

## CPP 28: Perovskite and Photovoltaics 3

Time: Wednesday 15:00–17:15

Location: H38

CPP 28.1 Wed 15:00 H38

**Optically-Induced Long-lived Chirality Memory in the Color Tunable Chiral Lead-Free Semiconductor (R)/(S)-CHEA4Bi2BrxI10-x ( $x = 0 - 10$ )** — ●SHANGPU LIU<sup>1</sup>, MARKUS HEINDL<sup>1</sup>, NATALIE FEHN<sup>2</sup>, SEBASTIÁN CAICEDO-DÁVILA<sup>1</sup>, SILVA KRONAWITTER<sup>2</sup>, GREGOR KIESLICH<sup>2</sup>, DAVID EGGER<sup>1</sup>, ARAS KARTOUZIAN<sup>2</sup>, and FELIX DESCHLER<sup>1</sup> — <sup>1</sup>Walter Schottky Institute and Department of Physics, TUM, Garching, Germany — <sup>2</sup>Catalysis Research Center, TUM, Garching, Germany

Hybrid organic-Inorganic networks that incorporate chiral molecules have attracted great attention due to their potential in semiconductor lighting applications and optical communication. Here we introduce the chiral organic molecules (R/S)-CHEA into bismuth-based structures with an edge-sharing octahedral motif, to synthesize chiral (R/S)-CHEA4Bi2BrxI10-x crystals and thin films. Using single-crystal X-ray diffraction measurements and density-functional theory calculations, we identify crystal and electronic band structures. We investigate the material optical properties and find circular dichroism, which we tune by the bromide-iodide ratio over a wide wavelength range from 300-500 nm. Further, we employ transient absorption spectra and time-correlated single photon counting to investigate charge carrier dynamics, which show long-lived excitations with unexpected optically-induced chirality memory up to 10s of nanosecond timescales. Our demonstration of chirality memory in a color-tunable and chiral lead-free semiconductor opens a new avenue for the discovery of high-performance spintronic materials with optical functionalities.

CPP 28.2 Wed 15:15 H38

**Time-Resolved Microwave Conductivity on ionic liquid doped Lead Halide Perovskites** — ●PATRICK DÖRFLINGER<sup>1</sup>, VALENTIN SCHMID<sup>1</sup>, YONG DING<sup>2</sup>, MOHAMMAD KHAJA NAZEERUDDIN<sup>2</sup>, and VLADIMIR DYAKONOV<sup>1</sup> — <sup>1</sup>Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — <sup>2</sup>Group for Molecular Engineering of Functional Materials, Institute of Chemical Sciences and Engineering, EPFL Valais, Sion 1950, Switzerland

In the past decade, perovskite solar cells evolved to one of the most promising photovoltaic materials with steadily rising power conversion efficiencies, now exceeding 25%. Nonetheless, Organolead Halide Perovskites suffer from insufficient long-term stability. Especially the stability under thermal stress is crucial towards commercialization. Ionic liquids as an additive into the precursor solution are candidates to overcome this issue. Besides the increased resistivity against higher temperatures, alterations of important material properties like mobility and lifetime are expected. Therefore, we used Time-Resolved Microwave Conductivity (TRMC) to determine the mobility and lifetime of photo-generated charge carriers in the perovskite layer. In addition, with Steady-State Microwave Conductivity (SSMC) we can provide insights into the predominating recombination pathways. Combined, we investigated the influence of the ionic liquids on the perovskite material properties and gain deeper understanding of the charge carrier dynamics.

CPP 28.3 Wed 15:30 H38

**Hidden interfaces: How ferroelastic domain walls affect the charge diffusion in perovskite solar cells** — ●ILKA M. HERMES<sup>1,2</sup>, ANDREAS BEST<sup>2</sup>, KALOIAN KOYNOV<sup>2</sup>, HANS-JÜRGEN BUTT<sup>2</sup>, and STEFAN A. L. WEBER<sup>2</sup> — <sup>1</sup>Leibniz Institute for Polymer Research Dresden e.V., Dresden, Germany — <sup>2</sup>Max Planck Institute for Polymer Research, Mainz, Germany

Ferroelastic domains form during phase transitions that change the crystal system. By arranging in domains with alternating unit cell orientation, the material lowers its overall strain. The walls that separate ferroelastic domains typically feature some structural anomalies, which can affect the electronic properties of the crystal by increasing the defect concentration, introducing dopants or forming a local electric polarization via the flexoelectric effect. Here, we explored the implications of ferroelastic domain walls for the photo-carrier transport in methylammonium lead iodide, a solar cell light absorber used in perovskite solar cells. Via correlative spatial and time-resolved photoluminescence microscopy and electromechanical atomic force microscopy, we could link the presence of domain walls to the occurrence of an anisotropic charge diffusion, where charges move faster parallel to do-

main walls than perpendicular. Moreover, the ferroelastic nature of the domains promises a targeted engineering of the domain wall arrangement using the application of external stress or heat treatments across the material's cubic-tetragonal phase transition: a perpendicular alignment of the domain walls with respect to the extraction layer interfaces should facilitate faster and more efficient charge extraction.

