

CPP 61: Perovskite and photovoltaics III (joint session HL/CPP)

Time: Wednesday 9:30–12:30

Location: POT 251

CPP 61.1 Wed 9:30 POT 251

Efficiency dependence on incident angle for CIGS solar cells — ●LILÉN VÖHRINGER¹, JANET NEERKEN¹, HIPPOLYTE HIRWA¹, JÖRG OHLAND¹, ALFONS WEBER², ROBERT LECHNER², THOMAS DALIBOR², SASCHA SCHÄFER¹, and STEPHAN HEISE¹ — ¹Ultrafast Nanoscale Dynamics, Institute of Physics, University of Oldenburg, D-26111 Oldenburg, Germany — ²Avancis GmbH, Otto-Hahn-Ring 6, D-81739 München, Germany

Facing climate change, renewable energies are becoming more and more relevant. Hence, understanding their mechanisms in detail is important to improve their use. In photovoltaics, solar cells are used to convert solar energy into electrical energy. In general, the efficiency of a solar cell is measured and compared under standard test conditions, which may vary vastly from real conditions. Hence, it is important to investigate the dependence of the efficiency on different parameters, in order to find the best solar cell for each case of non-standard conditions. One of these parameters is the incident angle of light, which varies according to the sun's position, but also depends on the orientation of the solar cell. Its influence on the efficiency is being tested in this study for Cu(In,Ga)(S,Se)₂ (CIGS) solar cells using IV-measurements. CIGS solar cells are thin-film solar cells which can reach efficiencies up to 23%. In particular, the role of the front glass for the angular-dependent efficiency is studied by investigating different front glass variations. The measurements show that the efficiency dependence on the incident angle cannot be explained by the reduced photon flux only.

CPP 61.2 Wed 9:45 POT 251

Reaching Efficiency Limits for Blue CsPbBr₃ based Light Emitting Diodes — ●TASSILO NAUJOKS¹, THOMAS MORGENSTERN¹, CAROLA LAMPE², ALEXANDER URBAN², MATTHEW JUROW³, YI LIU³, and WOLFGANG BRÜTTING¹ — ¹University of Augsburg, 86135 Augsburg, Germany — ²Ludwig-Maximilians-Universität München, 80539 Munich, Germany — ³Lawrence Berkeley National Laboratory, Berkeley, CA 94720, United States of America

The unique optical properties of lead halide perovskites have drawn significant attention towards their application in light emitting devices. While quantum yield, emission wavelength and stability are already in the focus of many research groups, the orientation of the emissive transition dipoles is rarely investigated.

In this work, we investigate CsPbBr₃ nanoplatelets of variable thickness and determine the orientation of their transition dipole moments from thin film radiation patterns.

We use a thickness variation for nanoplatelets reaching from 2 to 6 monolayers to systematically study the tunability of the TDM orientation and the concomitant color shift, while the emission peak stays as narrow as it is for the green emitting nanocubes. Together with high photoluminescent quantum yields the efficiency limit of lead-halide perovskite based light emitting diodes can be re-estimated.

The present data reveal very promising new efficiency limits, for solution-processed light emitting diodes: A solution-processed, highly efficient blue emitter with strong horizontal orientation can be made of CsPbBr₃ nanoplatelets.

CPP 61.3 Wed 10:00 POT 251

Frenkel-Holstein Hamiltonian Applied to Quaterthiophene-based 2D Hybrid Organic-Inorganic Perovskites — ●SVENJA M. JANKE¹, MOHAMMAD B. QARAI², VOLKER BLUM¹, and FRANK C. SPANO² — ¹Duke University, Durham, NC, USA — ²Temple University, Philadelphia, PA, USA

In two-dimensional hybrid organic-inorganic perovskites (HOIPs), both the organic and inorganic components can contribute to the electronic properties at the electronic frontier levels and hence open up a wide area for design of new materials with high tunability. For development of new devices like solar cells or light emitting diodes, the understanding of electronic excitations and their photophysical signatures play a fundamental role. Here, we show at the example of quaterthiophene-based lead-halide HOIPs that the organic contribution to 2D HOIP absorption and emission spectra can be theoretically investigated employing a Frenkel-Holstein Hamiltonian that treats electronic coupling and electron-phonon coupling on equal footing. We relate changes in the spectra to structural changes in the

organic layer that in turn are caused by variation of the halide anion. Furthermore, we take first steps towards including the contribution of the Wannier exciton on the inorganic component into the framework of the Frenkel-Holstein Hamiltonian. Supported by the German Science Foundation (DFG), grant number 393196393.

