

CPP 72: Hybrid and Perovskite Photovoltaics I

Time: Thursday 15:00–18:00

Location: C 264

Invited Talk

CPP 72.1 Thu 15:00 C 264

Ionic (in)homogeneity in metal-halide perovskites — ●EVA UNGER — Helmholtz Zentrum Berlin für Materialien und Energie, Albert Einstein Strasse 16, 12489 Berlin — Lunds Universitet, Naturvetarvägen 14, Lund, Schweden

Metal-Halide Perovskites are highly ionic semiconductors, which gives rise to some intriguing material properties. Alloys with increasing complexity have evolved during the past years in the attempt to tune the material band gap and synthesize perovskite semiconductors with increased stability. In mixed-cation and mixed-anion alloys, ionic (in)homogeneity and photo- or bias-induced ion migration can limit the device performance and give rise to strong transient capacitive effects in current-voltage measurements giving rise to hysteresis. This talk will reflect on ionic (in)homogeneity in metal halide perovskites as it evolves from the complex chemistry in solution to the consequence of ionic entropy on crystallization kinetics and how intrinsic ionic homogeneity or externally induced ion redistribution affect device performance.

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Interaction of mobile ions and electronic charge carriers in organic-inorganic perovskites revealed by in-situ photoluminescence and Kelvin probe measurements — ●SUSANNE T. BIRKHOOLD^{1,2}, JAKE PRECHT¹, HONGBIN LIU¹, RAJIV GIRIDHARAGOPAL¹, GILES E. EPERON¹, XIASONG LI¹, LUKAS SCHMIDT-MENDE², and DAVID S. GINGER¹ — ¹Department of Chemistry, University of Washington, Seattle, Washington 98195, United States — ²Department of Physics, University of Konstanz, 78464 Konstanz, Germany

The mixed ionic-electronic conductivity of organic-inorganic perovskites is expected to be responsible for slow response times, current-voltage hysteresis, as well as stoichiometric changes under an electric bias. Here, we present an investigation of the interaction of mobile ions and electronic charges during electric poling of MAPbI₃ and FAPbI₃. We use in-situ photoluminescence and Kelvin probe microscopy on lateral electrodes to correlate temporal changes in radiative recombination with the spatial distribution of ionic and electronic species. While ion migration is observed using both charge injecting and insulating contacts, our results show that non-radiative recombination centers only form if both ion migration and charge injection are present in MAPbI₃. Combining these results with ab initio simulations reveals a complex interaction between ion migration and charge injection that determines defect energetics. Furthermore, temperature dependent SKPM measurements are applied to determine activation energies of ion migration in MAPbI₃ and FAPbI₃.

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Capacitance profiling of planar perovskite solar cells taking mobile charged defects into account — ●MATHIAS FISCHER¹, KRISTOFER TVINGSTEDT¹, VLADIMIR DYAKONOV^{1,2}, and ANDREAS BAUMANN² — ¹Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — ²Bavarian Center for Applied Energy Research (ZAE Bayern), 97074 Würzburg

Currently, numerous approaches are being pursued to generate intentionally doped hybrid perovskite semiconducting materials. The Mott-Schottky analysis is a standard method to determine the doping concentration and the built-in potential. It is based on the fact that the depletion layer thickness, and therefore the capacitance changes with an applied electric field. In perovskite solar cells, however, this is typically not the case. We show experimentally that mobile charged defects might lead to erroneous values when not being considered. Instead, charges accumulated at the interface between the perovskite and a transport layer lead to an inhomogeneous doping distribution which is reflected in an underestimated built-in potential and doping density. We present electrical impedance measurements on planar solution-processed methylammonium and formamidinium lead iodide solar cells in a p-i-n configuration. Thereby, we derived a new measurement routine to determine the depletion layer capacitance as well as the doping density and the built-in potential by means of Mott-Schottky analysis. Finally, we provide informations on intentional or unintentional doping profiles in these solar cells.

