find that careful tuning of the cation composition leads to a reduction in trap-assisted non-radiative recombination channels, which supports enhanced lifetimes and high luminescence yields. Unexpectedly, we further observe the reduction of a non-radiative bimolecular recombination channel, particularly upon inclusion of formamidinium. Using Raman and X-ray diffraction techniques, we study the effect of cation substitution on lattice order. We find that formamidinium inclusion, aided through the presence of Rb and Cs during fabrication, leads to a reduction of the tetragonal distortion, and an increased rigidity of the lattice. We attribute the enhanced luminescence yields to reduced defect formation through carrier trapping due to the reduced lattice disorder.

HL 18.6 Tue 10:45 EW 203

**Circular structured Distributed Feedback Laser in Br based organic-anorganic perovskite** — ●MATTHÄUS JÄCKLE<sup>1</sup>, HEIKO LINNENBANK<sup>1</sup>, MICHAEL SALIBA<sup>2</sup>, MARIO HENTSCHEL<sup>1</sup>, MICHAEL GRÄTZEL<sup>2</sup>, and HARALD GIESSEN<sup>1</sup> — <sup>1</sup>4th Physics Institute, University of Stuttgart — <sup>2</sup>Laboratory of Photonics and Interfaces, École polytechnique fédérale de Lausanne

Organic-anorganic perovskites are direct semiconductors which are emerging as a new type of solution-processable semiconductors for optoelectronic applications. One particular interesting characteristic is that the bandgap can be tuned over the whole visible spectrum by using different halides. Most of the present research on perovskites is aimed at their usage as solar cells because of their high absorption rate and favorable material properties. However, recent scientific publications also employ these materials for light-emitting applications such as LEDs or Lasers. Based on the intense research in the solar cell community, lasing from Iodide containing perovskites has been recently presented. As this material is designed to absorb at visible wavelengths it will emit light at red or infrared wavelengths. In this work we will in

contrast present stimulated emission of radiation from Bromide based structures, which radiate in the green part of the visible spectrum. We will demonstrate a circular distributed feedback (2D-DFB) laser, based on a lithographic structuring of the supporting substrate. This allows us to make use of the solution-processability of the perovskite as active material, as well as achieving a higher confinement compared to previously presented 1D-DFB structures.

HL 18.7 Tue 11:00 EW 203

**First-principles-based modeling of atomic processes in hybrid perovskites** — ●JINGRUI LI<sup>1</sup>, JARI JÄRVI<sup>1,2</sup>, MARIANA ROSSI<sup>3</sup>, and PATRICK RINKE<sup>1</sup> — <sup>1</sup>Department of Applied Physics, Aalto University, Finland — <sup>2</sup>Department of Physics, University of Helsinki, Finland — <sup>3</sup>Fritz Haber Institute of the Max Planck Society, Theory Department, Berlin, Germany

To further advance hybrid-perovskite-based photovoltaic technology, we need to understand these materials on the atomic scale, on which the light-to-energy conversion and transport processes occur. Currently, this atomic scale is riddled with controversies. For the detachment of methylammonium (MA) cations from the  $\text{PbI}_3$  cage in  $\text{MAPbI}_3$ , very low ( $\sim 10$  meV) as well as high ( $\sim 100$  meV) activation energies  $E_a$  have been reported. Quasi-elastic neutron scattering measurements (QENS) for the orthorhombic phase found  $E_a = 48$  meV, which was attributed to the axial rotation of the whole MA cation [1]. To shed light on this controversy, we performed density-functional theory calculations (PBE0 functional + van der Waals corrections + inclusion of nuclear quantum effects) for several rotational MA processes. For the rotation of  $\text{CH}_3$  against the  $\text{NH}_3$  unit which remains bound to the  $\text{PbI}_3$  cage, we obtain  $E_a = 42$  meV in good agreement with the QENS result. We therefore ascribe this barrier to this torsional motion. For the full axial rotation, which breaks three hydrogen bonds, we obtain a barrier of  $\sim 130$  meV which is much higher than the QENS results.

[1] Chen *et al.*, *Phys. Chem. Chem. Phys.* **17** 31278 (2015).

