

CPP 11: Poster: Hybrid and Perovskite Photovoltaics

Time: Monday 18:15–21:00

Location: Poster B2

CPP 11.1 Mon 18:15 Poster B2

Titania network structures prepared via spray coating for photovoltaic applications — ●BO SU¹, HERBERT A. CALLER-GUZMAN¹, VOLKER KÖRSTGENS¹, CHRISTOPH J. SCHAFER¹, YUAN YAO¹, STEPHAN V. ROTH², and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — ²DESY, Notkestr. 85, 22607 Hamburg, Germany

Due to a high surface to volume ratio and their bicontinuous morphology, foam-like network nanostructures are receiving increasing interest in photovoltaic applications. Controlling the pore size is crucial for devices, such as dye-sensitized solar cells (DSSCs) and solid state DSSCs. In this study, spray coating is used as deposition method since it is allowing for scaling-up to large scale production. A block copolymer template assisted sol-gel process is used to form the nanostructured titania films. The structure evolution is probed with in situ GISAXS during the spray coating process. The morphology of the sprayed films is characterized with SEM and optical microscopy. The crystalline structure of the titania films is probed with XRD. The optical properties and photoluminescence emission state of the mesoporous titania films are probed by UV vis and photoluminescence, respectively.

CPP 11.2 Mon 18:15 Poster B2

Crystallization behavior of hybrid perovskite films on mesoporous titania templates — ●MARKUS TRUNK, BO SU, and PETER MÜLLER-BUSCHBAUM — TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany

The tremendous efficiency improvement in organic-inorganic halide perovskite solar cells has attracted very high interest in the last years. Comparing the stability of methylammonium lead halide materials, methylammonium lead bromide (MAPbBr₃) is a promising candidate. To increase the device performance with respect to the hysteresis in current-voltage characteristics, we use mesoporous titania films as support layer for the perovskite. We manufactured nanostructured titania films with an additional superstructure in the micrometer-regime. The superstructure was first transferred to a silicon chip via optical lithography. Then, a PDMS stamp was used as a replica of this master stamp and the superstructure was superimposed to the mesoporous titania films via a wet imprinting method. The morphology of wet imprint films is probed by SEM and AFM. The perovskite films are prepared via a one-step method on top of the superstructured mesoporous titania layers. Electronic properties, optical properties and crystalline structure are characterized for these samples.

CPP 11.3 Mon 18:15 Poster B2

Nanostructured zinc oxide films for application in hybrid photovoltaics — ●KUN WANG, LIN SONG, and PETER MÜLLER-BUSCHBAUM — Physikdepartment E13 Lehrstuhl für Funktionelle Materialien Technische Universität München, James-Frank-Straße 1, München, Germany

Hybrid solar cells, a combination of conventional inorganic photovoltaic systems and organic solar cell technologies, offer outstanding potential due to their minor investment compared to inorganic solar cells and higher stability compared to organic solar cells. In this kind of cells, nanostructured inorganic metal oxides with tunable morphologies are of great importance. Among the many inorganic metal oxides, ZnO has been widely explored due to its outstanding electrical and optical properties and rich variety of morphologies. In order to improve the interfaces between ZnO and hole-conducting polymers, routes to tune the length scales of the nanostructures are explored. We use SEM and AFM to investigate the surface morphology of ZnO, while the nanostructure inside the films can be probed with GISAXS. The understanding of the film morphology is helpful for improving the power conversion efficiency. The optical properties are examined with UV/Vis spectroscopy and the film thickness is investigated by x-ray reflectivity measurements.

