

CPP 48: Focus: Fundamental Physics of Perovskites I - organized by Lukas Schmidt-Mende and Vladimir Dyakonov

Time: Wednesday 15:00–17:45

Location: C 130

Topical Talk

CPP 48.1 Wed 15:00 C 130

Long lifetimes and small phonon energies in metal-halide perovskite solar cells — ●THOMAS KIRCHARTZ^{1,2}, DAVID EGGER³, and UWE RAU¹ — ¹IEK5 Photovoltaik, Forschungszentrum Jülich GmbH, 52428 Jülich — ²Faculty of Engineering and CENIDE, University of Duisburg-Essen, Carl-Benz-Str. 199, 47057 Duisburg, Germany — ³Institute of Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany

Lead-halide perovskite solar cells have remarkably high open-circuit voltages and relatively long lifetimes as determined from e.g. transient photoluminescence or transient microwave photoconductivity. These long lifetimes lead to fairly good charge carrier collection properties and in addition a high internal luminescence yield that makes these materials suitable for photovoltaics and other optoelectronic applications. One agreed-upon reason for these long lifetimes is the defect tolerance of lead-halide perovskites and the subsequently low density of deep defects in the material. However, various other potential explanations for long lifetimes and high open-circuit voltages have been brought forward. Among them are the existence of an indirect band gap, low effective masses or polaronic effects. Here, we recall the classical theories for non-radiative recombination via emission of multiple phonons, which predict the capture cross sections as a function of microscopic parameters such as the phonon energy, the deformation potential constant and the frequency dependent permittivity. Based on these theories we discuss the impact of low phonon energies and the strongly frequency dependent permittivity on recombination.

CPP 48.2 Wed 15:30 C 130

Observation of coherent phonons upon photo-excitation in lead halide perovskite — ●VANDANA TIWARI¹, HONG-GUANG DUAN^{1,2,3}, AJAY JHA¹, PABITRA NAYAK⁴, MICHAEL THORWART^{2,3}, HENRY SNAITH⁴, and R. J. DWAYNE MILLER^{1,3,5} — ¹MPSD, Hamburg, Germany — ²I. Institut für Theoretische Physik, UH, Germany — ³CUI, Hamburg, Germany — ⁴University of Oxford, UK — ⁵University of Toronto, Canada

The unprecedented success of hybrid organolead halide perovskites in different cell designs demands the fundamental understanding of underlying microscopic mechanisms for photoinduced charge generation. Electronic dynamics of perovskite upon photo-excitation has provided deep insights into its optoelectronic behavior, but the contribution of lattice vibrations is still to be deciphered. We have employed ultrafast transient grating spectroscopy to probe impulsively excited vibrational modes of CH₃NH₃PbI₃ in thin films. We distinctly observe the ground and excited state vibrational modes at room temperature. The interplay of strongly coupled dominant vibrational modes to ultrafast carrier generation process will be discussed.

CPP 48.3 Wed 15:45 C 130

Impact of Temperature Induced Structural Dynamics on the Optical Properties of Hybrid Perovskites — ●FABIAN PANZER and ANNA KÖHLER — Experimental Physics II, University of Bayreuth

There is still a need in the field of hybrid perovskites to fundamentally understand how changes in the structure, be it the crystal structure, material composition or surface morphology impact on their electronic structure, i.e. their optical properties. Due to their soft nature, hybrid perovskites are prone to changes in their structure, which, for example, can be induced by changing the temperature of the sample, be it realized by cooling in a cryostat,[1] or by local heating due to laser irradiation.[2] Here we present detailed temperature dependent absorption and photoluminescence characterizations on both, polycrystalline thin films and single crystals of the prototypical perovskite methylammonium lead iodide. From our measurements we distinguish between different crystal structures, phase transitions and investigate the influence of disorder on the electronic structure.[3] Furthermore we identify the existence of additional recombination pathways already in the high temperature tetragonal phase of the material. We show that it is possible to induce this phase also at lowest temperatures by local laser heating. This allows to distinguish between the emission features from distinct crystal phases and defect states, to gain full information about the optical properties of the investigated perovskites.