CPP 28.4 Wed 15:45 H38

**Degradation mechanisms of perovskite solar cells under vacuum and one atmosphere of nitrogen** — ●RENJUN GUO<sup>1</sup>, WEI CHEN<sup>1</sup>, LENNART K. REB<sup>1</sup>, MANUEL A. SCHEEL<sup>1</sup>, MATTHIAS SCHWARTZKOPF<sup>2</sup>, STEPHAN V. ROTH<sup>2</sup>, and PETER MÜLLER-BUSCHBAUM<sup>1</sup> — <sup>1</sup>Technische Universität München, Garching, Germany — <sup>2</sup>Deutsches Elektronen-Synchrotron, Hamburg, Germany

Extensive studies have focused on improving the operational stability of perovskite solar cells. Only a few studies survey the fundamental degradation mechanisms related to the device performance, and these studies were executed under various experimental conditions. Thus, we investigate the degradation mechanisms of high-efficiency perovskite solar cells under vacuum and a nitrogen atmosphere, as based on the International Summit on Organic Photovoltaic Stability protocols. We use synchrotron radiation-based operando grazing-incidence X-ray scattering methods. Unlike what was seen in previous reports, we find that the perovskite lattice can also experience a lattice shrinkage under operation. Moreover, we reveal that the atmosphere has a paramount influence on phase segregation, lattice distortion, and morphology deformation during operation of mixed cation lead mixed halide perovskite solar cells. This, in turn, degrades the performance of the respective perovskite solar cells. Our discoveries emphasize the importance of different types of inert atmospheres as critical parameters, which must be considered in future scientific studies and the industrial screening of longevity for photovoltaic modules.

CPP 28.5 Wed 16:00 H38

**Determination of the Optimum Dead Area Width of Laser-Patterned, Series-Interconnected Perovskite Solar Cells** — ●NICOLAS OTTO<sup>1</sup>, CHRISTOF SCHULTZ<sup>1</sup>, GUILLERMO FARIAS BASULTO<sup>2</sup>, JANARDAN DAGAR<sup>3</sup>, MARKUS FENSKER<sup>1</sup>, RUTGER SCHLATMANN<sup>1,2</sup>, EVA UNGER<sup>3</sup>, and BERT STEGEMANN<sup>1</sup> — <sup>1</sup>HTW Berlin - University of Applied Sciences, Wilhelminenhofstr. 75A, D-12459 Berlin — <sup>2</sup>HZB für Materialien und Energie, PVcomB, Schwarzschildstr. 3, D-12489 Berlin — <sup>3</sup>HZB für Materialien und Energie, Young Investigator Group Hybrid Materials Formation and Scaling, Kekuléstraße 5, D-12489 Berlin, Germany

Based on recent work on minimizing the interconnection width of laser patterned perovskite solar cells the optimum dead area width was determined. In order to use the largest possible aperture area, the dead area width should be as small as possible while still providing full electrical functionality. For this purpose the width between the P2 and the P3 scribes was varied ranging from overlapping to pattering with safety area. By also reducing the P1/P2 spacing an optimum dead area width can be achieved. The detailed scribe line characterization was done by optical microscopy imaging, electrical j-V measurements and compositional analyses. Minimodules with three in series connected cells were then produced. The results show that overlapping scribe lines as well as included safety areas cause avoidable electrical losses. Consequently, an optimum is achieved for arranging the scribe lines as closely as possible. In our study an optimal scribe line width of about 230 micrometres was realized.

CPP 28.6 Wed 16:15 H38

**Performance of Perovskite and Organic Solar Cells in Space** — ●LENNART REB<sup>1</sup>, MICHAEL BÖHMER<sup>2</sup>, BENJAMIN PREDESCHLY<sup>1</sup>, SEBASTIAN GROTT<sup>1</sup>, LUKAS SPANIER<sup>1</sup>, CHRISTIAN WEINDL<sup>1</sup>, GORAN IVANDEKIC<sup>1</sup>, RENJUN GUO<sup>1</sup>, CHRISTOPH DREISSIGACKER<sup>3</sup>, JÖRG DRESCHER<sup>3</sup>, ROMAN GERNHÄUSER<sup>2</sup>, ANDREAS MEYER<sup>3</sup>, and PETER MÜLLER-BUSCHBAUM<sup>1,4</sup> — <sup>1</sup>TU München, Physik-Department, Lehrstuhl für Funktionelle Materialien, Garching, Germany — <sup>2</sup>TU München, Physik-Department, Zentrales Technologielabor, Garching, Germany — <sup>3</sup>Deutsches Zentrum für Luft- und Raumfahrt (DLR), Institut für Materialphysik im Weltraum, Köln, Germany — <sup>4</sup>Heinz Maier-Leibnitz-Zentrum, Garching, Germany