CPP 11.4 Mon 18:15 Poster B2

Tuning the interface of hybrid thin films for PV applications — ●NURI HOHN¹, LIN SONG¹, MIKE BOONE², ERIC RIVARD², and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — ²University

of Alberta, Department of Chemistry, Edmonton, Alberta, Canada

Organic materials have been found to offer various, promising advantages for photovoltaic (PV) devices like flexibility and the potential of low-cost/large scale production. The major challenge to overcome the limited lifetime of such devices can be addressed via the substitution of an organic component with the respective inorganic counterpart for chemical/physical stability. Hence, a conjugated polymer serves as electron donor whereas n-type inorganic nanocrystals are deployed as electron conducting material. In such devices the surface-to-volume ratio is an indicator for both loss factors due to recombination as well as for efficiency gain through an increased amount of interface. Titanium dioxide nanostructures are obtained from sol-gel synthesis coupled with diblock copolymer templating to optimize the structure/interface between the donor and acceptor material. To improve the conditions for an efficient energy conversion in a PV cell primary investigations of the above mentioned systems correspond to spectral as well as morphological characterization via SEM and XRD.

CPP 11.5 Mon 18:15 Poster B2

Thermodynamic stability of mixed Pb:Sn methylammonium halide perovskites — ●KSENIA KORSHUNOVA, LARS WINTERFELD, WICHARD J.D. BEENKEN, and ERICH RUNGE — Institut für Physik und Institut für Micro- und Nanotechnologie, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Using density functional theory, we investigate systematically mixed $MA(Pb:Sn)X_3$ perovskites, where MA is $CH_3NH_3^+$, and X is I , Br or Cl . Ab initio calculations of the orthorhombic, tetragonal and cubic perovskite phases show that the substitution of lead by tin has a much weaker influence on both structure and cohesive energies than the substitution of the halogen. The thermodynamic stability of the $MA(Pb:Sn)X_3$ mixtures at finite, non-zero temperatures is studied within the Regular Solution Model.

We predict that it will be possible to create $MA(Pb:Sn)I_3$ mixtures at any temperature. This poster presents detailed numerical results supplementary to the results outlined in the talk given by our group.

CPP 11.6 Mon 18:15 Poster B2

Optoelectronic properties of mixed Pb:Sn methyl-ammonium halide perovskites — ●LARS WINTERFELD, KSENIA KORSHUNOVA, WICHARD J.D. BEENKEN, and ERICH RUNGE — Institut für Physik, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Using ab initio calculations, we investigate systematically the band structures of mixed $MA(Pb : Sn)X_3$ perovskites, where MA is $CH_3NH_3^+$, and X is Cl , Br or I . Here, we focus on the thermodynamically stable mixed structures in the high-temperature cubic phase and compare both DFT and post-DFT methods (including self-consistent GW) with and without spin orbit coupling. Interestingly, the optoelectronic properties are not just a linear combination of the non-mixed parent structures and are not limited by the non-mixed values, which allows band gap engineering. This poster presents detailed numerical results and a selection of over 150 different band structures supplementary to the results outlined in a talk given by our group.

CPP 11.7 Mon 18:15 Poster B2

Spectroscopic investigation of the nitrogen role in organic-inorganic perovskite films — ●MALGORZATA SOWIŃSKA¹, CHITTARANJAN DAS¹, KONRAD WOJCIECHOWSKI², HENRY SNAITH², and DIETER SCHMEISSER¹ — ¹Brandenburgische Technische Universität Cottbus-Senftenberg, Angewandte Physik-Sensorik, Konrad-Wachsmann-Allee 17, 03046 Cottbus, Germany — ²Clarendon Laboratory, University of Oxford, Parks Road, Oxford, OX13PU, UK

Over the past few years, a wide range of device architectures employing organic-inorganic metal halide perovskite absorbers has been reported, with efficiencies exceeding 20%. Despite the tremendous progress, a number of key issues must be resolved before the wide-spread commercialization will be possible. Some of the primary challenges include lead toxicity, long-term stability, and fast degradation upon exposure to humid atmosphere. Recent computational and experimental studies suggest that hybrid metal-halide perovskites act as an ionic-electronic conductor. The study of vacancy-mediated migration of I^- , Pb^{2+} and $CH_3NH_3^+$ ions and their relative activation energies suggests that migration of halide vacancies, to and from the interfaces

in the solar cell during its operation, is the main conduction mechanism. In this work, we are presenting high resolution synchrotron-based spectroscopic study, which indicates that the contribution of nitrogen into the conduction mechanism of methyl ammonium lead iodide-based ($\text{CH}_3\text{NH}_3\text{PbI}_3$) perovskite films should not be neglected. The N1s core level and resonant X-ray photoelectron spectroscopy at the N1s-edge of the $\text{CH}_3\text{NH}_3\text{PbI}_3$ films are discussed in detail.