CPP 61.4 Wed 10:15 POT 251

Environmental Stability of High Efficiency PbS Quantum Dot Solar Cells — ●DAVID BECKER-KOCH^{1,2}, MIGUEL ALBALADEJO-SIGUAN^{1,2}, VINCENT LAMI³, FABIAN PAULUS², HENGYANG XIANG⁴, ZHUOYING CHEN⁴, and YANA VAYNZOF^{1,2} — ¹IAPP, TU Dresden, Germany — ²cfaed, TU Dresden, Germany — ³KIP, Uni Heidelberg, Germany — ⁴ESPCI, CNRS, Université Pierre et Marie Curie, Paris, France

Colloidal inorganic quantum dot (CQD) solar cells (SCs) are an emerging class of photovoltaics, which can be processed from solution at low temperature and their optoelectronic properties can easily be tuned by changing their size, shape and surface passivation. While power conversion efficiencies of ~12% have been demonstrated by employing lead sulphide (PbS) CQDs, their stability remains an unresolved issue preventing them from being integrated into industrial applications. In this work we focus on the influence of different atmospheres on the performance of high efficiency PbS CQDs SCs. We find that while N₂ and humidity lead to a quick decline in performance, oxidation dominates the initial improvement and the subsequent deterioration of the device function. By applying a range of spectroscopic methods, we identify the pivotal layer for these processes and furthermore, we propose a model for the performance evolution. We conclude that the stability and performance can be improved by exchanging the extraction layer (EL) ubiquitously used in these devices. Finally, we present several promising organic, semiconducting replacement ELs and show preliminary results of their application as ELs in PbS CQDs solar cells.

CPP 61.5 Wed 10:30 POT 251

How does strain impact the solar cell performance at grain boundaries? — ●MICHAEL STUCKELBERGER¹, IRENE CALVO-ALMAZÁN², MARTIN HOLT², MEGAN HILL³, SIDDHARTH MADDALI², MARIANA BERTONI⁴, XIAOJING HUANG⁵, HANFEI YAN⁵, EVGENY NAZARETSKI⁵, YONG CHU⁵, ANDREW ULVESTAD², and STEPHAN HRUSZKEWYCZ² — ¹DESY, Hamburg, Germany — ²ANL, Lemont IL, USA — ³Northwestern University, Evanston IL, USA — ⁴ASU, Tempe AZ, USA — ⁵BNL, Upton NY, USA

Grain boundaries (GB) often limit the conversion efficiency of polycrystalline solar cells. Strain is particularly detrimental there, as it enhances the defect concentration and band fluctuations, leading to increased recombination rates. Unfortunately, standard methods cannot easily measure the strain distribution in working thin-film devices.

Based on nanodiffraction experiments, we demonstrate the assessment of the strain distribution at sub-100-nm resolution. In a multimodal detector design, we combined nanodiffraction with X-ray fluorescence (XRF) and X-ray beam induced current (XBIC) measurements. Mapping individual grains, this enabled us to correlate point-by-point the strain with composition and performance within grains and at GB.

In CIGS solar cells, we found that the strain increases towards GB, which is accompanied by an increase of the charge collection efficiency. In contrast, we found a decreasing lattice constant towards GB in CdTe solar cells. Similar correlative experiments are ongoing on perovskite solar cells, and we will present the latest results.

30 min. break

CPP 61.6 Wed 11:15 POT 251

Tuning Perovskite Halide Content to Engineer Environmental Stability — ●KATELYN P. GOETZ^{1,2}, FABIAN THOME^{1,2}, PAUL FASSL^{1,2}, LUKAS M. FALK^{1,2}, VINCENT LAMI^{1,2}, ALEXANDER D. TAYLOR^{1,2}, QINGZHI AN^{1,2}, FABIAN PAULUS^{1,2}, and YANA VAYNZOF^{1,2} — ¹IAPP, Technical University of Dresden, Germany — ²CFAED, Technical University of Dresden, Germany

The presence of surface defects in perovskite films has been linked to their stability; however, many questions remain regarding details of the degradation process. Here, we incrementally tune the iodine or

bromide content in MAPbI₃ or MAPbBr₃ thin-films and examine the impact on optoelectronic properties. X-ray photoelectron spectroscopy is used to identify the density and type of surface defect. We examine the interaction of the defect with the environment by exposing the films to controlled levels of oxygen and humidity under light, and monitor changes to the films via photoluminescence (PL) spectroscopy. Here, we observe that, while halide-rich films exhibit lower PL quantum efficiency (PLQE) than halide-poor films, exposure to low levels of oxygen enhances the luminescence of all films. In solar cells, iodine-poor MAPbI₃ samples show a tremendous drop in the short-circuit current after exposure to oxygen, while those with excess show no change. The MAPbBr₃ solar cells show little dependence of the initial photovoltaic performance on the halide content, but upon exposure to air and light, bromide-deficient solar cells undergo a large J_{sc} boost, resulting in a near tripling of their initial PCE. These results highlight the strong role that chemical composition plays in stability.