Perovskite and organic solar cells have become a hot research topic in the last few years. The lightweight thin-film solar cells exhibit an exceptional power per mass that exceeds their inorganic counterparts by magnitudes, particularly interesting for space applications. Recently, we launched perovskite and organic solar cells to space on a suborbital rocket flight for the first time [1, 2]. The perovskite and organic solar cells operate in space conditions and produce reasonable power per area of up to 14 and 7 mW cm<sup>-2</sup>, respectively. Here we derive, with a detailed solar irradiation reconstruction, the irradiation-dependent solar cell performance parameter evolutions, and conclude the solar cell efficiency under strong AM0 irradiation. [1] L. Reb et al., *Joule* 4,1880-1892 (2020), doi.org/10.1016/j.joule.2020.07.004. [2] L. Reb et al., *Rev. Sci. Instrum.* 92 (2021), doi.org/10.1063/5.0047346.

### 15 min. break

CPP 28.7 Wed 16:45 H38

**Quantum Efficiency Enhancement of Lead-Halide Perovskite Nanocrystal LEDs by Organic Lithium Salt Treatment** — ●ROSHINI JAYABALAN<sup>1</sup>, TASSILO NAUJOKS<sup>1</sup>, CHRISTOPHER KIRSCH<sup>2</sup>, FENGSHUO ZU<sup>3</sup>, MUKUNDHA MANDAL<sup>4</sup>, JAN WAHL<sup>2</sup>, MARTIN WAIBEL<sup>1</sup>, ANDREAS OPITZ<sup>3</sup>, NORBERT KOCH<sup>3,5</sup>, DENIS ANDRIENKO<sup>4</sup>, MARCUS SCHEELE<sup>2</sup>, and WOLFGANG BRÜTTING<sup>1</sup> — <sup>1</sup>Universität Augsburg, 86135 Augsburg, Germany — <sup>2</sup>Universität Tübingen, 72076 Tübingen, Germany — <sup>3</sup>Institut für Physik & IRIS Adlershof, Humboldt-Universität zu Berlin, Germany — <sup>4</sup>Max Planck Institut für Polymerforschung, 55128 Mainz, Germany — <sup>5</sup>Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, 12489 Berlin, Germany

Owing to large specific surface area in lead halide perovskite nanocrystals, surface passivation using ligands is crucial to attain high photoluminescent quantum yield (PLQY). With respect to device fabrication, such passivation methods must also enable balanced charge injection to achieve high efficiency and operational stability. In this regard, this talk will discuss on the results of post-passivation treat-

ment of CsPbBr<sub>3</sub> nanocrystals with LiTFSI, an organic lithium salt. The results from such treatment have proven to be propitious for the nanocrystals - yielding higher PLQY, longer exciton lifetime and improved light outcoupling. Consequently, a significant improvement is observed in the devices fabricated using such post post-treated nanoparticles. Lastly, photoelectron spectroscopy and density functional theory modelling is employed to understand the impact of LiTFSI post-treatment on the performance of a perovskite based LED.

CPP 28.8 Wed 17:00 H38

**Tunable mesoporous and optoelectronics properties of zinc titanate films using sol-gel technique** — ●YANAN LI<sup>1</sup>, NIAN LI<sup>1</sup>, APOSTOLOS VAGIAS<sup>2</sup>, and PETER MÜLLER-BUSCHBAUM<sup>1</sup> — <sup>1</sup>Physics Department, Technical University of Munich, 85748 Garching, Germany — <sup>2</sup>Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, 85748 Garching, Germany

Mesoporous films consisting of zinc titanate have high potential applications in photocatalysis, solar cells, and sensors due to tailoring their semiconductive properties. In the present work, we investigate the morphologies of mesoporous zinc titanate films obtained by changing the ratio of two inorganic precursors after calcining hybrid films consisting of organic-inorganic materials. The amphiphilic diblock copolymer poly(styrene)-*b*-poly(ethyleneoxide) PS-*b*-PEO self-assembles into core-shell micelles in a mixture of N,N-dimethylformamid/hydrogen chloride playing the role as structure directing template. The inorganic precursors, zinc acetate dehydrate and titanium tetraisopropoxide, are loaded in the micellar shell due to hydrogen bonds between PEO and precursors. We use slot-die and spin-coating methods to prepare hybrid films, and investigate the influence of the different deposition methods on the film morphologies. Moreover, we investigate how mesoporous structures and crystal phases depend on calcination temperatures. The morphologies of the hybrid films are characterized using grazing incidence small-angle X-ray scattering (GISAXS) and scanning electronic microscopy (SEM).