15 min. break.

HL 18.8 Tue 11:30 EW 203

**Light and Temperature Modulated Magneto-Transport in hybrid Lead Halide Perovskites** — ●MASOUMEH KESHAVARZ<sup>1</sup>, STEFFEN WIEDMANN<sup>2</sup>, HAIFENG YUAN<sup>1</sup>, ELKE DEBROYE<sup>1</sup>, MAARTEN ROEFAERS<sup>3</sup>, and JOHAN HOFKENS<sup>1</sup> — <sup>1</sup>Molecular Imaging and Photonics, Department of Chemistry, KU Leuven, 3001 Leuven, Be — <sup>2</sup>High Field Magnet Laboratory, Radboud University, 6525 ED Nijmegen, NI — <sup>3</sup>Department of Molecular and Microbial Systems, KU Leuven, 3001 Heverlee, Be

Hybrid lead-halide perovskites exhibit exceptional properties such as high carrier mobility and long diffusion lengths providing a variety of applications as the absorbing layer in solar cells, LEDs and photodetectors. In spite of their rapid evolution in devices, knowledge of the nature and microscopic origin of the intrinsic optical, electrical and structural properties is only just emerging. Using temperature-dependent magneto-transport and Hall measurements on single crystals of  $\text{MAPbI}_3$  and  $\text{MAPbBr}_3$  in magnetic fields up to 30 T, we have identified different transport regimes [1]. For temperatures up to 25 K, transport is determined by thermally-activated hopping of charge carriers reflected in a diverging zero-field resistance. Above 25 K, acoustic phonon scattering is the dominant charge transport evident in the temperature dependence of both zero and high-field resistance. Our findings shed new light on the fundamental charge carrier dynamics under steady-state illumination and emphasize the need for a comprehensive theoretical model for perovskite based devices. [1] M Keshavarz, *et al.*, *ACS Energy Lett.* **2018**, *3*, 39-45.

HL 18.9 Tue 11:45 EW 203

**From the Very Beginning: Linking Photovoltaic Evolution and Crystal Formation by the Example of Perovskite Solar Cells** — ●VITA MERGNER<sup>1,2</sup>, LUKAS WAGNER<sup>1</sup>, SIMONE MASTROIANNI<sup>1</sup>, ULI WÜRFEL<sup>1</sup>, CARMEN SANCHEZ-VALLE<sup>2</sup>, and ANDREAS HINSCH<sup>1</sup> — <sup>1</sup>Fraunhofer Institute for Solar Energy Systems ISE, Heidenhofstraße 2, D-79110, Freiburg, Germany — <sup>2</sup>Institute for Mineralogy, Universität Münster, Corrensstraße 24, D-48149, Münster, Germany

We present an experimental approach, which, for the first time, allows an observation of the photovoltaic effect in semiconductor devices during crystallization. The examination is facilitated by a nano-porous

contact scaffold for the extraction of the charge carriers within which a precursor solution is infiltrated as the final processing step to form a methylammonium lead iodide absorber layer in the perovskite solar cell. With this approach, we were able to simultaneously relate radiative recombination and transport of the photo-excited charges to the perovskite formation process. [1] Thereby, the former perovskite crystallization model could be refined by providing the crystallization stages associated with the photovoltaic performance in real-time as well as microscopically resolved real-time imaging of the photoluminescence. The results provide deeper understanding in the evolution of crystal growth of the perovskites and electrical coupling to the contact material which are key parameters for an optimization of perovskite solar cells. [1] Wagner, Mundt *et al.* *Scientific Reports* (2017). DOI: 10.1038/s41598-017-13855-6

HL 18.10 Tue 12:00 EW 203

**Large scale compositional and electronic inhomogeneities in  $\text{MAPbI}_3$  perovskite films** — ●QING SUN<sup>1,2</sup> and YANA VANYZOF<sup>1,2</sup> — <sup>1</sup>Kirchhoff Institute für Physik, Universität Heidelberg — <sup>2</sup>Center for Advanced Material, Universität Heidelberg