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In-Situ Investigation of Ion Migration and Aggregation in Organolead Halide Perovskite Films — ●YU ZHONG¹, CARLOS ANDRES MELO LUNA², RICHARD HILDNER², CHENG LI¹, and SVEN HUETTNER¹ — ¹Macromolecular Chemistry I, University of Bayreuth, Bayreuth, Germany — ²Experimental Physics IV, University of Bayreuth, Bayreuth, Germany

During current-voltage(J-V) measurements, perovskite solar cells(PSCs) exhibit a certain photo-induced instability and hysteresis phenomenon. Firstly, we study the light-induced behavior in CH₃NH₃PbI₃-xCl_x film in-situ, by employing wide-field photoluminescence(PL) microscopy to obtain both the spatially- and temporally-resolved PL image. Along with the increase of the PL intensity under continuous illumination, some areas render PL inactive. A faster and more obvious PL decay process was observed with a higher excitation energy. By characterizing this excitation energy dependent PL decay, we suggest that the PL quenching can be ascribed to an aggregation of iodide ions. Secondly, by introducing phenyl-C61-butyric acid methyl ester(PCBM) in PSCs, hysteresis phenomenon is suppressed. The results of wide-field PL image and temperature dependent J-V curve measurement confirm that PCBM molecules decrease the mobility and increase the activation energy of iodide ions. This real-time investigation of the light soaking of perovskite films provides more details to improve the performance of PSCs. The suppression of the iodide ions movement, e.g. involving PCBM, is a concern for better performance and stability of PSCs.

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Correlation of ion migration and charge carrier trap states in organic-inorganic lead halide perovskites — ●SUSANNE KOCH, SUSANNE T. BIRKHOOLD, and LUKAS SCHMIDT-MENDE — Department of Physics, University of Konstanz, Konstanz, 78457, Germany

While the efficiencies of organic-inorganic perovskite solar cells have seen a strong rise in recent years, the understanding of physical processes inside the material is still limited and devices face stability issues. Many observed phenomena, like current-voltage hysteresis, have been attributed to mobile ions and their interaction with charge carriers. Additionally charge carrier trap states are known to have a strong impact on the carrier dynamics inside the perovskite. Since both ion migration and charge carrier trapping occur simultaneously and are influenced by common material modifications, a correlation between them is possible and could provide information on their origins and contribution to conduction processes. To characterize this possible coupling and to understand electronic and ionic conduction in the perovskite material, the energetic distribution of electronic trap states is studied by measuring thermally stimulated current, while temperature-dependent impedance spectroscopy measurements are employed to extract activation energies for the movement of ionic charges in the material. Using both techniques on comparable systems, where the perovskite is modified targeting specific trap states, should give insights into the correlation of ion migration and trap state distribution.

15 min. break

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Defect spectroscopy in triple-cation hybrid perovskites — ●DAVID DIERING¹, CHARLES HAGES¹, SERGIU LEVCENCO¹, CHRISTIAN WOLFF², DIETER NEHER², and THOMAS UNOLD¹ — ¹Helmholtz-Zentrum Berlin, Germany — ²Universität Potsdam

High power-conversion efficiencies have been observed for hybrid perovskite solar cells based on multi-cation materials, containing methylammonium (MA), formamidinium (FA), cesium (Cs). Thus, the question arises how the presence of these cations alters the absorbers optoelectronic properties and defect physics. Capacitance spectroscopy such as thermal admittance is an established method to search for defects, which may contribute to non-radiative recombination.

In this study, the impact of cesium incorporation in (FAPbI₃)₈₃(MAPbBr₃)₁₇ with cesium contents ranging from 0% to 15% was investigated for a series of solar cells. We performed detailed temperature-dependent admittance measurements, temperature-dependent current-voltage and EQE measurements. The results are correlated with numerical device modelling as well as the

opto-electronic properties of the respective pure absorbers, i.e. charge carrier lifetimes.

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Reducing recombination and enhancing open circuit voltage by Strontium-alloying in multiple cation perovskite solar cells — ●PIETRO CAPRIOGLIO^{1,3}, FENGSHUO ZU², CHRISTIAN M. WOLFF¹, MARTIN STOLTERFROT¹, NORBERT KOCH², BERND RECH³, STEVE ALBRECHT³, and DIETER NEHER¹ — ¹University of Potsdam — ²Humboldt-Universität, Berlin — ³Helmholtz-Zentrum Berlin

State of the art perovskite solar cells still suffer from too low fill factor and open circuit voltage (Voc), which has been related to non-radiative losses mostly happening at the surface. Here, we present the enhancement of the Voc by addition of Strontium (Sr) to a quadruple cation perovskite Rb₅(Cs₅(MA_{0.17}FA_{0.83})Pb(I_{0.83}Br_{0.17})₃)₉₅95. The resulting material displays significantly enhanced photoluminescence (PL) lifetime and absolute PL yield together with a larger splitting of the quasi-Fermi levels. These findings are confirmed by the increase in Voc and in electroluminescence efficiency observed in actual devices. As a result, the power conversion efficiency increases, reaching a PCE of 20.3% under AM1.5G illumination. We show through various photoelectron spectroscopy techniques (UPS/XPS and IPES), how the addition of Sr induces a more n-type surface and enables better contact selectivity. Such a change in energetics is responsible for a substantial suppression of surface and interface recombination. Morphology characterization shows that Sr is mostly segregated close to the charge transport layers, affecting only the interfaces. In conclusion, we propose that Sr-addition enables an appropriate interface modification that helps to reduce Voc losses.

