

## DS 5: Fundamentals of Perovskite Photovoltaics I (jointly with CPP)

Time: Monday 10:15–13:00

Location: ZEU 222

**Invited Talk**

DS 5.1 Mon 10:15 ZEU 222

**The Versatility of Mesoscopic Solar Cells** — ●ANDERS HAGFELDT — Laboratory of Photomolecular Science, Swiss Federal Institute of Technology Lausanne (EPFL), CH-1015, Lausanne, Switzerland

In our work on solid-state dye-sensitized solar cells (ssDSSC) we have recently [1] shown that copper phenanthroline complexes can act as an efficient hole transporting material, achieving power conversion efficiencies of more than 11%.

In our work on perovskite solar cells (PSC) we have achieved efficiencies above 20% with a mixed composition of iodide/bromide and methyl ammonium/formamidinium. With the use of SnO<sub>2</sub> compact underlayers as electron acceptor contacts we have constructed planar perovskite solar cells with a hysteresis free efficiency above 20% [2]. We have taken the cation mixing of the perovskite film further by including Cs<sup>+</sup> and Rb<sup>+</sup>. Larger grains grown in a monolithic manner are observed and for example reproducibility and device stability are improved [3]. At the meeting we will discuss our champion data; up to 22% efficiency with an external electroluminescence of 4%, and an outstanding open-circuit voltage of 1.24 V at a band gap of 1.63 eV. Furthermore, we will report a breakthrough in stability at 85 °C for 500 h under full solar illumination.

References [1]\*Freitag et al., *Energy & Envir. Sci.*, DOI:10.1039/C5EE1204J [2]\*Correa et al., *Energy & Envir. Sci.*, DOI:10.1039/C5EE02608C [3]\*M. Saliba et al., *Science* 10.1126/science.aah5557 (2016)

DS 5.2 Mon 10:45 ZEU 222

**Impact of Preparation Conditions on Properties of Perovskite Thin Films** — ●ALEXANDER HINDERHOFER<sup>1</sup>, M. IBRAHIM DAR<sup>2</sup>, JAN HAGENLOCHER<sup>1</sup>, NEHA ARORA<sup>2</sup>, MICHAEL GRÄTZEL<sup>2</sup>, and FRANK SCHREIBER<sup>1</sup> — <sup>1</sup>Institute of Applied Physics, University of Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany — <sup>2</sup>Laboratory of Photonics and Interfaces, EPFL, CH-1015 Lausanne, Switzerland

The performance of light emitting and light harnessing perovskite thin film devices depend strongly on their structural features. The so-called two-step conversion for preparing perovskite thin films, involves the deposition of lead halide precursor onto a substrate and the subsequent transformation of the resulting films into the perovskite phase by spin coating (drop casting) or dipping into an isopropanol solution containing a defined amount of methylammonium halide (CH<sub>3</sub>NH<sub>3</sub>X) (X=I,Br). It is well-known that the morphology and structural properties of perovskite depend strongly on the exact preparation conditions.

We applied grazing incidence wide angle x-ray scattering (GIWAXS) to determine the domain size and preferred orientation in several perovskite thin films. We will discuss the impact of different solvents and preparation methods (spin coating, dip coating) on the structure and morphology of the different perovskite films and we comment on the device performance. Finally, we will comment on the time scale of the crystallization process in CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub> perovskite thin films, which is accessible by in situ real time x-ray scattering.

DS 5.3 Mon 11:00 ZEU 222

**Analysis of electronic trap states in methylammonium lead halide perovskite solar cells via thermally stimulated current** — ●PHILIPP RIEDER<sup>1</sup>, DAVID KIERNASCH<sup>1</sup>, MATHIAS FISCHER<sup>1</sup>, KRISTOFER TVINGSTEDT<sup>1</sup>, ANDREAS BAUMANN<sup>1,2</sup>, and VLADIMIR DYAKONOV<sup>1,2</sup> — <sup>1</sup>Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — <sup>2</sup>Bavarian Center for Applied Energy Research ZAE, 97074 Würzburg

While power conversion efficiencies already exceeding 22% have been achieved for organo lead halide perovskite solar cells, a complete understanding of its fundamental working principles is still missing, but nonetheless essential to further improve this type of thin film photovoltaic. To address the impact of electronic trap states on device performance, we probed solution processed methylammonium lead halide perovskite solar cells via thermally stimulated current (TSC) analysis. Thereby, after cooling the sample down to 10 K, possible trap states are filled optically and gradually released again by heating the sample back up to 300 K. This causes a weak current to flow, which allows to draw conclusions about the trap state density as well its energetic

depth. We probed perovskite solar cells in normal as well as inverted device configuration to identify the influence of different transport layers on the energetic trap landscape and observe a substantial addition in the case of the commonly used TiO<sub>2</sub>. Additionally, we studied the effect of incorporating bromine as well as chlorine to partly replace the iodine on the electrically active trap state distribution of the photoactive semiconductor.