CPP 11.8 Mon 18:15 Poster B2

Observation of ionic- and trapped charges at interfaces in an operating perovskite solar cell — ●VICTOR BERGMANN¹, YUNLONG GUO², HIDEYUKI TANAKA², ILKA HERMES¹, DAN LI¹, ALEXANDER KLASSEN¹, SIMON BRETSCHNEIDER¹, EIICHI NAKAMURA², RÜDIGER BERGER², and STEFAN WEBER^{1,3} — ¹MPI for Polymer Research, Mainz — ²University of Tokyo, Japan — ³Johannes Gutenberg University Mainz, Germany

Optimization of solar cell devices requires efficient charge extraction. With cross section Kelvin probe force microscopy (KPFM), we were able to locally study the potential distribution inside a mesoporous device under working conditions (DOI:10.1038/ncomms6001). Here, we used frequency modulation KPFM to investigate cross sections of planar perovskite solar cells. In particular, we performed experiments in dark and under illumination on an operating planar $\text{CH}_3\text{NH}_3\text{PbI}_3$ device, in short circuit and open circuit conditions, respectively. Thereby, we found an experimental proof that both ion migration and trapped interfacial charges can be present in a perovskite device and demonstrate that cross sectional FM-KPFM is able to distinguish between the two effects.

CPP 11.9 Mon 18:15 Poster B2

Structure analysis on hybrid organic-inorganic perovskite solar cells — ●FLORIAN SOUTSCHEK¹, HARIKESH P. CHOLAKKAL², SJÖERD A. VELDHUIS², EVA M. HERZIG¹, PETER MÜLLER-BUSCHBAUM³, DHARANI SABBA², and NRIPAN MATHEWS² — ¹Technische Universität München, Munich School of Engineering, 85748 Garching, Germany — ²Energy Research Institute @NTU (ERI@N), Research Techno Plaza, 637553, Singapore — ³TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany

The desire to efficiently convert solar into electric energy has led to increasing activity in the associated field of scientific research in the last decades. Due to major advantages, as low material costs and the applicability of mass production techniques, solution processed solar cells have long been of particular interest; disadvantages such as comparatively low efficiency and fast degradation inhibited mass production so far. Combining advantages of organic and inorganic systems, perovskite solar cells - as hybrid organic-inorganic cells - have shown a skyrocketing rise in efficiency for the last years to currently around 20 %. However, little is known about the formation of the perovskite film under different conditions on a crystal size level, which is of key importance for the understanding of how to further improve this type of solar cells. Therefore the aim of this project is to use multiple measurement techniques, in particular Grazing Incidence Wide Angle X-ray Scattering (GIWAXS), on perovskite films with standard and systematically altered production procedures to learn about the film formation and possibilities of specific manipulation.

CPP 11.10 Mon 18:15 Poster B2

Fabrication and characterisation of solution processed perovskite solar cells with various transport layers — ●MARVIN GRÜNE¹, STEFAN VÄTH¹, ANDREAS BAUMANN², and VLADIMIR DYAKONOV^{1,2} — ¹Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — ²Bavarian Center for Applied Energy Research (ZAE Bayern), 97074 Würzburg

Perovskite solar cells are considered to be the upcoming star of thin film solar cells, exhibiting rapidly rising power conversion efficiencies (PCE). The active layer consist of the organic-inorganic perovskite structure $\text{CH}_3\text{NH}_3\text{PbI}_3$. The perovskite is sandwiched between a electron and hole transport layers which allows the selective extraction of the different types of charge carriers to the respective contacts of the solar cell. In this study different structures of solar cells, including different combinations of selective transport layers such as PEDOT:PSS and MoO_3 for hole transport or BCP, BPhen and Ca for electron transport were investigated concerning efficiency, hysteresis and long-term stability. Finally, the device stability of silver and gold as cathode material was inspected.

