

## HL 60: Perovskite and photovoltaics V (joint session HL/ CPP)

Time: Thursday 9:30–12:00

Location: POT 251

HL 60.1 Thu 9:30 POT 251

**Surface Properties of  $\text{FA}_x\text{Cs}_{1-x}\text{Pb}(\text{I}_y\text{Br}_{1-y})_3$**  — ●JULIAN GEBHARDT<sup>1</sup>, DANIEL URBAN<sup>1</sup>, and CHRISTIAN ELSÄSSER<sup>1,2</sup> — <sup>1</sup>Fraunhofer IWM, Wöhlerstraße 11, D-79108 Freiburg — <sup>2</sup>FMF Universität Freiburg, Stefan-Meier-Straße 21 D-79104 Freiburg

Since the rise of hybrid perovskites as promising material for photovoltaic applications inspired by  $\text{MAPbI}_3$  ( $\text{MA}=\text{CH}_3\text{NH}_3^+$ ), many research efforts have been directed towards overcoming practical issues of such light absorbing layers. Apart from replacing silicon as absorber in single-junction solar cells, a promising route is to combine perovskites with established materials in multi-junction tandem cells. For these applications, hybrid perovskite design, i.e., mixing inorganic and organic ions in order to balance stability and light absorbing properties, changes in terms of target properties. This search temporarily concluded in materials of the type  $\text{FA}_x\text{Cs}_{1-x}\text{Pb}(\text{I}_y\text{Br}_{1-y})_3$  ( $\text{FA}=\text{HC}(\text{NH}_2)_2^+$ ), with  $x \approx 0.8$  and  $y \approx 0.7$ . During the extensive search for perovskite based absorber materials, theoretical understanding has proven vital to navigate the huge combinatorial space. Naturally, such investigations focused on bulk properties. This neglects the important step from lab scale absorber materials design towards working devices that require contacting and possibly passivation.

We present an investigation of surface properties of the  $\text{FA}_x\text{Cs}_{1-x}\text{Pb}(\text{I}_y\text{Br}_{1-y})_3$  family by electronic-structure theory to guide future interface optimization for these and other absorber materials. Focusing on non-polar surfaces, we investigate the stability and effects on the electronic-structure.

HL 60.2 Thu 9:45 POT 251

**Theoretical analysis of ultrathin  $\text{Cu}(\text{In,Ga})\text{Se}_2$  solar cells with  $\text{Zn}(\text{O,S})$  buffer layer** — ●GABIN LANDRY MBOPDA TCHEUM<sup>1,3</sup>, ARIEL TEYOU NGOUPO<sup>1</sup>, NARNGAR GUIRDJEBAYE<sup>1</sup>, SOUMAILA OUEDRAOGO<sup>2</sup>, and JEAN-MARIE B. NDJAKA<sup>1</sup> — <sup>1</sup>University of Yaounde I, Yaounde, Cameroon — <sup>2</sup>Université Joseph Ki-ZERBO, Ouagadougou, Burkina Faso — <sup>3</sup>Friedrich-Schiller-Universität, Jena, Germany

The optimisation of Cd-free buffer layer, for CIGS based solar cells, appears as an ingenious way to reduce the absorber thickness without compromising the solar cell's performance. Therefore, we discuss and present simulated electrical properties of CIGS solar cells with  $\text{Zn}(\text{O,S})$  buffer layers. We present the electrical performance of this type of thin films solar cells with ultra thin absorber and buffer layers. However, as ultra thin absorber leads to increasing recombinations at the back contact, we introduced SnSe and a highly doped CIGS layer (known as p+-CIGS layer) as back surface field between the Mo layer and CIGS absorber. Here, we discussed their impact on the cell's efficiency and on the band alignment.

HL 60.3 Thu 10:00 POT 251

**A comprehensive argument for the defect tolerance of metal-halide perovskite solar absorbers** — ●ANOOP CHANDRAN, IRENE AGUILERA, CHRISTOPH FRIEDRICH, THOMAS KIRCHARTZ, UWE RAU, and STEFAN BLÜGEL — PGI-1, IAS-1 and IEK-5, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Charge transport and recombination probabilities are related to the defects in a semiconductor. Reduction of scattering centres is essential to preserve the optoelectronic properties of solar absorbers. The ability of semiconductors to retain its properties in the presence of defects or the elimination of defects by a self-reorganisation mechanism is collectively known as defect tolerance.