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Structural and Compositional Analyses of Perovskite-like Cesium Lead Halides — ●HANNAH FUNK¹, SEBASTIAN CAICEDO-DAVILA¹, ROBERT LOVRINCIC², CHRISTIAN MÜLLER², MICHAEL SENDNER², FREDERIKE LEHMANN¹, RENÉ GUNDEL¹, ALEXANDRA FRANZ¹, MARKUS WOLLGARTEN¹, BENEDIKT HAAS³, CHRISTOPH T. KOCH³, and DANIEL ABOU-RAS¹ — ¹Helmholtz-Zentrum Berlin, Hahn-Meitner-Platz 1, 14109 Berlin, Germany — ²InnovationLab GmbH, Speyerer Straße 4, 69115 Heidelberg, Germany — ³Humboldt-Universität zu Berlin, Unter den Linden 6, 10099 Berlin, Germany

Inorganic CsPbX₃ (X=I, Cl, Br) thin films are investigated as supposedly more stable alternative to methyl-ammonium-containing hybrid perovskite layers for thin-film solar cells. For the present contribution, wide band gap CsPbBr₃ thin films were synthesized by spin-coating and coevaporation. In addition, also corresponding powder samples were produced as reference. Structural properties were obtained by X-ray diffraction. To resolve the structure more locally high-resolution images as well as electron diffraction patterns were acquired with a transmission electron microscope. The elemental distributions were analyzed by means of energy-dispersive X-ray spectrometry. The evaluation of these results shows that - in contrast to the powder sample the CsPbBr₃ thin films are accompanied by secondary phases such as CsPb₂Br₅ or Cs₄PbBr₆. The present contribution will also report on electron beam damage and how to avoid it.

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Influence of Different Halides and Organic Cations on the Crystallization Dynamics of Perovskite Thin Films — ●ALESSANDRO GRECO, ALEXANDER HINDERHOFER, JAN HAGENLOCHER, and FRANK SCHREIBER — Institute of Applied Physics, University of Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany

The performance of hybrid perovskite thin films in photovoltaic and light emitting devices depends not only on their composition, but also their structural and morphological features.[1] Conventionally, the perovskite thin films in these devices are created with the so-called two-step conversion method, which involves the deposition of an isopropanol solution onto a lead halide precursor (PbX₂, X=I,Br,Cl) via drop casting. The solution contains a defined amount of either methylammonium halide (CH₃NH₃X) or formamidinium halide (CH(NH₂)₂X). The morphology and structural properties of perovskites depend strongly on their composition and the crystallization dynamics. We applied in situ grazing incidence wide angle X-ray scattering (GIWAXS) to determine the reaction rate, domain size and preferred orientation in several perovskite thin films over time. We will discuss how choosing different lead halide precursors in combination with different organic halide solutions can impact the quality and time scale of the structural and morphological development of the perovskite thin films.

[1] N. Arora et al. *Science*, **358**, 768 (2017).

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Topography-dependent phase-segregation in mixed-halide perovskite — ●XIAOFENG TANG, GEBHARD MATT, and CHRISTOPH BRABEC — Institute of Materials for Electronics and Energy Technology (i-MEET), Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany

Mixed-halide perovskites have emerged as promising materials for optoelectronics due to the merit of their tunable bandgap in the entire visible region. A challenge remains however in the instability of the bandgap. This bandgap instability is attributed to phase-segregation, which strongly affects the voltage attained in mixed-halide perovskite-based solar cells and seriously restricts the applications.

In this work, we provide an in-depth insight into this phenomenon with a combination of local-resolved and bulk investigations. We demonstrate phase-segregation in mixed-halide perovskite is topography-dependent. By using spatially-resolved photoluminescence spectroscopy, we show the gradual red-shift of the photoluminescence signal at the grain boundaries of mixed-halide perovskite during the consecutive illumination. Contrarily, we observe the spectrally stable emission exclusively stems from the grain centers. Such difference is further evidenced by bulk characterizations, showing the illuminated mixed-halide perovskite presenting double band-edge features. The above spatially selective halide separation provides a strong argument that ion migration indeed dominantly occurs along these boundaries and will support the development of better passivation strategies, ultimately allowing to process environmentally stable perovskite films.