

CPP 49: Poster Session II

Topics: Exploitation of Anisotropy in Organic Semiconductors (49.1-49.4); Hybrid and Perovskite Photovoltaics (49.5-49.20); In-situ probes toward better understanding of hybrid halide perovskites (49.21-49.24); Molecular Electronics and Excited State Properties (49.25-49.32); Organic Electronics and Photovoltaics (49.33-49.54).

Time: Tuesday 14:00–16:00

Location: P1A

CPP 49.1 Tue 14:00 P1A

The Influence of Side Chain Linkage on Bulk Structure and Orientation in Thin Films of Ethylene Glycol Substituted Polythiophenes — ●ROBERT KAHL¹, OLEKSANDR DOLYNCHUK¹, PHILIP SCHMODE², MUKUNDAN THELAKKAT², and THOMAS THURN-ALBRECHT¹ — ¹Experimental Polymer Physics, Martin Luther University Halle-Wittenberg, Germany — ²Applied Functional Polymers, University of Bayreuth, Germany

Polythiophenes with ethylene glycol side chains exhibit ionic as well as electronic charge transport, making them promising materials for application in organic electrochemical transistors (OECTs). In the present study, we investigated the effect of linkage of diethylene glycol side chains in polythiophenes on the structure formation and orientation in thin films. Three polythiophenes in which the diethylene glycol side chain is either directly linked to the thiophene backbone (P3MEET) or attached via a methylene (P3MEEMT) or an ethylene (P3MEEET) spacer were investigated in bulk (DSC, WAXS) and in thin films on Si/SiO₂ (GIWAXS, AFM). As seen in DSC and WAXS measurements, the molecular order in the bulk significantly decreases with decreasing spacer length. In confirmation to this, a clear lamellar morphology is only visible in AFM measurements of thin films of P3MEEET. GIWAXS measurements show, that all samples have a strong preference for edge-on orientation in thin films. From these results we conclude, that the length of the alkyl spacer has a significant influence on the molecular order, but little influence on the orientation in thin films.

CPP 49.2 Tue 14:00 P1A

Morphology Study of self-assembled Supramolecular Structures — ●ASENA CERHAN¹, CHRISTOPHER GREVE¹, MICHAEL BUCHHORN¹, RICHARD KELLNBERGER¹, BERND WITTMANN², FELIX WENZEL³, HANS-WERNER SCHMIDT³, RICHARD HILDNER^{2,4}, and EVA M. HERZIG¹ — ¹Dynamik und Strukturbildung - Herzig Group, Universität Bayreuth, Universitätsstr. 30, 95447 Bayreuth — ²Lehrstuhl für Spektroskopie weicher Materie, Universität Bayreuth, Universitätsstr. 30, 95447 Bayreuth — ³Makromolekulare Chemie I, Universität Bayreuth, Universitätsstr. 30, 95447 Bayreuth — ⁴Zernike Institute for Advanced Materials, University of Groningen, Nijenborgh 4 9747 AG Groningen, Netherlands

Organic, supramolecular systems can exhibit extraordinary transport properties [1]. Here we investigate the self-assembly of a carbonyl-bridged triarylamine (CBT) small molecule into helical supramolecular nanostructures [2]. The self-assembly is sensitive to environmental parameters like solvent type and temperature. Using x-ray scattering on the system in various solvents we are able to study the morphology of supramolecular nanostructures formed from CBT molecules. Examining the morphology further with temperature resolved measurements, as well as comparisons of behaviour in solution versus thin films, allows us to learn more about the intermolecular interactions, that are key for their functional properties. [1] Brixner, T., Hildner, R., Köhler, J., Lambert, C. & Würthner, F. *Adv. Energy Mater.* 7, 1700236 (2017). [2] Haedler, A. T. et al. *Nature* 523, 196-199 (2015).

CPP 49.3 Tue 14:00 P1A

Rotary Kelvin probe system to efficiently measure the giant surface potential of polarized organic films in completely dark condition — ●MASAHIRO OHARA¹, TATSUYA WATANABE², YUYA TANAKA^{2,3}, and HISAO ISHII^{2,3,4} — ¹Fac. Eng. Chiba Univ. — ²GSSE Chiba Univ. — ³CFS Chiba Univ. — ⁴MCRC Chiba Univ.

Amorphous organic films often show orientation polarization with giant surface potential (GSP). The polarization due to GSP often affects device performance; however, the origin of anisotropic orientation is still not well understood. One of the factors that hinders understanding this phenomenon is the difficulty in Kelvin probe (KP) experiment. GSP have been investigated by using conventional KP method. In this method, the repeated cycles of KP measurements and film deposi-

tions are quite time-consuming. In addition, ambient light illumination to sample film cannot be avoided at the switching between measurement and deposition, and it reduces the GSP more or less due to the compensation by photo-generated carriers. In this study, we have developed a surface potential measurement apparatus using the "Rotary KP method". It can solve the above problems by rotating the reference electrode. Since the reference electrode does not always cover the sample, the surface potential can be measured continuously even during the film deposition. Thus, GSP values free from light illumination can be efficiently measured. We will report on the details of our apparatus with the results of the surface potential of TPBi film prepared from its methanol solution to compare with the GSP of the vacuum evaporated film.