DS 5.4 Mon 11:15 ZEU 222

**Strong impact of processing parameters on morphology and crystal orientation of hybrid perovskite thin films for photovoltaic application** — ●JOHANNES SCHLIPF<sup>1</sup>, LUKAS OESINGHAUS<sup>1</sup>, YINGHONG HU<sup>2</sup>, NADJA GIESBRECHT<sup>2</sup>, SIGRID BERNSTORFF<sup>3</sup>, THOMAS BEIN<sup>2</sup>, PABLO DOCAMPO<sup>4</sup>, and PETER MÜLLER-BUSCHBAUM<sup>1</sup> — <sup>1</sup>TU München, Physik-Department, LS Funktionelle Materialien, James-Frank-Str. 1, 85748 Garching — <sup>2</sup>Department of Chemistry and CENS, LMU München, 80539 München — <sup>3</sup>Elettra-Sincrotrone Trieste S.C.p.A., Basovizza, 34149 Trieste, Italy — <sup>4</sup>Newcastle University, School of Electrical and Electronic Engineering, Newcastle upon Tyne NE1 7RU, UK

After five years of rapid research, power conversion efficiencies of hybrid perovskite solar cells (PSC) around 20% have become feasible for solution-processed polycrystalline thin films. However, photovoltaic performance, reproducibility and stability of PSC devices depend on crystal size and orientation which in turn are affected by processing parameters during synthesis. We investigate hybrid perovskite thin films with small and wide angle X-ray scattering (GISAXS, GIWAXS) and thereby identify key crystallization mechanisms that strongly influence film morphology and crystal orientation [1,2]. This not only shows the importance of rigorous control of processing parameters, but also renders film morphologies tunable which allows for a rational development of new synthesis methods for high efficiency PSC. [1] J. Schlipf et al., *J. Phys. Chem. Lett.* 2015, 6, 1265. [2] L. Oesinghaus et al., *Adv. Mater. Interfaces* 2016, 1600403.

**15 min break**

DS 5.5 Mon 11:45 ZEU 222

**Local Time-Dependent Charging in a Perovskite Solar Cell** — VICTOR W. BERGMANN<sup>1</sup>, ILKA M. HERMES<sup>1</sup>, DAN LI<sup>1</sup>, ALEXANDER KLASSEN<sup>1</sup>, SIMON BRETSCHNEIDER<sup>1</sup>, EIICHI NAKAMURA<sup>2</sup>, RÜDIGER BERGER<sup>1</sup>, and ●STEFAN A.L. WEBER<sup>1,3</sup> — <sup>1</sup>Max Planck Institute for Polymer Research, 55128 Mainz, Germany — <sup>2</sup>The University of Tokyo, Tokyo 113-0033, Japan — <sup>3</sup>Johannes Gutenberg University Mainz, 55128 Mainz, Germany

Efficient charge extraction within solar cells explicitly depends on the optimization of the internal interfaces. Potential barriers, unbalanced charge extraction or interfacial trap states can prevent cells from reaching high power conversion efficiencies. Furthermore, in perovskite solar cells, slow processes happening on timescales of seconds cause hysteresis. Here, we report on local and time-dependent potential measurements with Kelvin probe force microscopy (KPFM) on cross sections [1] of planar methylammonium lead iodide (MAPI) perovskite solar cells. The KPFM revealed distinct differences in the charging dynamics at interfaces of the MAPI to adjacent layers [2]. Illumination experiments showed that more than one process is involved in hysteresis. By locally resolving these processes we found distinct differences in the charging dynamics in different regions of the device. Our results support the scenario of mobile ions and interfacial trap states for explaining the hysteresis in our device. [1] *Nat. Commun.* 2014, 5. [2] *ACS Appl. Mater. Interfaces*, 2016, 8 (30), 19402.

DS 5.6 Mon 12:00 ZEU 222

**Effect of Thermal and Structural disorder on Electronic Structure in Methylammonium Lead Halide Perovskites** — ●CHENG LI<sup>1</sup>, SHIVAM SINGH<sup>2</sup>, FABIAN PANZER<sup>3</sup>, K. L. NARASIMHAN<sup>2</sup>, YU ZHONG<sup>1</sup>, ANNA GRÄSER<sup>1</sup>, TANAJI GUJAR<sup>1</sup>, MUKUNDAN THELAKKAT<sup>1</sup>, ANNA KÖHLER<sup>3</sup>, DINESH KABRA<sup>2</sup>, and SVEN HUETTNER<sup>1</sup> — <sup>1</sup>Macromolecular Chemistry I, Universität Bayreuth, Universitätsstr. 30, 95447 Bayreuth, Germany — <sup>2</sup>Indian Institute of Technology Bombay, Powai, 400076 Mumbai, India — <sup>3</sup>Experimentalphysik II, Universität Bayreuth, Universitätsstr. 30,

95447 Bayreuth, Germany

In this work, to understand the structure of perovskite materials, we investigate the temperature dependence of optical properties of perovskite from room temperature (300K) to 6K. Unlike typical inorganic semiconductor, in both tetragonal ( $T > 163\text{K}$ ) and orthorhombic ( $T < 163\text{K}$ ) phases of MAPbI<sub>3</sub>, the band gap decreases with decrease in temperature. We indicate that this temperature dependence of the band gap is governed by the lattice expansion term instead of the electron-phonon interaction. The exciton linewidth is homogeneously broadened in both phases. The absorption, at the low energy edge of the exciton absorption, increases exponentially with energy, i.e reminiscent of Urbach tail absorption. The Urbach energy which is used to characterize order of structure, is modelled using thermal and static disorder for both phases separately. This work provides important insights to the electronic and structural properties of MAPbI<sub>3</sub> based perovskites, and this method is transferable to many related perovskites.