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Revealing the structural properties of p-DTS(FBTTh₂)₂ with the help of MD-simulations — ●AXEL BOURDICK and STEPHAN GEKLE — Universität Bayreuth

With the advent of organic photovoltaics promising materials for organic solar cells have become a strong focus of research. One particular interesting manufacture strategy is the push-pull chromophore design, whereby an electron rich donor unit and an electron deficient acceptor unit are placed alternating on the same molecule.^[1,2] With the help of MD-Simulations we simulate the system p-DTS(FBTTh₂)₂. In particular we investigate the structure and conformation of aggregated states in different solvents, and various physical properties, like the free energy of the system in dependence of the distance between molecules.

[1]: Gendron, D.; Leclerc, M. New Conjugated Polymers for Plastic Solar Cells. *Energy Environ. Sci.* 2011, 4, 1225-1237.

[2]: Duan, C.; Huang, F.; Cao, Y. Recent Development of Push-Pull Conjugated Polymers for Bulk-Heterojunction Photovoltaics: Rational Design and Fine Tailoring of Molecular Structures. *J. Mater. Chem.* 2012, 22, 10416-10434.

CPP 11.12 Mon 18:15 Poster B2

X-Ray Absorption Spectroscopy of Hybrid Organic-Inorganic Perovskites: Theory and Experiment — ●C. VORWERK¹, C. HARTMANN², C. COCCHI¹, G. SADOUGH³, S. HABISREUTINGER³, R. FÉLIX², R.G. WILKS^{2,4}, H. SNAITH³, P. BECKER², J. JUST², T. UNOLD², K. HANNEWALD^{1,5}, M. BÄR^{2,4,6}, and C. DRAXL^{1,5} — ¹Institut für Physik, Humboldt-Universität zu Berlin, 12489 Berlin, Germany — ²Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, 14109 Berlin, Germany — ³Clarendon Laboratory, Department of Physics, University of Oxford, Oxford OX1 3PU, United Kingdom — ⁴Energy Materials In-Situ Laboratory Berlin (EMIL), Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, 12489 Berlin, Germany — ⁵Fritz-Haber-Institut der Max-Planck-Gesellschaft, 14195 Berlin, Germany — ⁶Institut für Physik und Chemie, Brandenburgische Technische Universität Cottbus-Senftenberg, 03046 Cottbus, Germany

We present a joint experimental and theoretical study of the x-ray absorption spectra (XAS) of the hybrid organic-inorganic perovskite methyl ammonium lead triiodide $\text{CH}_3\text{NH}_3\text{PbI}_3$ - a promising material for photovoltaic energy conversion. The Pb M_{4,5} and I L_{2,3} absorption edges of the perovskite were measured in partial fluorescence and total electron yield modes at the HiKE endstation located at the KMC-1 beamline of the BESSY II light source. The corresponding *ab-initio* calculations are performed using all-electron many-body theory (DFT+BSE), as implemented in the **exciting** code.

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Impact of PbI₂ on excited state dynamics in hybrid lead halide perovskites — ●TOBIAS MEIER¹, FABIAN PANZER^{1,2,3}, TANAJI GUJAR⁴, THOMAS UNGER^{1,2}, MUKUNDAN THELAKKAT⁴, and ANNA KÖHLER^{1,2} — ¹Experimental Physics II — ²Bayreuth Institute of Macromolecular Research (BIMF) — ³Department of Functional Materials — ⁴Applied Functional Polymers, Macromolecular Chemistry, University of Bayreuth, 95440 Bayreuth, Germany

Hybrid lead halide perovskites have emerged as novel and highly efficient active material in different applications such as solar cells, or light emitting device. They also yield the possibility for cheap and simple processing which makes this class of material currently highly attractive and prominent. Depending on the processing method, it is known that PbI₂ incorporations can be present in the perovskite material after perovskite formation took place. Here a fundamental understanding on how and in which extend PbI₂ interacts with the perovskite domains and how this impacts on device performance is still missing. We therefore performed temperature dependent steady-state absorption and emission measurements, as well as transient absorption spectroscopy to investigate the impact of PbI₂ incorporations on the excited state dynamics in different $\text{CH}_3\text{NH}_3\text{PbI}_3$ samples.