CPP 49.4 Tue 14:00 P1A

Structure Formation and Optical Emission of Organic Binary Mixed Thin Films — ●OLEG VLADIMIROV, NADINE RUSSEGGER, ALEXANDER HINDERHOFER, and FRANK SCHREIBER — Institut für Angewandte Physik, Universität Tübingen, Tübingen 72076, Germany

We present a comprehensive investigation of the charge transfer (CT) effect in weakly interacting organic semiconductors by means of planar heterostructures and mixtures. The donor-acceptor pairs diindenoperylene (DIP) with N,N*-Dimethyl-3,4,9,10-perylenetetracarboxylic diimide (PTCDI-C1), 2,9-Dipropylantra[2,1,9-def:6,5,10-d*e*f*]diisoquinoline-1,3,8,10(2H,9H)tetrone (PTCDI-C3) and N,N*-Dipentyl-3,4,9,10-perylenedicarboximide (PTCDI-C5) have been chosen for this purpose in order to investigate the structure and CT characteristics in dependence of the chain length of the respective molecules. The binary mixtures of PTCDI derivatives have already been studied for different mixing ratios in reference [V.Belova *J. Am. Chem. Soc.* 2017, 139, 25, 8474-8486]. A wide range of experimental methods, for instance atomic force microscopy, x-ray reflectometry, photoluminescence spectroscopy, UV-Vis spectroscopy and ellipsometry were used in order to characterize the structural, optical, electronic, and device properties of the intermolecular interactions. We observed that the mixtures with PTCDI-C1 phase separate due to their short chain length and form crystal structures when grown at high temperature, whereas mixtures with PTCDI-C3 show the formation of a co-crystal with pronounced CT.

CPP 49.5 Tue 14:00 P1A

Investigation of polymer templated silicon-germanium nanostructures for hybrid photovoltaics — ●CHRISTIAN L. WEINDL¹, MICHAEL A. GIEBEL², MATTHIAS SCHWARTZKOPF³, THOMAS F. FÄSSLER², STEFAN V. ROTH^{3,4}, and PETER MÜLLER-BUSCHBAUM^{1,5}

— ¹Technische Universität München, PhysikDepartment, Lehrstuhl für Funktionelle Materialien, James-Frank-Straße 1, 85748 Garching, Germany — ²Technische Universität München, Chemie-Department, Lehrstuhl für anorganische Chemie mit Schwerpunkt Neue Materialien, Lichtenbergstr. 4, 85748 Garching, Germany — ³Deutsches Elektronen-Synchrotron DESY, Noetkestraße 85, 22607 Hamburg, Germany — ⁴Royal Institute of Technology KTH, Teknikringen 34-35, 10044 Stockholm, Sweden — ⁵Heinz Maier-Leibniz Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany

Latest research in the field of hybrid photovoltaics focuses on the benefits of inorganic and organic materials. Flexibility, low cost, and large-scale production are the most valuable properties of organic components whereas the inorganic components add chemical and physical stability. In this work, we analyze thin films with optical, electrical and morphological measurement techniques to understand and control the corresponding properties. An amphiphilic diblock copolymer templating with polystyrene-b-polyethylene oxide (PS-b-PEO) and a potassium-semiconductor-semiconductor precursor is used to prepare porous thin films via sol-gel synthesis. The focus is to implement these mesoporous nanostructures into hybrid photovoltaics.

CPP 49.6 Tue 14:00 P1A

Key factors study in amphiphilic block copolymer-oriented porous SnO₂ synthesis process — ●SHANSHAN YIN¹ and PETER MÜLLER-BUSCHBAUM^{1,2} — ¹TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — ²Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, D-85748 Garching, Germany

SnO₂, as a crucial material in the field of energy storage, has always been the focus of scientific research. For organic-inorganic halide perovskite solar cells (PSCs) or dye-sensitized solar cells (DSSCs), SnO₂ contributes a high electron mobility and superior chemical stability amongst the various metal oxides. Moreover, as an alternative anode material for lithium ion battery, it possesses a decent theoretical specific capacity of 1494 mAhg⁻¹. Compared with conventional bulk materials, mesoporous SnO₂ with high specific surface area affords more advantages when applied on either solar cells or lithium-ion batteries. In the present work, a novel amphiphilic block copolymer assisted sol-gel chemistry is used for the synthesis of porous SnO₂ nanostructure. Different kinds of solvent are used as good solvent for both PS and PEO polymer chains, HCl is utilized as a selective poor solvent for PS chains and catalyst for the hydrolytic condensation reaction of SnCl₄ precursor. For removing the organic polymer template, the composite thin films are calcined at 500 °C for two hours under ambient condition. The obtained nanostructures are characterized by scanning electron microscope (SEM), X-ray diffraction (XRD) and grazing-incidence small-angle X-ray scattering (GISAXS) measurement.

