

CPP 31: Hybrid and Perovskite Photovoltaics III (joint session CPP/DF/DS/HL, organized by DS)

Time: Wednesday 9:30–11:45

Location: H11

CPP 31.1 Wed 9:30 H11

Impact of Preparation Conditions on the Ionization Energy and Electronic Structure of CH₃NH₃PbI₃ Perovskites — ●JENNIFER EMARA¹, TOBIAS SCHNIER¹, NEDA POURDAVOUD², THOMAS RIEDL², KLAUS MEERHOLZ¹, and SELINA OLTHOFF¹ — ¹University of Cologne, Institute for Physical Chemistry, Luxemburger Straße 116, 50939 Köln, Germany — ²Institute of Electronic Devices, University of Wuppertal, Rainer-Grünter-Straße 21, 42119 Wuppertal, Germany

Hybrid organic/inorganic halide perovskites have lately been a topic of great interest in the field of solar cell applications, with the potential to achieve device efficiencies exceeding other thin film device technologies. Yet, large variations in device efficiency and basic physical properties are reported. This is due to unintentional variations during film processing, which have not been systematically investigated so far. We therefore conducted an extensive study of the electronic structure of a large number of CH₃NH₃PbI₃ perovskite films produced by different preparation methods and by varying precursor ratios. We show that variations in film stoichiometry lead to vast changes in the density of states (DOS), and changes in ionization energy, which can be intentionally tuned by almost 1 eV. Using x-ray diffraction measurements, we find the variations in film stoichiometry are not due to the formation of separate phases, but that interstitials and vacancies are homogeneously distributed within the material. Implementing the prepared perovskite layer materials in solar cells, we find a clear correlation between the changes in DOS with the overall power conversion efficiency.

CPP 31.2 Wed 9:45 H11

Two dimensional organometal halid perovskite nanosheets in light emitting application — ●RUI WANG¹, ZHENDONG FU¹, VITALIY PIPICH¹, ALEXANDROS KOUTSIOMPAS¹, STEFAN MATTAUCH¹, PETER MÜLLER-BUSCHBAUM², and HENRICH FRIELINGHAUS¹ — ¹Jülich Center for Neutron Science, outstation at FRM II, Lichtenbergstr. 1, 85747 Garching — ²TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching

Two dimensional functional materials have created intensive research interest for high efficiency solar cells. Recently low dimensional perovskite nanocrystals, such as 2D perovskite nanosheets have been reported to possess reduced fluorescence decay times, an increased exciton binding energy and low conductivity in certain crystallographic directions. Consequently, these lower dimensional perovskites can be utilized for light emitting applications. In the present work, 2D nanosheet perovskites are formed by using octylamine bromide as capping ligands. GISANS combined with neutron reflectivity (NR) are applied to investigate the structure buried inside the thin films. GISANS had proven to be a powerful technique for thin film morphology investigations. NR guarantees that information about nanometer sized layers can be accessed. We present the determined structures in terms of optical properties, grain size information and stacked layered characteristic.

CPP 31.3 Wed 10:00 H11

Morphology and crystal orientation of hybrid perovskite thin films for application in high efficiency solar cells — ●JOHANNES SCHLIPF¹, LUKAS OESINGHAUS¹, NADJA GIESBRECHT², YINGHONG HU², SIGRID BERNSTORFF³, THOMAS BEIN², PABLO DOCAMPO², and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — ²Department of Chemistry and CENS, LMU München, 80539 München, Germany — ³Elettra-Sincrotrone Trieste S.C.p.A., Basovizza, 34149 Trieste, Italy

Organo-metal halide perovskites mark a paradigm shift in photovoltaic research, as they combine high efficiencies challenging conventional inorganic solar cells with easy processing and cheap abundant precursor materials. Recent reports of power conversion efficiencies around 20% are possible due to remarkable material properties and their highly crystalline nature even when processed from solution. However, photovoltaic performance is directly linked to film morphology which in turn depends on the fabrication method. We investigate hybrid perovskite thin films of high efficiency solar cells prepared by various synthe-

sis protocols with X-ray diffraction, GIWAXS and GISAXS. Thereby, we evidence different crystallization mechanisms that lead to certain morphologies and crystal orientations reflecting the chosen synthesis method [1]. We link these findings to the photovoltaic performance and aim at a rational development of new synthesis methods for high efficiency perovskite solar cells.

