CPP 33: Hybrid and Perovskite Photovoltaics I

Time: Wednesday 16:30–18:00 Location: H 0106

CPP 33.1 Wed 16:30 H 0106

Structure and morphology investigations on printed perovskite quantum dot films — •Manuel A. Reus[1], Ahmed Krifa[1], David P. Kosbahn[1], Quinten A. Akkerman[2], Alexander Biewald[3], Lennart K. Reb[1], Matthias Schwartzkopf[4], Andrei Chumakov[4], Stephan V. Roth[4], Achim Hartschuh[3], Jochen Feldmann[2], and Peter Müller-Buschbaum[1,5] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching — [2]Nano-Institut München und Fakultät für Physik, LMU, 80539 München — [3]Department Chemie und CeNS, LMU, 81377 München — [4]DESY, 22607 Hamburg — [5]MLZ, TUM, 85748 Garching

Solar cells based on thin-film architectures offer potentially cheaper production, semi-transparency, and flexibility. Slot-die coating is one of the most promising scalable and roll-to-roll compatible deposition method for thin-film solar cells. Printing thin-film layers from colloidal quantum dot solution offers the advantage of decoupling the crystallization from the deposition process. Perovskite quantum dots are one option for high-quality next-generation perovskite solar cells. We demonstrate the feasibility of fabricating solar cells from printed quantum dots as the active layer. Extensive characterization by SEM and grazing-incidence X-ray scattering gives insights into the morphology, structure, and texture. SEM, FLIM, PL, and transient PL measurements shed light on the optoelectronic properties of the solar cell printed from colloidal hybrid perovskite quantum dot solution.

CPP 33.2 Wed 16:45 H 0106

Time-resolved structure formation in perovskite thin films and powders — •Christopher Greve[1], Konstantin Schötz[2], Philipp Ramming[2], Fabian Panzer[2], Anna Köhler[2], Helen Grüninger[3], and Eva M. Herzig[1] — [1]Dynamik und Strukturbildung - Herzig Group — [2]Lehrstuhl für Optoelektronik weicher Materie — [3]Inorganische Chemie III - all Universität Bayreuth, 95440 Bayreuth

To shift from a trial-and-error optimization methodology to a more systematic approach in optimizing metal halide perovskite (MHP) processing, it is imperative to enhance the understanding of MHP formation and the subsequent dynamical processes. To improve the understanding of thin film formation from solution we can utilize in situ PL, light scattering and absorption measurements to track the crystallization processes.[1] However, subsequent dynamic processes within the final MHP film also play a major role, as they define material stability. One example is phase segregation in mixed halide MHP, which we can track with in-situ XRD measurements at various temperatures.[2] Another tool to study dynamics in MHP films is grazing incidence X-ray correlation spectroscopy, which bulk-sensitive application to films results in altered correlation functions. We present an approach within the sDWBA to identify suitable measurement parameters for the application to MHP thin films.[3] [1]: Schötz, Greve et al., 10.1002/adom.202101161; [2] Greve, Ramming et al., 10.1021/acsenergylett.3c01878; [3]: Greve et al., 10.1021/acs.langmuir.3c00669

CPP 33.3 Wed 17:00 H 0106

Simulation of the Impact of Processing Conditions on the Perovskite Film Morphology — •Martin Majewski[1], Shudi Qui[2], Olivier Ronsin[1], Larry Lüer[2], Tian Du[2], Hans-J. Egelhaaf[2], and Jens Harting[1] — [1]Forschungszentrum Juelich GmbH, Helmholtz Institute Erlangen- Nuernberg (IEK-11), Dynamics of Complex Fluids and Interfaces, Cauerstraße 1, 91058 Erlangen, Germany — [2]Department of Materials Science and Engineering, Friedrich-Alexander-Universitaet Erlangen-Nuernberg, Erlangen, Germany

The solution-processed perovskite layer forms complex structures during drying. This morphology of the dry film heavily influences the efficiency of the final solar cell. The impact of the physical mechanisms on the morphology, like for example nucleation and evaporation rate, in a drying, crystallizing wet film is not really understood yet. Therefore a better understanding of the interplay of these phenomena is needed.

We present phase field simulations which are capable to describe the main physical processes: evaporation, diffusion, spontaneous nucleation, crystal growth and advection. The evaporation rate is modified in the experiment (by gas quenching) and simulation. The simulation is successfully validated against the experiments. With help of the simulation, the formation pathways for all investigated evaporation rates are uncovered. The ratio between evaporation and crystallization rate is identified as the main driver for the morphological transition from pinhole prone to pinhole free perovskite thin films.