[1] F.Panzer et al., Adv. Energy Mater, 7, 2017, 1700286; [2]

F.Panzer et al., Adv. Optical Mater. 6, 2016, 917; [3] S.Singh, C.Li, F.Panzer et al., J. Phys. Chem. Lett, 7, 2016, 3014

CPP 48.4 Wed 16:00 C 130

The influence of solvent engineering on the fundamental functionality of organolead triiodide perovskite solar cells — ●JULIAN HÖCKER², PHILIPP RIEDER¹, DAVID KIERSMASCH¹, ANDREAS BAUMANN², and VLADIMIR DYAKONOV^{1,2} — ¹Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — ²Bavarian Center for Applied Energy Research (ZAE Bayern), 97074 Würzburg

The organic and hydrophobic polymer poly[N, N'-bis(4-butylphenyl)-N, N'-bis(phenyl)-benzidine] (pTPD) is a representative hole transport layer (HTL) for its use in hybrid perovskite solar cells. Due to its beneficial energy levels, whereby its highest occupied molecular orbital (HOMO) level matches with the valence band level of methylammonium lead iodide perovskite, an efficient hole extraction can be achieved. In this study, we demonstrate highly efficient planar p-i-n perovskite solar cells using pTPD as HTL and CH₃NH₃PbI₃ processed from 2-step interdiffusion as the active layer. We found that the wettability of DMF strongly depends on the preparation method of pTPD. With varying the solvent and material concentrations we increased the wettability of the perovskite layer which lead to an increase in power conversion efficiency (PCE) of the corresponding solar cell devices. Our solvent engineering approach demonstrates that in this case no further interface modifications is needed for the preparation of efficient perovskite solar cell devices.

CPP 48.5 Wed 16:15 C 130

Time-resolved structural analysis of humidity assisted crystallization in printed mesoscopic organometal halide perovskite solar cells — ●OLIVER FILONIK¹, MARGRET EVA THORDARDOTTIR^{1,2}, JENNY LEBERT², STEPHAN PRÖLLER², SEBASTIAN WEISS², JIA HUR LEW³, ANISH PRIYADARSHI³, NRIPAN MATHEWS³, PETER MÜLLER-BUSCHBAUM², and EVA M. HERZIG⁴ — ¹TU München, Munich School of Engineering, Herzig Group, 85748 Garching, Germany — ²TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — ³Energy Research Institute @ NTU (ERI@N), Research Techno Plaza, 637553 Singapore, Singapore — ⁴Universität Bayreuth, Physikalisches Institut, Herzig Group - Dynamik und Strukturbildung, 95440 Bayreuth, Germany

Organometal halide perovskite based solar cells have emerged as the fastest-advancing photovoltaic technology to date. However, in-depth knowledge about the perovskite crystal formation and optimal processing protocols is still lacking. In the presented work, we fabricate a mesoscopic scaffold comprised of a triple-layer of titania, zirconia and carbon by screenprinting. We further investigate the influence of humidity on the perovskite formation inside the scaffold by time-resolved grazing incidence wide angle X-ray scattering. The experimental data reveal the formation of intermediate solvent phases in solution due to humidity, altering the perovskite formation route. Our results grant us a better understanding of the humidity assisted perovskite crystallization processes and are of key importance for further developments.

15 min. break

CPP 48.6 Wed 16:45 C 130

Investigation of Photon Recycling in Perovskites by Spatially-Resolved Confocal Photoluminescence — ●MILENA MERKEL², LIUDMILA KUDRIASHOVA¹, VALENTIN BAIANOV², SIMON BERGER¹, GEORGY V. ASTAKHOV¹, ANDREAS BAUMANN², and VLADIMIR DYAKONOV^{1,2} — ¹Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — ²Bavarian Center for Applied Energy Research (ZAE Bayern), 97074 Würzburg

Methylammonium lead iodide (MAPI) perovskites were shown to combine long diffusion lengths (up to 10 μm) with high carrier recombination rates (~10⁶ s⁻¹). Coexistence of these competing properties can be explained by efficient interplay between photons and electron-hole pairs in the perovskite film with multiple absorption-diffusion-emission events occurring, namely by photon recycling. Here we implement confocal double-objective photoluminescence (PL) spectroscopy to study

the photon recycling in MAPI. Analysis of steady-state PL spectra at various distances from excitation spot was performed. We show that photon recycling takes place in thin MAPI films, while its efficiency strongly depends on film morphology defined by preparation approach. Additionally, we discuss here the observed light-soaking effects.