Defect states formation is dictated by the bonding behaviour of the band extremes. Compression or dilation of lattice from its equilibrium configuration results in the change of energy levels. Rate of this change can be used to measure the deformation potential and thereby defect tolerance of materials. We develop a turn-key solution for the automated computing of the deformation potential combining the FLEUR codes[1] with the open science platform AiiDA[2] to study metal-halide perovskites using density-functional-theory (DFT).

[1] www.flapw.de

[2] G. Pizzi et al. Comp. Mat. Sci. 111, 218-230 (2016)

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HL 60.4 Thu 10:15 POT 251

**Differences between vacuum deposition and solution processing of lead halide perovskites** — ●MARTIN KROLL, RAN JI, ZONGBAO ZHANG, TIM SCHRAMM, CHANGSOON CHO, FREDERIK NEHM, YANA VAYNZOF, and KARL LEO — TU Dresden, IAPP, Nöthnitzer Straße 61, 01187 Dresden

Vacuum deposition is the preparation technique of choice for large scale production of organic thin film solar cells, due to the superior control it offers over film formation and deposition of multilayers. It is also possible to deposit perovskite materials by thermal evaporation, however motivated by its simplicity and low associated costs, most research groups focus on solution processed perovskites. Nevertheless, recent reports show that power conversion efficiencies of vacuum deposited perovskite solar cells surpassed 20%, making them comparable to solution processed devices. The fabrication of perovskite thin films by thermal evaporation in vacuum faces different challenges that solution processing and often results in different film properties. We compare the properties and performance of perovskites fabricated by the two methods and report on the deviations we observe in morphology, stability and photovoltaic device performance. We discuss the influence of processing conditions during vacuum and solution processing on the properties of the perovskites films as well as their effect on the device performance, stability and reproducibility.

30 min. break

HL 60.5 Thu 11:00 POT 251

**Tuning the Grain Size and Porosity of  $\text{MAPbI}_3$  Perovskite films for High Efficiency Solar Cells** — ●QINGZHI AN<sup>1,2</sup>, FABIAN PAULUS<sup>1,2</sup>, and YANA VAYNZOF<sup>1,2</sup> — <sup>1</sup>Integrated Center for Applied Photophysics and Photonic Materials, TU Dresden, Germany — <sup>2</sup>Center For Advancing Electronics Dresden (cfaed), TU Dresden, Germany

In this work, a facile approach to control perovskite grain size and porosity is introduced. By slightly tuning the amount of  $\text{H}_3\text{PO}_2$  (HPA) in the perovskite precursor solution, we demonstrate that the average perovskite grain size can be enlarged by one magnitude regardless of the underlying charge extraction layer. We correlate these microstructural changes to the photovoltaic performance of devices and demonstrate that optimal HPA concentration leads to open circuit voltages of 1.16 V and a power conversion efficiency of 19 %. We also demonstrate that further increase in the HPA amount in perovskite precursor solution results in the formation of a regular, porous perovskite networks with highly degree of crystalline orientation. Such porous structures can be of great interest to application in light-emitting diodes or semi-transparent photovoltaic devices. This work demonstrates that tuning the fraction of HPA in perovskite precursor solution is an effective method to control the perovskite grain size and layer topology.

HL 60.6 Thu 11:15 POT 251

**Charge Carrier Transport in Halide Perovskites Investigated by Optical-Pump Terahertz-Probe Spectroscopy** — HANNES HEMPEL<sup>1</sup>, ●ANDREI PETSUK<sup>1</sup>, MARTIN STOLTERFOHT<sup>2</sup>, PASCAL BECKER<sup>1</sup>, DIETER NEHER<sup>2</sup>, RAINER EICHBERGER<sup>1</sup>, and THOMAS UNOLD<sup>1</sup> — <sup>1</sup>Helmholtz Zentrum Berlin für Materialien und Energie GmbH — <sup>2</sup>Institute of Physics and Astronomy, Universität Potsdam