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Understanding excited state dynamics in hybrid lead halide perovskites by temperature dependent time resolved spectroscopy — ●MARIUS JAKOBY¹, THOMAS UNGER^{1,2}, FABIAN PANZER^{1,2,3}, TANAJI GUJAR⁴, MUKUNDAN THELAKKAT⁴, and ANNA KÖHLER^{1,2} — ¹Experimental Physics II — ²Bayreuth Institute of Macromolecular Research (BIMF) — ³Department of functional Materials — ⁴Applied functional Polymers, Macromolecular Chemistry,

University of Bayreuth, 95440 Bayreuth, Germany

Within the last few years, hybrid lead halide perovskites have emerged as highly attractive active layers in solar cells and in light emitting devices. Here remarkably long charge carrier diffusion lengths in the range of several micrometers combined with the typically low binding energies of excited states are important material properties, which lead to high device efficiencies. Despite these high device efficiencies that were reported, there is still a lack in fundamental understanding the excited state dynamics of this class of material. For instance, there is still no clear consensus about the physical origin of additional emission features that are often observed at low temperature. To identify and characterise the dynamics of these different excited states we performed temperature dependent time resolved emission spectroscopy on different hybrid lead halide perovskite samples using a Streak-Camera setup. The results enable us to identify the nature of the different excited states and explore to which extend the morphology of the material controls their excited states dynamics.

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X-Ray analysis towards highly stable, superior efficiency perovskite solar cells — ●SHAMBHAVI PRATAP, JOHANNES SCHLIPF, and PETER MÜLLER-BUSCHBAUM — TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany

Perovskite solar cells represent the new wave in the field of photovoltaics and show a lot of promise. The technology has seen a meteoric rise with device performances crossing the 20% mark in just half a decade since its' inception.

The major challenge in the field remains the stability of these cells. The science of the response of the perovskite materials to atmospheric conditions of moisture and temperature demands considerable investigation before commercialization of these cells is feasible.

We aim to understand the structural changes occurring in the material with controlled humidity and temperature conditions, and to enhance the stability by the addition of functional additives and the use of novel solvent media during the synthesis of the perovskite crystals.

Grazing-incidence wide angle X-ray scattering (GIWAXS) aids us to understand the stability of the perovskite structure of the material and help us to gain insight for the fabrication of high-efficiency, long term stable perovskite solar cells.

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Charge Extraction in Organometallic Perovskite Solar Cells — ●CHRISTIAN M. WOLFF, ANDREAS PAULKE, NATALIE SCHÖN, and DIETER NEHER — Institute of Physics and Astronomy, University of Potsdam, Karl-Liebknecht-Str.24-25, D-14476 Potsdam-Golm, Germany

We present a study on transfer and extraction of charge carriers in working hybrid perovskite solar cells. With a toolbox comprising transient absorption (TAS), time-resolved PL (TRPL) and spectroscopic-electronic pump-probe experiments including time-delayed collection field (TDCF) and bias-assisted charge extraction (BACE) we follow the fate of charge carriers after excitation. We look at internal processes, such as recombination in the active layer, as well as external processes, such as extraction of charges to the transport layers. Whereas most previous studies have primarily investigated only sections of the solar cells, we apply the outlined techniques to working solar cells with all-organic (e.g. PEDOT and PCBM) or metal oxide (e.g. NiOx and ZnO) extraction layers. With these methods we gain insight into elementary processes in these high efficiency devices. For example, we find that electron transfer to PCBM occurs on a ns-time scale corresponding to mean extraction lengths of less than 20 nm. This finding is consistent with the interpretation, that PCBM molecules penetrate into the cracks between grains [1], in contrast to the picture of flat layers with sleek interfaces.

[1] Paulke, A. et al. Charge Carrier Recombination Dynamics in Perovskite and Polymer Solar Cells. *Submitt. Publ.* (2016).

