

HL 53: Fundamentals of Perovskite Photovoltaics V (joint session CPP/DS/HL)

Time: Wednesday 10:15–12:45

Location: ZEU 250

Invited Talk

HL 53.1 Wed 10:15 ZEU 250

Light-induced degradation of methylammonium and formamidinium PbI₃ perovskites — ●NORBERT H. NICKEL, FELIX LANG, VICTOR V. BRUS, and JÖRG RAPPICH — Helmholtz-Zentrum Berlin für Materialien und Energie, Institut für Silizium Photovoltaik, Kekuléstr. 5, 12489 Berlin

We investigate the stability of methylammonium (CH₃NH₃⁺ - MA) and formamidinium (HC(NH₂)₂⁺ - FM) lead iodide perovskite films using visible and ultra violet light in oxygen atmosphere and in vacuum. Insight into the degradation mechanisms was obtained from in-situ Fourier-transform infrared absorption (FT-IR), photoluminescence, and gas effusion measurements. We revisited the light-induced degradation of MAPbI₃ in the presence of oxygen. Illumination in O₂ atmosphere results in a swift degradation. Isotope experiments clearly show that O₂ acts as a catalyst decomposing MA ions into CH₃NH₂ and hydrogen. In case of FMPbI₃ perovskites illumination in the presence of O₂ results in a more complex reaction; decomposition of the FM ions occurs at the N-C-N bonds and as a result CO₂ and C = O molecules are formed that rapidly diffuse out of the crystalline lattice.

In addition, we present experimental evidence of a hitherto unknown but fundamental degradation mechanism of MAPbI₃ and FMPbI₃ perovskite layers due to exposure to visible and ultra violet light. This degradation mechanism does not require the presence of oxygen or other constituents. Our data indicate that the molecular orbitals of the organic ions are not in resonance with the energy bands of the perovskite.

HL 53.2 Wed 10:45 ZEU 250

Degradation Studies of Methylammonium Lead Iodide under Controlled Exposure to Oxygen and Light — ●PAUL FASSL, QING SUN, DAVID BECKER-KOCH, ALEXANDRA BAUSCH, and YANA VAYNZOF — Kirchhoff-Institute for Physics / Centre for Advanced Materials, Heidelberg University, Germany.

Despite the remarkable increase in the power conversion efficiency of hybrid organometal-halide perovskite solar cells reaching 22% to date, the low environmental stability of the material remains only partly understood. While the instability of methylammonium lead iodide (CH₃NH₃PbI₃) in humid atmospheres has been studied experimentally as well as theoretically, degradation in the presence of oxygen and light has just recently been reported.

In this work, planar pinhole-free perovskite films are degraded under dry conditions with precisely controlled exposure to various oxygen levels and simulated sunlight using our environmental stability testing rig and then characterized by multiple techniques such as XPS, PDS, PL, AFM and SEM. These results are then correlated to the efficiency decay of photovoltaic devices (ITO/PEDOT:PSS/CH₃NH₃PbI₃/PCBM/BCP/Ag), where the bare perovskite film has been first degraded under identical conditions.

Our results show that exposure to oxygen and light is one of the major reasons for the fast degradation of unencapsulated perovskite solar cells at ambient conditions and that the morphology and defect density of the pristine perovskite film has a considerable impact on the rate of degradation.

HL 53.3 Wed 11:00 ZEU 250

Real-Time Observation of Iodide Ion Migration in Methylammonium Lead Halide Perovskites — ●CHENG LI¹, ANTONIO GUERRERO², YU ZHONG¹, ANNA GRÄSER¹, CARLOS ANDRES MELO LUNA³, JÜRGEN KÖHLER³, JUAN BISQUERT², RICHARD HILDNER³, and SVEN HUETTNER¹ — ¹Macromolecular Chemistry I, Universität Bayreuth, Universitätstr. 30, 95447 Bayreuth, Germany — ²Institute of Advanced Materials (INAM), Universitat Jaume I, 12006 Castell, Spain — ³Experimental Physics IV and Bayreuth Institute of Macromolecular Research, Universität Bayreuth, Universitätstr. 30, 95447 Bayreuth, Germany