[1] Schlipf et al: J. Phys. Chem. Lett, 6, 1265-1269, 2015.

CPP 31.4 Wed 10:15 H11

Influence of annealing time on crystal structure and composition of CH₃NH₃PbI₃-xCl_x mixed halide perovskite film — ●MARYLINE RALAIARISOA¹, YAN BUSBY², JOHANNES FRISCH¹, INGO SALZMANN¹, JEAN-JACQUES PIREAUX², and NORBERT KOCH¹ — ¹Humboldt-Universität zu Berlin, Institut für Physik, Brook-Taylor-Str. 6, 12489 Berlin, Germany — ²Research Center in the Physics of Matter and Radiation, Laboratoire Interdisciplinaire de Spectroscopie Electronique (LISE), University of Namur, 5000 Namur, Belgium

Thermal annealing is a crucial step for the formation of crystalline perovskite films from precursor solution. However, the structural evolution during perovskite film formation and particularly its composition during annealing have not been thoroughly characterized yet. Such characterization is essential to understand the mechanisms leading to the complete conversion to perovskite. Using ToF-SIMS, we monitored the changes in composition and structure of CH₃NH₃PbI₃-x Cl_x perovskite films after two different annealing stages, that is, before and after complete perovskite crystallization. At the early stage of annealing, our results show phase separation throughout the entire film depth into one where perovskite was formed and another where mostly the inorganic precursor PbCl₂ was detected. After sufficiently long annealing, we found a single perovskite phase of homogeneous composition on the micrometer scale. By means of UPS, we further observed that perovskite films become more n-type for longer annealing time, which correlates the morphological evolution and the surface electronic structure.

15 min. break.

CPP 31.5 Wed 10:45 H11

Ferroelasticity in methylammonium lead halide perovskite? — ILKA HERMES¹, SIMON BRETSCHNEIDER¹, VICTOR BERGMANN¹, DAN LI¹, ALEXANDER KLASSEN^{1,2}, JULIAN MARS¹, WOLFGANG TREMEL², FRÉDÉRIC LAQUAI¹, HANS-JÜRGEN BUTT¹, MARKUS MEZGER^{1,2}, RÜDIGER BERGER¹, BRIAN RODRIGUEZ³, and ●STEFAN WEBER^{1,2} — ¹MPI for Polymer Research, Mainz — ²Johannes Gutenberg University, Mainz — ³University College Dublin, Ireland

Methylammonium lead halide (MAPbX₃) perovskite materials show an outstanding performance in photovoltaic devices. However, some material properties, especially the possible ferroic behavior, remain unclear. We observed distinct nanoscale periodic domains in the piezoresponse of MAPbI₃(Cl) grains. The structure and the orientation of these striped domains is indicating ferroelasticity as their origin. By correlating vertical and lateral piezoresponse force microscopy experiments performed at different sample orientations with x-ray diffraction, the preferred domain orientation was assigned to the $a_1 - a_2$ -phase. The observation of the twin domains appears to strongly depend on the preparation route and the film texture and is thought to be induced by internal strain during the cubic-tetragonal phase transition.