CPP 11.17 Mon 18:15 Poster B2

Spectroscopic Imaging of Perovskites Thin Films — ●SEBASTIAN BADERSCHNEIDER^{1,2}, FABIAN PANZER^{2,3}, THOMAS UNGER^{2,3}, TANAJI GUJAR⁴, MUKUNDAN THELAKKAT⁴, JÜRGEN KÖHLER^{1,2}, ANNA KÖHLER^{2,3}, and RICHARD HILDNER^{1,2} — ¹Experimentalphysik IV, Universität Bayreuth — ²Bayreuther Institut für Makromolekülforschung — ³Experimentalphysik II, Universität Bayreuth — ⁴Applied Functional Polymers, Makromolekulare Chemie I, Universität Bayreuth

The efficiency of perovskite solar cells has increased within a few years up to more than 20%. Responsible for the remarkable success of this class of solar cells are, among others, the high extinction coefficient over the whole visible range and low binding energies of the excited states allowing for efficient generation of charge carriers. Though mixed halide perovskites yield the possibility to be solution processed in a simple and cheap way, they show a high degree of crystallinity which ensures high diffusion lengths in the range of μm for both electrons and holes. Employing 2-dimensional spectroscopic imaging on thin polycrystalline perovskite films, we show that at low temperatures the crystal structure can be reversibly switched between the tetragonal and the orthorhombic phase. Moreover, we address the question whether the photoluminescence stems predominantly from the grain boundaries or the crystallites.

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Charge Transport Properties in Perovskite Photovoltaic Devices Incorporating Carbon Nanotube Hole Transport Layers — ANDREW ROWBERG, MATTHIAS HANDLOSER, KATHRIN BADER, PABLO DOCAMPO, and ●ACHIM HARTSCHUH — Ludwig-Maximilians-Universität München, München, Deutschland

Hybrid thin-film perovskite photovoltaic devices have attracted considerable interest due to their high efficiency and affordable fabrication. [1] However, the small molecule spiro-OMeTAD, the most often used hole transporting material in perovskite devices, suffers from a poor intrinsic charge mobility. Networks of semiconducting carbon nanotubes (s-CNTs), which possess excellent charge mobility properties, [2] offer a potential replacement and have been demonstrated as hole-transport layers in lead halide perovskite devices. [3] However, the mechanisms behind the functionality of perovskite devices incorporating s-CNT networks have not been thoroughly explored. This work examines the intrinsic charge transport properties in such devices through laser excitation at unique wavelengths corresponding to the absorption of each layers. A confocal optical microscope is used to raster-scan the samples or detection positions for fixed excitation and to generate photoluminescence (PL) maps, while charge carrier decay and transport dynamics are studied on the sub-nanosecond scale by time-correlated single photon counting (TCSPC) through rapid pulsed laser excitation.

[1] Hodes, G. et al. *Nat. Phot.* 8, 87-88 (2014). [2] Jariwala, D. et al. *Chem. Soc. Rev.* 42, 2824-2860 (2013). [3] Habisreutinger, S. et al. *Nano Lett.* 14, 5561-5568 (2014).

CPP 11.19 Mon 18:15 Poster B2

Ferroelectric organic layers for solar cell applications — ●MALGORZATA WAWRZYŃIAK-ADAMCZEWSKA¹ and MALGORZATA WIERZBOWSKA² — ¹Faculty of Physics, A. Mickiewicz University, Umultowska 85, 61-614 Poznan, Poland — ²Institute of Physics, Polish Academy of Sciences (PAS), Al. Lotnikow 32/46, 02-668 Warszawa, Poland

Organic ferroelectric layers and molecular columns, arranged between the graphene sheets, are discussed for the solar cell application. The proposed layers possess many advantageous properties: 1) the cascade energy-levels alignment, 2) simultaneous donor and acceptor character depending on the charge-carrier direction, 3) the charge-transfer excitonic type, 4) the induced polarization of the electrodes, leads to a substantial work-function change (± 1.5 eV) of the anode and cathode. The separate-path electron and hole transport is theoretically predicted for the layers and molecular columns. The carrier separation effect allows to deal with the charge recombination problem. The building molecules contain the mesogenic flat aromatic part and the terminal dipole groups which make the system ferroelectric. The diffusion path of the electrons cuts through the aromatic rings, while holes hop between the dipole groups. We verified that the separation of the diffusion paths is not destroyed by the application of the graphene leads. These features make the systems suitable for the efficient solar cells. (arXiv:1510.05220) This work has been supported by The National Science Centre of Poland: the Projects No.2013/11/B/ST3/04041 and DEC-2012/07/B/ST3/03412.