CPP 48.7 Wed 17:00 C 130

Transient Photoluminescence Studies of $\text{CH}_3\text{NH}_3\text{PbI}_3/\text{PC}_{61}\text{BM}$ Heterojunctions — •BENEDIKT KROGMEIER¹, FLORIAN STAUB¹, DAVID GRABOWSKI¹, UWE RAU¹, and THOMAS KIRCHARTZ^{1,2} — ¹IEK5-Photovoltaik, Forschungszentrum Jülich, 52425 Jülich, Germany — ²Faculty of Engineering and CENIDE, University of Duisburg-Essen, Carl-Benz-Str. 199, 47057 Duisburg, Germany

Lead-halide perovskites have shown long bulk lifetimes in thin film photovoltaics, which implies that devices are limited by the interfaces and that studying the selectivity of contacts can lead to further improvement. One method proposed for obtaining interface properties is studying the transient photoluminescence of a lead-halide perovskite and an electron- or hole-transfer material layer. Previous studies analyze the photoluminescence transients using either rate equations or analytical solutions to the diffusion equation and do not take nonlinearities caused by charge accumulation at the interface into account. Therefore we use numerical drift-diffusion simulations of the transient photoluminescence of $\text{CH}_3\text{NH}_3\text{PbI}_3/\text{PC}_{61}\text{BM}$ heterojunctions which enables us to study the impact of laser fluence and interface properties without neglecting the non-linearities. The results show that charge accumulation can have a major impact on the lifetime measured with transient photoluminescence. Comparing simulated photoluminescence with measured data gives us insight into the dominating charge carrier loss mechanisms at different laser fluences and an analysis of the uniqueness of our result enables us to obtain an interfacial recombination velocity of 200 cm/s.

CPP 48.8 Wed 17:15 C 130

Tunable Anisotropic Photon Emission from Self-Organized CsPbBr_3 Perovskite Nanocrystals — •THOMAS MORGENSTERN¹, MATTHEW J. JUROW², ERIKA PENZO², JUN KANG², MATTHEW A. KOC³, THOMAS ZECHEL¹, ZACHARY NETT², MICHAEL BRADY², LINWANG WANG², A.PAUL ALIVISATOS^{2,3,4}, STEFANO CABRINI², YI LIU², and WOLFGANG BRÜTTING¹ — ¹Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — ²Lawrence Berkeley National Laboratory, Berkeley, California 94720, United States — ³College of Chemistry, University of California, Berkeley, California

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The introduction of preferentially aligned transition dipole moment vectors (TDMVs) is a common concept in the field of organic light emitting diodes. However, in the literature of perovskites and especially CsPbBr_3 nanocrystals this effect has rarely been reported.

In this work the anisotropy factor, correlating to the alignment of the transition dipoles within the nanocubes, for several CsPbBr_3 nanocrystal systems has been determined. [1] The results indicate a preferential alignment in vertical direction to the underlying surface. Using theoretical predictions the observed effect can be attributed to a charge redistribution originating from the contact of the nanocrystal to its underlying surface. Thus, a suitable choice of the substrate material can be used to further control the anisotropic emission properties, giving further potential to improve emission properties for light emitting devices. [1] M. JUROW, ET. AL.: *Nano Lett.* **17(7)** (2017), 4534-4540

CPP 48.9 Wed 17:30 C 130

Circular photogalvanic effect in single-crystal $(\text{CH}_3\text{NH}_3)\text{PbI}_3$ — •DANIEL NIESNER¹, MARTIN HAUCK², SHREETA SHRESTHA³, IEVGEN LEVCHUK³, GEBHARD J. MATT³, ANDRES OSVET³, MIROSLAW BATENTSCHUK³, CHRISTOPH J. BRABEC^{3,4}, HEIKO B. WEBER², and THOMAS FAUSTER¹ — ¹Lehrstuhl für Festkörperphysik, Univ. of Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen, Germany — ²Lehrstuhl für Angewandte Physik, Univ. of Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen, Germany — ³Institute of Materials for Electronics and Energy Technology (I-MEET), Univ. of Erlangen-Nürnberg, Martensstr. 7, D-91058 Erlangen, Germany — ⁴Bavarian Center for Applied Energy Research (ZAE Bayern), Haberstr. 2a, D-91058 Erlangen, Germany

The mechanisms underlying the remarkable phototransport properties of organic-inorganic perovskite compounds (OIPCs), such as carrier diffusion lengths $> 1 \mu\text{m}$ despite the moderate carrier mobilities, remain a matter of ongoing debate. Rashba and Dresselhaus spin-splittings have been predicted to enhance both carrier lifetimes and electron-acoustic-phonon coupling. Spin-splittings at the surface of an OIPC were measured using photoelectron spectroscopy, but little information exists to quantify their occurrence in bulk material. In a system with spin-split bands, the direction of diffusive photocurrents excited with circularly polarized light is reversed when the helicity of the light is changed. The phenomenon is known as the circular photogalvanic effect. We demonstrate this effect in $(\text{CH}_3\text{NH}_3)\text{PbI}_3$ single-crystal devices and discuss its relationship to optical properties.