DS 5.7 Mon 12:15 ZEU 222

**Impact of bromine doping on recombination kinetics in perovskite solar cells** — ●DAVID KIERMASCH<sup>1</sup>, PHILLIP RIEDER<sup>1</sup>, KRISTOFER TVINGSTEDT<sup>1</sup>, ANDREAS BAUMANN<sup>2</sup>, and VLADIMIR DYAKONOV<sup>1,2</sup> — <sup>1</sup>Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — <sup>2</sup>Bavarian Center for Applied Energy Research (ZAE Bayern) Bayern, 97074 Würzburg

Organo metal halide perovskite solar cells exhibit exceptionally good power conversion efficiency values exceeding already 20%. To allow further improvements it is important to understand the limiting processes e.g. charge carrier recombination in this new photovoltaic technology. Most of the recombination studies presented so far have been focused on perovskite films or crystals but only a few have studied the charge carrier dynamics in solar cell devices. We report on charge carrier lifetime values in bromine containing planar perovskite solar cells with varying the bromine content. The lifetime and corresponding charge carrier density has been derived from transient photovoltage (TPV) and charge carrier extraction (CE) experiments. We found increased lifetime values in solar cells with bromine (MAPb(I<sub>3-x</sub>Br<sub>x</sub>)<sub>3</sub>) compared to pure methylammonium lead iodide (MAPbI<sub>3</sub>). Furthermore, the CE signals from the bromine containing solar cells can be divided in two different extraction parts on different time scales leading to anomalously high extracted charge values. We discuss the experimental findings in regard of possible different contributions to the CE signal.

DS 5.8 Mon 12:30 ZEU 222

**Reduced Recombination for High-Open-Circuit Voltages in CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub> Solar Cells** — ●CHRISTIAN M. WOLFF<sup>1</sup>, FENG-

SHUO ZU<sup>2</sup>, ANDREAS PAULKE<sup>1</sup>, LORENA PERDIGON TORO<sup>1</sup>, NORBERT KOCH<sup>2</sup>, and DIETER NEHER<sup>1</sup> — <sup>1</sup>Universität Potsdam, Institut für Physik und Astronomie — <sup>2</sup>Humboldt-Universität zu Berlin, Institut für Physik

Perovskite solar cells with all-organic transport layers have shown efficiencies rivalling their counterparts that employ inorganic transport layers while avoiding high temperature processing. We investigate how the choice of the fullerene derivative employed in the electron-transporting layer of inverted perovskite cells affects the open circuit voltage. Non-radiative recombination mediated by the electron-transporting layer is the determining factor for the open-circuit voltages in our cells. By inserting an ultra thin layer of an insulating polymer between the active CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub> perovskite and the fullerene layer, external radiative efficiencies of up to 0.3%, open-circuit voltages (V<sub>oc</sub>) as high as 1.16V and with efficiencies up to 19.4% were realised. Our results show that reduction of non-radiative recombination due to charge-blocking at the perovskite/organic interface is more important than proper alignment in the search for ideal selective contacts for high V<sub>oc</sub>.

DS 5.9 Mon 12:45 ZEU 222

**On the chemical origins of crystalline preferred orientations in hybrid organometallic lead halide perovskite thin films** — ●SHAMBHAVI PRATAP, JOHANNES SCHLIFF, and PETER MÜLLER-BUSCHBAUM — TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching

Solar cells based on organometallic lead halide perovskites have established themselves as a promising alternative to commercial thin film solar cells. The crystallographic versatility of the material allows the possibility of extensive chemical tuning, which manifests in the material as a spectra of properties that may be obtained. This entices research on hybrid perovskite structures combining different organic and inorganic groups into a crystalline framework. Preferential orientations of the crystalline hybrid perovskites (1) are reported and correlated to their morphological and chemical characteristics by grazing incidence wide angle x-ray scattering (GIWAXS). Remarkably, perovskite thin films prepared by the same methodologies displayed varying behaviors of preferred orientations, as their chemical composition was varied. Moreover, the route and rate of crystallization (2) is known to radically influence crystalline preferred orientations as well, giving rise to information regarding kinetic and thermodynamic orientations. These results, for the first time propose the possibility of controlling crystallinity of spin-coated thin films by tuning the ingredients of and the treatment of the solution used for spin coating.

(1) Oesinghaus et al., Adv. Mater. Interfaces 2016, 3, 1600403

(2) Giesbrech et al., ACS Energy Lett. 2016, 1, 150-154