CPP 61.7 Wed 11:30 POT 251

Enabling Versatile High-Efficiency Perovskite Photovoltaics by Charge-Selective Contact Design — ●AMRAN AL-ASHOURI¹, ARTIOM MAGOMEDOV², MARCEL ROSS¹, MARKO JOŠT¹, MARTYNAS TALAİKIS³, GANNA CHRISTIAKOVA¹, JOSÉ M. PRIETO¹, EIKE KÖHNEN¹, ERNESTAS KASPARAVIČIUS², BERND RECH¹, TADAS MALINAUSKAS², THOMAS UNOLD¹, LARS KORTE¹, GEDIMINAS NIAURA³, VYTAUTAS GETAUTIS², and STEVE ALBRECHT¹ — ¹HZB, Berlin, Germany — ²KTU, Kaunas, Lithuania — ³FTMC, Vilnius, Lithuania

By establishing a simple, low-cost and robust perovskite solar cell device structure that employs self-assembled monolayers (SAMs) [1], we realized power conversion efficiencies of over 21 % for single junction cells, over 23 % for CIGSe/perovskite and well over 27 % for silicon/perovskite tandem solar cells. Using time-resolved and absolute photoluminescence spectroscopy together with an analysis of the energetic alignment between hole-selective contact and absorber, we identify design guidelines for an hole-selective interface without non-radiative recombination losses. A SAM model system further allows to study voltage and fill factor losses for an increased understanding of how to experimentally explore pathways towards theoretical efficiency limits.

[1] Al-Ashouri et al. *Energy Environ. Sci.* 2019, **12**, 3356

CPP 61.8 Wed 11:45 POT 251

Anharmonicity, short-range correlated disorder, and small Urbach energies in halide perovskites — ●CHRISTIAN GEHRMANN and DAVID A. EGGER — Department of Physics, Technical University Munich, 85748 Garching, Germany.

Halide perovskites (HaPs) are known to show complex nuclear dynamics and structural effects. But seemingly in contrast to this effects, a low amount of disorder is implied by measurements of small Urbach energies and sharp optical absorption edges. Using density functional theory (DFT) and DFT-based molecular dynamics, we calculated spatial correlations in the disorder potential induced for electronic states due to nuclear dynamics in representative HaPs [1]. We find sizeable anharmonicity in the nuclear vibrations and a dynamic shortening of

correlations in the disorder potential: the motion of especially A-site and X-site ions are found to have an important impact on the length of spatial correlations in the disorder potential, such that they become as short as atomic bonds in the material. We explicitly establish that these short-range correlated disorder potentials lead to narrow band-energy distributions, which imply small Urbach energies. We conclude that effective collection of sunlight in HaP based photovoltaic devices, as indicated by small Urbach energies and sharp optical absorption edges, is facilitated by this mechanism.

[1] C. Gehrman & D. A. Egger, *Nat. Commun.* 10, 3141 (2019).

CPP 61.9 Wed 12:00 POT 251

Combined Multi-Photon-Excitation and Multi-Exciton-Generation Processes in CsPbBr₃ Supercrystals — ●ANJA BARFÜSSER¹, ALEXANDER F. RICHTER¹, AURORA MANZI¹, SHIXUN WANG², HE HUANG¹, ANDREY L. ROGACH², and JOCHEN FELDMANN¹ — ¹Chair for Photonics and Optoelectronics, Nano-Institute Munich and Department of Physics, Ludwig-Maximilians-Universität (LMU), Königinstr. 10, 80539 Munich, Germany — ²Department of Materials Science and Engineering and Centre for Functional Photonics (CFP), City University of Hong Kong, Kowloon, Hong Kong

A fundamental problem limiting the power conversion efficiency of solar cells are photons with energies below the band gap, as they cannot be absorbed by linear processes, and above the band gap, as the excess energy typically is lost as heat. Multi-photon-excitation (MPE) and multi-exciton-generation (MEG) target this issue. Up to now, these processes have only been observed independently. Here, their combined effect is demonstrated for bulk-like CsPbBr₃ perovskite nanocubes forming a superlattice. For below-band-gap excitation energies (0.5-0.8 E_g) nonlinear absorption is observed. Interestingly, when the energy of multiple below-band-gap photons resonantly matches the energy of multiple excitons, a strong photoluminescence enhancement of up to 10⁵ takes place. Excitation power dependent measurements reveal a high-order absorption process deviating from the typical two-photon absorption.

CPP 61.10 Wed 12:15 POT 251

The Versatility of Polyelemental Perovskite Compositions — ●MICHAEL SALIBA — TU Darmstadt

Perovskites have emerged as low-cost, high efficiency photovoltaics with certified efficiencies of 22.1% approaching already established technologies. The perovskites used for solar cells have an ABX₃ structure where the cation A is methylammonium (MA), formamidinium (FA), or cesium (Cs); the metal B is Pb or Sn; and the halide X is Cl, Br or I. Unfortunately, single-cation perovskites often suffer from phase, temperature or humidity instabilities. This is particularly noteworthy for CsPbX₃ and FAPbX₃ which are stable at room temperature as a photoinactive *yellow phase* instead of the more desired photoactive *black phase* that is only stable at higher temperatures. Moreover, apart from phase stability, operating perovskite solar cells (PSCs) at elevated temperatures (of 85 °C) is required for passing industrial norms.