To investigate the origin of current-voltage (J-V) hysteresis characteristic in perovskite solar cells (PSC), we utilize correlated time-resolved photoluminescence (PL) microscopy and impedance spectroscopy (IS) on perovskite films to in-situ investigate both the spatial and temporal evolution of these PL inactive areas under external optical/electrical fields. We attribute the formation of PL inactive domains to the migration and accumulation of iodine ions under external electrical

fields. Furthermore, we fabricate and characterize PSC incorporating phenyl-C61-butyric acid methyl ester (PCBM) and PCBM polymer to investigate the influence of diffusions of PCBM molecules on the hysteretic behavior. Following that, the step-wise temperature dependent J-V measurement demonstrates the reduction of migration with the aid of PCBM molecules. Hence, it is proposed that the elimination/alleviation of J-V curve hysteresis is ascribed to the diffusion of PCBM molecules, which passivate the iodide related defects.

HL 53.4 Wed 11:15 ZEU 250

Polarization of Methylammonium Lead Halide Perovskite Films on Microstructured Arrays — ●MARTINA STUMPP^{1,3}, RAFAEL RUESS^{1,3}, JAN MUESSENER^{2,3}, and DERCK SCHLETTWEIN^{1,3} — ¹Justus-Liebig-University Giessen, Institute of Applied Physics — ²Justus-Liebig-University Giessen, 1st Physics Institute — ³Justus-Liebig-University Giessen, Laboratory for Materials Science

Despite the great advances of methylammonium lead halide perovskites in photovoltaics, many properties such as the I-V hysteresis of such films are not fully understood and, therefore, need detailed investigation. In the current study, CH₃NH₃PbI₃ and CH₃NH₃Pb(I_{3-x}Cl_x)₃ films were prepared on microstructured gold or platinum electrode arrays on SiO₂/Si wafers in order to use symmetric contacts and widely inert substrates. The perovskite films were poled with high voltages and the current was measured under variation of ambient parameters and analyzed in detail. Following the poling of the samples, voltage sweeps were performed. The I-V characteristics during these sweeps showed clearly that the perovskite films were polarized and that the polarization had a persistent character. Additionally, different hysteresis characteristics were observed. The origin of regular and inverted characteristics will be discussed.

15 min break

HL 53.5 Wed 11:45 ZEU 250

Characterization of the perovskite solar cells containing atomic layer deposited Al₂O₃ buffer layer. — ●MALGORZATA KOT¹, KONRAD WOJCIECHOWSKI², HENRY SNAITH², and DIETER SCHMEISSER¹ — ¹BTU Cottbus-Senftenberg, Konrad-Wachsmann-Allee 17, 03046 Cottbus, Germany — ²Clarendon Laboratory, University of Oxford, Parks Road, Oxford, OX13PU, UK

Hybrid perovskites have potential to overcome performance limits of the current solar cell technologies and achieve low cost and high versatility. Nonetheless, they are prone to degradation in presence of moisture within a couple of hours or days. In this work, we use the atomic layer deposition (ALD) of Al₂O₃ on the CH₃NH₃PbI₃ perovskite at room temperature in order to verify if this thin ALD layer may protect the perovskite film against moisture degradation and to check the impact of the Al₂O₃ on the solar to power conversion efficiency (PCE). Depth profiling X-ray photoelectron spectroscopy study shows that the ALD precursors are chemically active only at the perovskite surface and the film bulk is not affected. The perovskite film coated with Al₂O₃ layer has enhanced moisture stability. Solar cells with a fresh-made CH₃NH₃PbI₃ perovskite film have shown PCE of 15.4%, while the one with 50 days aged perovskite only 6.1%. However, when the aged perovskite is covered with RT-ALD-Al₂O₃ the PCE value is clearly enhanced.[1]

[1] M. Kot et al., Room temperature ALD impact on efficiency, stability and surface properties in perovskite solar cells, ChemSusChem, accepted.

