

CPP 7: Hybrid and Perovskite Photovoltaics I (joint session CPP/DF/DS/HL, organized by CPP)

Time: Monday 15:00–17:30

Location: H38

CPP 7.1 Mon 15:00 H38

Effect of phase transition on photoluminescence polarization of single perovskite nano-objects — •DANIELA TÄUBER¹, ALEXANDER DOBROVOLSKY¹, RAFAEL CAMACHO^{1,2}, and IVAN SCHEBLYKIN¹ — ¹Chemical Physics, Lund University, Lund, Sweden — ²Department of Chemistry, University of Leuven, Leuven, Belgium

We use 2D polarization resolved microscopy to study the polarization of single $CH_3NH_3PbI_3$ perovskite nano-objects in excitation and emission at 295, 152 and 77 K. Depending on size and shape, polarization of up to 70% was observed at 77 K in emission, while it is in general smaller in excitation, and it decreases with increasing temperature. For wire-shaped objects the polarization is along the long axis, which points to contributions from antenna effects and crystal growth direction in combination with asymmetric crystal structures. The difference seen in excitation and emission may be caused by the band structure and the excitation wavelength at 448 nm.

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CPP 7.2 Mon 15:15 H38

Energy Levels at Perovskite/Electron Transport Layer Interfaces — •FENGSHUO ZU¹, JOHANNES FRISCH¹, LIANGSHENG LIAO², and NORBERT KOCH¹ — ¹Institut für Physik & IRIS Adlershof, Humboldt-Universität zu Berlin, Brook-Taylor-Str. 6, 12489 Berlin, Germany — ²FUNSOM, Soochow University, Jiangsu 215123, China

organometal halide perovskites attract substantial attention for high-efficiency thin film solar cells. Numerous studies are focused on film processing and device configuration variation in order to further improve device efficiency, but the fundamental physics in particular regarding interfacial energy level alignment with charge transport materials (e.g., fullerene derivatives) are yet poorly understood. It is generally believed that perovskites form type-II p-n junctions with C60 or PCBM, which would favor the charge separation process at the interface. To substantiate this proposition, we performed TRPL and UPS measurements to investigate the interface energy levels and the charge separation process at perovskite/fullerene junctions. However, contrary to the common believe, our measurements show that both junctions exhibit n-n type-I level alignment. TRPL results show no different decay channels with or without fullerene layers, which indicates the perovskite/fullerene interface does not provide a driving force for charge separation. Nonetheless, our solar cells with PCBM junctions show reasonable performance, with a power conversion efficiency of 9.30%. In contrast, the perovskite/C60 solar cells show much lower efficiency, which we attribute to upward band bending within perovskite when in contact with C60.

CPP 7.3 Mon 15:30 H38

The influence of hole transporting materials on the charge transport in stacked perovskite-based systems — •KATHRIN BADER^{1,2}, MICHIEL PETRUS^{1,2}, THOMAS BEIN^{1,2}, PABLO DOCAMPO^{1,2}, MATTHIAS HANDLOSER^{1,2}, and ACHIM HARTSCHUH^{1,2} — ¹Department of Chemistry and CeNS, LMU Munich — ²Nanosystems Initiative Munich (NIM)

Hybrid metal halide perovskites have become a focal point of the photovoltaic community as promising candidates for next-generation solar cells. Extremely fast progress in this field has taken efficiencies to over 20% [1] and lead to the development of a large variety of material compositions, preparation techniques and device structures [2]. Although the fabrication of the perovskite absorber itself is comparably cheap, latest device architectures incorporate the expensive hole transporting material (HTM) spiro-OMeTAD. To reduce the overall production costs for perovskite-based devices alternative organic HTMs have been developed [3]. Here we use a contact-less technique based on time-resolved laser scanning confocal microscopy [4] to visualize the influence of different HTMs on $CH_3NH_3PbI_3$ thin films. We investigate charge carrier transport properties and photoluminescence lifetimes of individual HTM layers as well as stacked perovskite/HTM systems and identify potential candidates to replace the expensive spiro-OMeTAD in the device structure. [1] Green, M. A. et al., Prog. Photovolt: Res. Appl. 2015, 23, 805-812. [2] Green, M. A. et al., Nature Photon. 2014, 8, 506-514. [3] Petrus, M. L. et al., J. Mater. Chem. A 2015, 3, 12159-12162. [4] Bader, K. et al., ACS Photonics 2015, under review.