CPP 31.6 Wed 11:00 H11

XPS study of the ALD growth of Al₂O₃ on the CH₃NH₃PbI₃ — ●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

Organic-inorganic lead halide perovskites have emerged as very attractive absorber materials for the fabrication of low cost and high efficiency solar cells, but a delicate nature of these films is one of the main challenges for a successful commercialization. Typically, when exposed to air or moisture, perovskite films degrade within a cou-

ple of hours or days. Moreover, the methylammonium lead triiodide ($\text{CH}_3\text{NH}_3\text{PbI}_3$) perovskite cannot sustain a prolonged annealing at temperatures around 85°C . In this work, we are investigating stability (upon air and thermal exposure) of a $\text{CH}_3\text{NH}_3\text{PbI}_3$ perovskite film coated with a thin layer of Al_2O_3 deposited by atomic layer deposition (ALD). In particular, the chemical and electronic changes occurred at the $\text{Al}_2\text{O}_3/\text{CH}_3\text{NH}_3\text{PbI}_3$ interface during the first 50 ALD cycles were monitored ex-situ by high-resolution and surface-sensitive synchrotron-based X-ray photoelectron spectroscopy (SR-XPS). The advantage of the ALD as a deposition method is that it can produce extremely dense layers with a very precise thickness control at room temperature. Detailed SR-XPS data analysis and a stability test of the perovskite film with alumina will be presented.

CPP 31.7 Wed 11:15 H11

Water based hybrid solar cells: spray deposition of the active layer monitored with x-ray scattering methods — ●VOLKER KÖRSTGENS¹, CHRISTOPH MAYR¹, STEPHAN V. ROTH², HRISTO IGLEV³, REINHARD KIENBERGER³, and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching — ²DESY Photon Science, Notkestr. 85, 22607 Hamburg — ³TU München, Physik-Department, LS Laser- und Röntgenphysik, James-Franck-Str. 1, 85748 Garching

Spray-coating is a technique suitable for the large-scale and cost-effective preparation of hybrid photovoltaics. Unique environmentally friendly processing of hybrid solar cells can be realized with systems based on the solvent water. Using an active layer consisting of laser-ablated titania nanoparticles and water-soluble poly[3-(potassium-6-hexanoate)thiophene-2,5-diyl] (P3P6T) hybrid solar cells were realized. [1] For the performance of these devices the morphology of the active layer is of major importance. We followed the development of the morphology in situ with high spatial and temporal resolution. The mesoscale was probed with GISAXS and the crystallinity of the poly-

mer and the inorganic component was probed with GIWAXS. The changes of the morphology of the active layer with increasing thickness and the dependence on the blocking layer chosen as the initial substrate are discussed and implications for an improved spray protocol will be given.

[1] Körstgens et al., *Nanoscale* 7, 2900 (2015).

CPP 31.8 Wed 11:30 H11

A low temperature route towards hierarchically structured titania films for thin hybrid solar cells — ●LIN SONG¹, AMR ABDELSAMIE¹, CHRISTOPH J. SCHAFFER¹, VOLKER KÖRSTGENS¹, WEIJIA WANG¹, NICOLA HÜSING², PAOLO LUGLI³, and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — ²Materialchemie, FB Chemie und Physik der Materialien, Universität Salzburg, Hellbrunnerstr. 34, 5020 Salzburg, Austria — ³TU München, Department of Electrical Engineering and Information Technology, Institute for Nanoelectronics, 80333 München, Germany

Fabricating titania based solar cells at low temperature has a high significance regarding energy efficacy, since most of photovoltaic devices with titania require high-temperature calcination. Moreover, a low-temperature process offers the potential for flexible solar cells. However, this kind of solar cells has a low efficiency. In order to improve the device performance, we make superimposed structural order on titania films from nanometer to submicrometer length scales. Hierarchical structural order enhances light harvesting in solar cells, thereby enhancing the photovoltaic performance. Titania nanostructures are obtained via PS-b-PEO template assisted sol-gel processing. Nanoimprint lithography (NIL) provides ordered submicrometer patterns as a superstructure over nanostructured titania films. SEM and AFM measurements map the film surface morphology, and GISAXS measurements yield information about the bulk film morphology. The optoelectronic properties are examined by UV/Vis spectroscopy.