HL 53.6 Wed 12:00 ZEU 250

Influence of the grain size on electronic properties of methylammonium lead iodide — ●OLEKSANDRA SHARGAIEVA, FELIX LANG, JÖRG RAPPICH, THOMAS DITTRICH, BERND RECH, and NORBERT NICKEL — Helmholtz-Zentrum Berlin, Institute for Silicon Photovoltaics, Kekulestr. 5, D-12489 Berlin (Germany)

Recently, hybrid perovskites have drawn the attention of researchers due to huge potential as absorbers in photovoltaic devices. The biggest advantage of such materials is the ease of the preparation within low costs leading to highly efficient solar cells. However, the solution based processing often lacks a control over crystal quality of obtained material. Despite the numerous reports showed different methods to

improve morphology of perovskite layer, the influence of microscopic structure on properties of the material is not fully understood.

In this work we present a new approach to tune the grain size of CH₃NH₃PbI₃ perovskite from 150 to 1000 nm with about 100 nm step. The new method is based on solid-phase recrystallization and provides a reliable way to control the grain size and hence, systematically study the influence of the grain size on optical and electrical properties of the material. The recrystallized perovskite layers were characterized using photoluminescence spectroscopy and surface photovoltage measurements. The recrystallized samples demonstrated a pronounced increase of the PL intensity due to lower defect density in treated material. Furthermore, our study showed a direct correlation between grain size and the transport length, L, with the maximum value of 900 nm.

HL 53.7 Wed 12:15 ZEU 250

Investigation of novel material systems for hybrid photovoltaics - alternatives for the paradigm — •NURI HOHN¹, 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. Hybrid devices combine these advantages with the chemical/physical stability of inorganic materials and, thus, overcome the issue of limited lifetimes of purely organic cells. Poly(styrene-block-ethylene oxide) templated sol-gel chemistry is used to synthesize high surface-to-volume ratio, mesoporous titania thin films, which allows for precise structure control and an increased amount of interface. The n-type, electron conducting titania thin film serves as a basis for novel organic material studies. The studies aim to

introduce new material combinations to the field of hybrid PV and to open up pathways for enhanced efficiency in terms of energy conversion and band alignment. Thin film spectral absorption characterization is carried out via UV/Vis measurements. Furthermore, morphological characterization is realized via SEM and XRD to address to surface structure and the crystallinity of the material.

HL 53.8 Wed 12:30 ZEU 250

Water-processed hybrid solar cells: deposition of the active layer with vertical composition gradient — •VOLKER KÖRSTGENS¹, FLORIAN BUSCHEK¹, MARTIN WÖRLE², HRISTO IGLEV², WIEBKE OHM³, STEPHAN V. ROTH³, REINHARD KIENBERGER², and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik-Department, LS Funktionelle Materialien, James-Frank-Str. 1, 85748 Garching — ²TU München, Physik-Department, LS Laser- und Röntgenphysik, James-Frank-Str. 1, 85748 Garching — ³DESY, Notkestr. 85, 22607 Hamburg

Particular environmentally friendly processing of hybrid solar cells with the solvent water is feasible with an active layer consisting of laser-ablated titania and a water-soluble polythiophene [1]. One way to optimize conversion efficiencies of these devices is the introduction of a vertical compositional gradient of the two components of the active layer. Dip-coating and spray-coating have been utilized as techniques which are suitable for the cost-effective preparation of hybrid photovoltaics. We followed the development of the morphology during spray deposition in situ with high spatial and temporal resolution. The mesoscale was probed with GISAXS and the crystallinity of the polymer and the inorganic component was probed with GIWAXS. The changes of the morphology and the influence on photovoltaic performance with the introduction of a compositional gradient are discussed. [1] Körstgens et al., *Nanoscale* 7, 2900 (2015).