CPP 11.20 Mon 18:15 Poster B2

Crystalline Structure and Stability Studies of Differently Processed Hybrid Perovskite Films -Towards Stability under Ambient Conditions — ●TANAJI GUJAR and MUKUNDAN THELAKKAT — Applied Functional Polymers, Department of Macromolecular Chemistry I, University of Bayreuth, 95440 Bayreuth, Germany
Organic-inorganic halide perovskite-based thin film solar cells show excellent PCE. However, high PCE values have often been reached

with poor air-stability. The degradation of its performance in moisture has attracted great attention, but the specific mechanism is not yet fully established. In this work, we used three different processing methods for the perovskite films preparation under N₂ atmosphere and observed that the processing methods have a strong influence on the film structural properties and stability in ambient condition. Intensive characterizations including SEM, XRD and UV-Visible with aging of perovskite films in ambient conditions are carried out for understanding the structural and morphological relation with stability. Here we show that the films prepared by MAI-Vapor assisted method have compact, dense and pore-free with stability more than one month in ambient conditions. This also indicates that the formation of film morphology and structure could prevent water infiltration into the perovskite and increase the stability, thus enabling possibilities toward perovskite solar cells with long device lifetimes and a resistance to humidity. A comparison of the materials for their solar cell performance is also carried out. This work suggests important pathway to understand the degradation of the perovskite structure under normal humidity condition.

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Effect of Thermal and Structural disorder on Electronic Structure of Hybrid Perovskite Semiconductor CH₃NH₃PbI₃ — CHENG LI¹, SHIVAM SINGH², K. L. NARASIMHAN², FABIAN PANZER³, TANAJI GUJAR⁴, MUKUNDAN THELAKKAT⁴, ANNA KÖHLER³, DINESH KABRA², and SVEN HÜTTNER¹ — ¹Organic and Hybrid Electronics, Makromol. Chemie I, Universität Bayreuth — ²Indian Institute of Technology Bombay, Powai, Mumbai — ³Experimentalphysik II, Universität Bayreuth — ⁴Angew. Funktion-spolymere, Makromol. Chemie I, Universität Bayreuth

We investigate the temperature dependence of optical properties of methylammonium lead iodide (MAPbI₃ = CH₃NH₃PbI₃) from room temperature to 6K. In both tetragonal (T > 163K) and orthorhombic (T < 163K) phases of MAPbI₃, the band gap decreases with decrease in temperature in contrast to what is normally seen for many inorganic semiconductors. We show that the temperature dependence of the band gap is determined by the lattice expansion term rather than 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 - reminiscent of Urbach tail absorption. The Urbach energy is a measure of the disorder, which is modelled using thermal and static disorder for both the phases separately. The static disorder component is small, which is consistent with the observed homogeneous broadening of the exciton with temperature. Both these features are a measure of the high crystal quality of the perovskite films.

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Ion Migration in Perovskite based Solar Cells — •CHENG LI¹, YU ZHONG¹, ANNA GRÄSER¹, RICHARD HILDNER², and SVEN HÜTTNER¹ — ¹Organic and Hybrid Electronics, Makromol. Chemie I, Universität Bayreuth — ²Experimentalphysik IV, Universität Bayreuth