CPP 7.4 Mon 15:45 H38

Substrate-dependent electronic structure and film formation of MAPbI₃ perovskites — •SELINA OLTGHOF and KLAUS MEERHOLZ — University of Cologne, Institute for Physical Chemistry, Luxemburger Straße 116, 50939 Köln, Germany

Hybrid organic / inorganic perovskite materials have attracted significant attention in the past years. However, little is known so far about the electronic structure and, more importantly, the energetic alignment at interfaces. Here, we present the investigation of the interface formation between the perovskite MAPbI₃ and various substrate materials. The perovskite films are incrementally evaporated in situ while the electronic structure is evaluated using photoelectron spectroscopy (PES). The results show a deviation from the commonly assumed flat band condition, and that dipole formation and band bending dominate the interfaces. More importantly, we find a deviation from the expected perovskite stoichiometry at the interface due to a wide variety of chemical interaction taking place, which are highly dependent on the nature of the substrate material. On metal oxides the perovskite film formation is hindered and it takes up to 30 nm for the density of states of perovskite to emerge in the PES measurements. Therefore, the nature of the substrate not only changes the energetic alignment of the perovskite, but can hinder film formation and introduce gap states as well.

CPP 7.5 Mon 16:00 H38

In-Situ Investigation of Optoelectronic Properties during One-Step Synthesis of MAPbI_{3-x}Cl_x Perovskite — •KLARA SUCHAN, JUSTUS JUST, MARTIN KÄRGELL, DAN R. WARGULSKI, PASCAL BECKER, and THOMAS UNOLD — Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Hahn-Meitner-Platz 1, 14109 Berlin, Germany

Organometal halide perovskites have emerged as promising absorber materials for solid state solar cells since 2012. With the fast improvement in power conversion efficiency to over 20%, perovskites have high prospects for low-cost, high efficiency solar cell production. $CH_3NH_3PbI_{3-x}Cl_x$ layers are prepared by a one-step solution based process using $PbCl_2$ and MAI precursors dissolved in DMF. Since solution based processes do not need cost intensive vacuum technology and no high-temperature annealing steps, they yield high potential for industrial implementation. However, little is known about the exact mechanisms during synthesis, leading to poor reproducibility. Employing in-situ photoluminescence and reflection imaging as well as spectroscopy we monitor the growth process. The evolution of optoelectronic properties for various temperature profiles and annealing durations is analysed. Additional X-ray diffraction measurements during various stages of the process are used to evaluate structural changes occurring during film formation.

CPP 7.6 Mon 16:15 H38

Reversible Laser induced Amplified Spontaneous Emission from Coexisting Tetragonal and Orthorhombic Phases in Hybrid Lead Halide Perovskites — •FABIAN PANZER^{1,2,3}, SEBASTIAN BADERSCHNEIDER^{2,4}, TANAJI GUJAR⁵, THOMAS UNGER^{1,2}, HEINZ BÄSSLER², RALF MOOS³, MUKUNDAN THELAKKAT⁵, RICHARD HILDNER^{2,4}, and ANNA KÖHLER^{1,2} — ¹Experimental Physics II — ²Bayreuth Institute of Macromolecular Research (BIMF) — ³Department of Functional Materials — ⁴Experimental Physics IV — ⁵Applied Functional Polymers, Macromolecular Chemistry I, University of Bayreuth, 95440 Bayreuth, Germany

Organic-inorganic mixed halide perovskites received enormous attention over the last few years due to their outstanding performances when used as absorber material in solar cells or in light emitting devices, while offering the possibility for low cost production, e.g. by solution-processing. Furthermore it is known that most halide perovskite materials can exist in different crystal structures, depending on environmental conditions such as temperature. Here we show that a coexistence of tetragonal and orthorhombic phases within the same crystalline grain can be optically induced into the halide perovskite $CH_3NH_3PbI_3$ at low temperatures, leading to amplified spontaneous emission simultaneously at two distinct wavelengths. The emission feature associated with the tetragonal phase can be reproducibly written,

read-out, and erased at 5 K by choosing appropriate laser fluences or raising the temperature. Finally we show to which extend our findings can be exploited for use as an all optical data storage device.