Metal-halide hybrid perovskites exhibit excellent optoelectronic properties except for their rather moderate charge carrier mobilities. The origin of these moderate mobilities has been attributed to several (contradicting) effects, such as the formation of large and small polarons, dynamic disorder due to the soft nature of these materials, slow rotational modes of the organic molecules, as well as to the confinement of charge carriers in grains, ferroelectric domains or nanostructures. To clarify the nature of the charge carrier transport, we probed different hybrid and inorganic halide perovskites thin films and nano-crystals by temperature dependent Optical-Pump Terahertz-Probe (OPTP) spectroscopy. We find a strongly increasing mobilities with lower temperature, thus excluding small polaron formation and hopping transport. Instead, this behavior can be modeled by conventional large polaron theory and Fröhlich-type electron-phonon scattering.

HL 60.7 Thu 11:30 POT 251

**Singlet Fission Processes in Hybrid Organo-Metal Halide Perovskites Semiconductors** — ●KARUNANANTHARAJAH PRASHANTHAN<sup>1,2</sup>, KLAUS LIPS<sup>1</sup>, SIMONE RAOUX<sup>1</sup>, and ROWAN MACQUEEN<sup>1</sup> — <sup>1</sup>Institute for Nanospectroscopy, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH — <sup>2</sup>Department of Physics, University of Jaffna, Jaffna, Sri Lanka

Solar cells made from Organo-Metal Halide Perovskites show power conversion efficiency very close to the record efficiency of commercially available thin film technologies. Looking to the future of these devices, there exists promising approaches to push the efficiency beyond the Shockley-Queisser single junction thermodynamic limit. Singlet fission is a quantum mechanical process which occurs in various organic molecules, whereby a photogenerated high-energy singlet exciton spontaneously splits into two lower-energy triplet excitons. In this work, we present the possible routes and challenges involved in combining singlet fission materials with low bandgap hybrid metal halide perovskite solar cells. Using time-resolved photoluminescence spectroscopy we investigate the dynamic processes involved in singlet fission and the subsequent injection of energy and charge into the perovskite layer. The objective is to form augmented photovoltaic devices which can efficiently harvest triplets from a singlet fission layer, substantially reducing the energy loss to carrier thermalization.

HL 60.8 Thu 11:45 POT 251

**Manganese Doping Induced Quantum Confinement in the**

**Perovskite Nanocrystals via Ruddlesden-Popper Defects** — ●KAVYA REDDY DUDIPALA, SHARMISTHA PAUL, TUSHAR DEBNATH, JOCHEN FELDMANN, and LAKSHMINARAYANA POLAVARAPU — Chair for Photonics and Optoelectronics, Nano-Institute Munich and Department of Physics, Ludwig-Maximilians-Universität (LMU), Königinstr. 10, 80539 Munich, Germany

The concept of doping manganese ions ( $\text{Mn}^{2+}$ ) into II-VI semiconductor nanocrystals (NCs) has recently been extended to perovskite NCs. The transfer of the exciton energy from a semiconductor host to  $\text{Mn}^{2+}$  dopants leads to orange emission from a spin-forbidden 4T1-6A1 Mn d-d transition. To date, most studies on  $\text{Mn}^{2+}$  doped NCs focused on enhancing the emission related to the  $\text{Mn}^{2+}$  dopant via an energy transfer mechanism. Here, we show that the doping of  $\text{Mn}^{2+}$  ions into  $\text{CsPbCl}_3$  NCs not only results in a  $\text{Mn}^{2+}$ -related orange emission, but also strongly influences the excitonic properties of the host NCs. We observe for the first time that  $\text{Mn}^{2+}$  doping leads to the formation of Ruddlesden-Popper defects and thus induces quantum confinement in host perovskite NCs. We find that a slight doping with  $\text{Mn}^{2+}$  ions improves the size distribution of the NCs, which results in a prominent excitonic peak. However, with increasing the  $\text{Mn}^{2+}$  concentration, the number of Ruddlesden-Popper planes increases leading to smaller single crystal domains. The enhanced confinement and crystal inhomogeneity cause a gradual blue shift and broadening of the excitonic transition.