Solution processed Inorganic-organic halide organometal perovskite solar cells (e.g. CH₃NH₃PbI₃ - xCl_x and CH₃NH₃PbI₃) have demonstrated remarkable efficiencies recently. However, there is still a large space toward the theoretical limitation - the Shockley-Queisser Limit (33%). Hence, more and more interests are concentrated on factors which hinder the approach towards the limit. We employ different methods to especially address the issue of ion migration in perovskite based solar cells: electroabsorption (EA) spectroscopy explores the built-in potential in the working photovoltaic devices and temperature dependent dynamic processes are characterized by their current-

voltage behavior in different temperatures. Furthermore, photoluminescence (PL) characterization, especially fluorescence microscopy (FM), is a powerful tool to investigate the trap states, excited states, charge carrier dynamics and etc., within the individual crystalline grains. We find that the PL blinking behavior in the whole film under the increasing intensity background. In addition, we also observe the process of PL decay during light illumination. We propose that this PL decay is associated with the migration of ions, especially the iodide ions, which are driven by the local electrical field induced by the light illumination.

CPP 11.23 Mon 18:15 Poster B2

Electric characterization of single crystalline and polycrystalline Copper-Zinc-Tin-Sulfide — •MARTIN HANDWERG^{1,2}, RÜDIGER MITDANK¹, JUSTUS JUST², SEGEJ LEVCENCO², THOMAS UNOLD², and AN SASKIA F. FISCHER¹ — ¹AG Neue Materialien, Humboldt-Universität zu Berlin, 12489 Berlin, Germany — ²Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, 14109 Berlin, Germany

Copper Zinc Tin Sulfide (CZTS) is investigated as absorption layer for solar cells to increase their efficiency. To understand the electrical transport mechanism in this material system, temperature dependent electrical conductivity measurements are carried out. Here, the temperature dependence of the electrical conductivity of single crystals and polycrystalline films is investigated. The composition of the polycrystalline films range from high copper (2.29 n_{Cu}/n_{Zn+Sn}) to low copper content (0.47 n_{Cu}/n_{Zn+Sn}), where as the single crystals have a stoichiometric composition. All measurements were performed between 4.2 K and 300 K and show an increase of conductivity with increasing temperature. Different hopping transport mechanism occur in different temperature regions: Nearest neighbor hopping at high temperatures, Mott variable range hopping at intermediate temperatures and Efros-Shklovskii hopping at low temperatures. Grain boundary scattering is detected in polycrystalline material as well. Also, the electrical conductivity increases with increasing copper content. Specific electrical applications can be designed by knowing these material properties.

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Hydrothermal synthesis of methylammonium lead halide perovskites CH₃NH₃PbX₃ (X = Br, Cl, I) — •IRINA ANUSCA, SABRINA IFFLÄNDER, SAMET DUMAN, VLADIMIR V. SHVARTSMAN, and DORU C. LUPASCU — Institute for Materials Science and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Universitätsstraße 15, 45141 Essen, Germany

Compounds with organic-inorganic perovskite structure continues to be in the photovoltaic focus area because these materials have the abilities to combine the properties of inorganic part (high carrier mobility, wide range of bandgaps) and those of organic part (high efficiency luminescence, mechanical properties [1,2]). In the present work we report the preparation of the organic-inorganic perovskites CH₃NH₃PbX₃ (X=Br, Cl, I) by low temperature (130°C) and autogenous pressure hydrothermal route and characterization by X-ray powder diffraction and optical UV-VIS spectroscopy. Keywords Hydrothermal synthesis; organic-inorganic perovskites; absorber solar cells Reference: [1]*KOJIMA, Akihiro ;TESHIMA, Kenjiro ; SHIRAI, Yasuo ; MIYASAKA, Tsutomu: Organometal halide perovskites as visible-light sensitizers for photovoltaic cells. In: Journal of the American Chemical Society 131 (2009), Nr. 17, S. 6050*6051 [2]*SNAITH, Henry J. ; ABATE, Antonio ; BALL, James M. ; EPERON, Giles E. ; LEIJTENS, Tomas ; NOEL, Nakita K. ; STRANKS, Samuel D. ; WANG, Jacob Tse-Wei ; WOJCIECHOWSKI, Konrad ; ZHANG, Wei: Anomalous Hysteresis in Perovskite Solar Cells. In: The Journal of Physical Chemistry Letters 5 (2014), Nr. 9, S. 1511*1515