CPP 33.4 Wed 17:15 H 0106

Deciphering the interplay of structure and charge carrier dynamics in reduced-dimensional perovskites — •Kun Sun[1], Renjun Guo[1], Shangpu Liu[2], Xiongzhuo Jiang[1], Yuxin Liang[1], Matthias Schwarzkopf[3], Felix Deschler[2], and Peter Müller-Buschbaum[1,4] — [1]TUM, TUM School of Natural Sciences, E13, Garching, Germany — [2]UOH, Physikalisch-Chemisches Institut, Heidelberg, Germany — [3]Desy, Hamburg, Germany — [4]TUM, MLZ, Garching, Germany

RDPs have advanced the development of PSCs due to their tunable energy landscape, structure, and orientation. Thus, we aim for an increase in the understanding of structure-photophysical properties of DJ and RP RDPs with different dimensionalities. Our findings reveal that RP RDPs with lower dimensionality exhibits a dominant n=2 phase, preferential out-of-plane orientation, and longer charge carrier lifetime compared with DJ RDPs, as evidenced by X-ray scattering technique and transient absorption spectroscopy. In addition, we unveil the film growth of respective RDPs by in-situ X-ray scattering, showing the stoichiometry-determined phase growth. The formation of lower-n phases in RP RDPs with higher dimensionality is thermodynamically favored, while those phases are likely in the form of intermediate phase, which bridge the 3d-like and lower-n phases in DJ RDPs. DJ RDPs with higher dimensionality demonstrate comparable phase purity, giving rise to more sufficient energy transfer and longer charge carrier lifetime. Our work paves the way for dictating the utilization of RDPs in both 3D and quasi-2D PSCs.

CPP 33.5 Wed 17:30 H 0106

Local Charge Carrier Dynamics in Lead Halide Perovskites by Nano Surface Photovoltage Spectroscopy — Yenal Yalcinkaya[1], Pascal Rohrbeck[1], Lukas Schmidt-Mende[2], and •Stefan A.L. Weber[1,3] — [1]MPI for Polymer Research, Mainz — [2]Department of Physics, University of Konstanz — [3]Institute for Photovoltaics, University of Stuttgart

Understanding electron and ion dynamics is an important task for improving lead halide perovskites based solar cells and related devices. Perovskite materials have a delicate nano- and micro structure that influences the device parameters. This study investigates the spatial defect distribution in the vicinity of grain boundaries (GB). To this end, we introduce Nano surface photovoltage spectroscopy (Nano-SPV) via time-resolved Kelvin probe force microscopy (tr-KPFM) [1,2]. By measuring the SPV decay on perovskite samples with small, large, and passivated grains, areas of increased charge carrier recombination, ion migration, and defects were locally detected [3]. Our results clearly show an improved uniformity of SPV and SPV decay distribution within the perovskite films upon passivation. Furthermore, the perovskite films with large grains show better recombination properties based on SPV decay and ideality factor values.

[1] Axt et al. Beilstein J. Nanotechnol. 9, 1809 (2018). [2] Weber et al., Energy Environ. Sci. 11, 2404 (2018). [3] Yalcinkaya et al. Adv. Opt. Mater. 2301318 (2023).

CPP 33.6 Wed 17:45 H 0106

CTAB assisted solvent-free mechanosynthesis of MAPbX3 nanocrystals: Stability, and photoresponse — •Gaurav Nim[1], Parul Bansal[2], and Prasenjit Kar[2] — [1]Department of Physics and Material Sciences Center, Philipps-Universität Marburg, Germany — [2]Department of Chemistry, Indian Institute of Technology Roorkee, India

In this work, hybrid metal halide perovskite, or HPs (MAPbX3, X = Br, I), was produced exclusively using multifunctional cetyl trimethylammonium bromide (CTAB) and the mechano-synthesis technique.* Equimolar amounts of MAX and PbX2 combined with a mmol quantity of CTAB were used to synthesize HPs. We did steady-state photoluminescence, X-ray diffraction (XRD), and time-correlated single-photon count (TCSPC) to look at the optical and structural properties of perovskite. The thermogravimetric analysis informs us about the

thermal stability of the nanocrystals. X-ray diffraction analysis reveals that mechanochemically synthesized HPs show high crystallinity and phase purity, with stability over a period of time. The photoinduced current response of the perovskite reveals an excellent increase in photoconductivity when exposed to light (with a 1 V bias). The device fabricated of perovskite witnessed prompt photoresponse under light illumination and temporally stable photocurrent over multiple cycles of light irradiation. Due to their phase purity, low bandgap, nanoscale size, long-term stability, and easy-to-synthesis approach, the synthesized materials are useful for photovoltaic applications.