Recently, hybrid organic-inorganic halide perovskites have gained significant attention in the field of thin film photovoltaics due to its rapid increase in power conversion efficiencies from 3.8% to around 22%. This tremendous progress is a result of the advantageous optoelectronic properties of perovskite materials and extensive research efforts dedicated to improving the layer microstructure and charge extraction layers. While significant amount of work had been performed to further improve the efficiency of the devices, much less attention has been focused on the large variations observed in the performance of identically prepared perovskite solar cells within single studies. Here, we perform macroscopic characterisation of the  $\text{CH}_3\text{NH}_3\text{PbI}_3$  films prepared by different methods and identify large scale inhomogeneities in the layer properties across each sample. After deposition of ETL and electrode and analyzing their current density-voltage curves, we are able to correlate the variation in PSCs performance to the inhomogeneities observed in the perovskite films.

HL 18.11 Tue 12:15 EW 203

**Exciton dynamics in quantum confined  $\text{CsPbBr}_3$  nanoplatelets** — ●MORITZ GRAMLICH, BERNHARD J. BOHN, YU TONG, LAKSHMINARAYANA POLAVARAPU, ALEXANDER S. URBAN, and JOCHEN FELDMANN — Chair for Photonics and Optoelectronics, Department of Physics, Ludwig-Maximilians-Universität, Munich, Germany

In contrast to bulk perovskite films, new reports have shown that in perovskite nanocrystals the excitonic absorption onset and photoluminescence (PL) peak exhibit a blue shift due to quantum confinement when their size in at least one dimension approaches the exciton Bohr radius of that material [1]. For decreasing thickness of organic-inorganic perovskite nanoplatelets – separated by centrifugation – increasing exciton binding energies and decreasing PL decay times have been observed [2]. Now a new method has been developed which enables the direct synthesis of quantum-confined inorganic  $\text{CsPbBr}_3$  nanoplatelets of uniform thickness. Here, transient absorption spectroscopy is applied to such nanoplatelets of different thickness varying from two to seven crystal layers to gain additional insight into confinement effects on fast charge carrier dynamics in these systems. A comparison to the results of organic-inorganic perovskite nanoplatelets is given to investigate the role of the A-site cation.

[1] J. A. Sichert, *et al.* *Nano letters* **2015**, *15*(10), 6521-6527. [2] V. A. Hintermayr, *et al.* *Advanced Materials* **2016**, *28*(43), 9478-9485.

HL 18.12 Tue 12:30 EW 203

**Effect of Varying the Density of Defects on the Properties of Organometallic Halide Perovskites** — ●PAUL FASSL<sup>1</sup>, VINCENT LAMI<sup>1</sup>, ALEXANDRA BAUSCH<sup>1</sup>, ZHIPING WANG<sup>2</sup>, HENRY SNAITH<sup>2</sup>, and YANA VAYNZOF<sup>1</sup> — <sup>1</sup>Kirchhoff-Institute for Physics, Heidelberg University — <sup>2</sup>Department of Physics, University of Oxford, UK

Organometallic halide perovskite solar cells have become a promising class of material with certified efficiencies up to 22.7 % to date. [1] However, reports investigating the fundamental mechanisms limiting the material and device stability remain scarce.

In our recent work we investigated the role of microstructure on the degradation rate of methylammonium lead triiodide ( $\text{MAPbI}_3$ ) perovskite films upon exposure to light and oxygen, however the role of the density of defects remains unknown. [2] In this work we therefore vary the density of defects in the films while keeping the microstructure

unchanged. We characterize the perovskite films using photoemission spectroscopy, x-ray diffraction, photoluminescence and photothermal deflection spectroscopy and correlate the findings to the photovoltaic parameters and stability of complete devices.

[1] Research Cell Efficiency Records: [https://www.nrel.gov/pv/assets/images/efficiency-](https://www.nrel.gov/pv/assets/images/efficiency-chart.png)

[chart.png](#) (accessed: December 2017)

[2] Q. Sun, P. Fassel, D. Becker-Koch, A. Bausch, B. Rivkin, S. Bai, P. E. Hopkinson, H. J. Snaith, Y. Vaynzof, *Adv. Energy Mater.* 2017, 7, 1700977.