15 min. break

CPP 7.7 Mon 16:45 H38

Iodine Migration and its Effect on Hysteresis in Perovskite Solar Cells — CHENG LI¹, STEFFEN TSCHUSCHER², FABIAN PAULUS³, PAUL HOPKINSON³, JOHANNES KIESSLING¹, ANNA KÖHLER², YANA VAYNZOF³, and •SVEN HÜTTNER¹ — ¹Organic and Hybrid Electronics, Makromol. Chemie I, Universität Bayreuth — ²Experimentalphysik II, Universität Bayreuth — ³Centre for Advanced Materials, Universität Heidelberg

Solution-processed organic-inorganic hybrid perovskite solar cells (e.g. $\text{CH}_3\text{NH}_3\text{PbI}_3-x\text{Cl}_x$) currently exhibit promising performances. However, the origin of the observed hysteresis in the current-voltage (J-V) curves, i.e. the sweeping-history-dependent electrical current, is still not sufficiently understood. To investigate its origin we employ electroabsorption (EA) spectroscopy to explore the built-in potential in working photovoltaic devices. Furthermore, we study the temperature dependent dynamic processes in perovskite solar cells by characterizing their current-voltage behavior at different temperatures. The electrical current relaxation process during temperature dependent J-V measurements provides the evidence of the migration of ions. In order to investigate the nature of these ions, we further present X-ray photoemission spectroscopy (XPS) experiments which shows the elemental redistribution after applying an electrical bias. The results give a concise picture that mainly iodide ions can be driven by an external electrical field and then accumulate at the respective perovskite/electrode interfaces. The migration and accumulation of iodide ions create a modulation of the respective interfacial barriers which is the origin of the hysteresis.

CPP 7.8 Mon 17:00 H38

The Importance of Hydrogen Defect Migration in Organic-Inorganic Perovskites — •DAVID A. EGGER¹, LEEOR KRONIK¹, and ANDREW M. RAPPE² — ¹Department of Materials and Interfaces, Weizmann Institute of Science, Rehovoth 76100, Israel — ²The Makineni Theoretical Laboratories, Department of Chemistry, University of Pennsylvania, Philadelphia, PA 19104-6323, USA

Solar cells based on organic-inorganic perovskites have been proven

to be remarkably efficient in recent years. However, they exhibit hysteresis in the current-voltage curves, and their stability properties, especially in the presence of water, are problematic. Both issues are possibly related to ionic diffusion phenomena occurring in the hybrid perovskite material. Using first-principles calculations based on density functional theory, we study the properties of an important defect in hybrid perovskites - interstitial hydrogen.[1] We show that differently charged defects occupy different sites in the hybrid perovskite crystal, which allows for an ionization-enhanced defect migration following the Bourgoin-Corbett mechanism. Our analysis further highlights the structural flexibility of organic-inorganic perovskites, where successive displacements of iodide combined with hydrogen bonding enables proton diffusion with low migration barriers. These findings indicate that hydrogen species can be highly mobile in hybrid perovskite solar cells and thus relevant for their performance.

[1] *Angew. Chem. Int. Ed.* 54, 12437 (2015)

CPP 7.9 Mon 17:15 H38

Humidity-induced hydration of methylammonium lead iodide perovskite: Understanding and prevention — •YINGHONG HU¹, PABLO DOCAMPO¹, AURÉLIEN LEGUY², and PIERS BARNES² — ¹Department of Chemistry, Ludwig-Maximilians-Universität, 81377 München, Germany — ²Physics Department, Imperial College, London, SW7 2AZ, United Kingdom

The long-term stability of hybrid metal halide perovskite solar cells is of paramount importance for the future of this emerging technology. In particular, solar cells composed of methylammonium lead iodide (MAPI) are notorious for their sensitivity to moisture. Here, we elucidate the humidity-induced degradation mechanisms occurring within the perovskite material and report on the development of a novel interlayer which improves the moisture stability of perovskite solar cells. Our results show that MAPI undergoes a stepwise transformation into two species of hydrated MAPI crystal phases upon exposure to moist air at room temperature. However, we show that this hydration process can be reversed when the material is subsequently dried in nitrogen. In contrast to water vapor, the presence of liquid water directly leads to the irreversible decomposition of MAPI to form lead iodide. Our developed functional moisture barrier significantly enhances the stability of the perovskite solar cells towards cycles of hydration and dehydration. We believe that our results open new possibilities for the design of moisture resistant, highly efficient perovskite solar cells.