CPP 49.7 Tue 14:00 P1A

In situ morphology study of printed ZnO photoanodes templated by block polymer for scalable fabrication of hybrid solar cells — ●TING TIAN¹, MATTHIAS SCHWARTZKOPF², STEPHAN V. ROTH^{2,3}, and PETER MÜLLER-BUSCHBAUM^{1,4} — ¹TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — ²DESY, Photon Science, 22607 Hamburg — ³KTH, Department of Fibre and Polymer Technology, 100 44 Stockholm, Sweden — ⁴Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, D-85748 Garching, Germany

Hybrid solar cells have attracted great attention due to the advantages of their short payback time, high stability and flexibility, which results from the combination of inorganic and organic materials. As photoanodes, mesoporous ZnO with a large surface area were widely employed to host the light-harvesting dyes and the organic molecular hole-transporters. For the synthesis of nanostructured ZnO, diblock copolymer assisted sol-gel approach has been corroborated by countless reports to be powerful in morphology tunability. The amphiphilic diblock copolymer assisted sol gel method and suitable printing parameters are used to fabricate nanostructured ZnO films. In situ grazing-incidence small-angle X-ray scattering (GISAXS) monitors continuously the inner film morphology in a destruction free manner. Based on printed nanostructured ZnO films, hybrid dye-sensitized solar cells are prepared and photovoltaic performance is investigated.

CPP 49.8 Tue 14:00 P1A

Quantification of Phase Purity in Formamidinium Based Multiple-Cation Perovskites by X-ray Scattering — ●LENA MERTEN, ALEXANDER HINDERHOFER, and FRANK SCHREIBER — Institut für Angewandte Physik, Universität Tübingen, Germany

During the last decade, the material class of hybrid organic-inorganic perovskites aroused huge interest in the solar cell community, leading to a substantial rise in photovoltaic efficiency and a promising perspective for relatively cheap and easy to manufacture solar cell materials. Formamidinium (FA) used as a central cation has the advantage of enhanced light harvesting due to a relatively small band gap, however, α -FAPbI₃ is unstable at room temperature and decays into hexagonal δ -FAPbI₃. Mixing various organic and inorganic cations within the perovskite material is investigated as one means to achieve enhanced phase purity of the photoactive cubic perovskite phase.

We used grazing incidence x-ray diffraction^[1] to examine mixed cation perovskite thin films on mesoporous TiO₂ substrates with regard to their ability to stabilize FA based perovskite.

Addition of the inorganic cations Cs and Rb to mixed MA:FA hybrid perovskites was found to significantly reduce the amount of hexagonal phases and excess lead iodide phase. By varying the probing depth, differences in phase composition between the film surface and the bulk material could be observed. The presence of inorganic cations also affected the degree of orientational order, crystallite size and the lattice

constant of the perovskite crystal structure.

[1] A. Greco et al., J. Phys. Chem. Lett. 2018, 9, 23, 6750-6754

CPP 49.9 Tue 14:00 P1A

Influence of Different Organic Cation and Halide Combinations on the Crystallization Dynamics of Perovskite Thin Films — ●EKATERINA KNESCHAUREK, ALEXANDER HINDERHOFER, and FRANK SCHREIBER — Institute for Applied Physics, University of Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany

Understanding the kinetic and energetic effects during organic-inorganic perovskite film growth is very important, since they determine how ions distribute in the structure, which affects the optoelectronic properties of the perovskite film. By tuning the composition of the perovskite films, the growth and formation of perovskite crystals and the extraordinary photophysical properties of perovskite materials can be significantly improved. The initial composition and formation mechanism define crystallization dynamics and structural properties of the resulting thin film. Samples with different compositions of MPbX₃ (M = CH₃NH₃⁺, CH(NH₂)₂⁺, Cs⁺ or Rb⁺ and X = Br⁻, I⁻ or a mixture) were produced using one-step conversion, a common fabrication technique. The perovskite crystal formation was induced by annealing. We applied in situ grazing incidence wide angle X-ray scattering (GIWAXS) to determine the reaction rate, intermediate phases during growth and perovskite unit cell parameter change in several perovskite thin films over time.[1] We discuss how combining lead halide precursors with different organic and inorganic halide solutions can impact the quality and time scale of the structural and morphological development of the spin-coated perovskite thin films.

1. A. Greco et. al., J. Phys Chem Lett., 2018, 6750

CPP 49.10 Tue 14:00 P1A

Fabrication on plasmonic nanostructures as light trapper in perovskite and organic solar cells — ●TIANFU GUAN, RENJUN GUO, XINYU JIANG, and PETER MÜLLER-BUSCHBAUM — TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany

Photovoltaic technology that can converting sunlight directly into electricity is one of the most promising technologies to harvest solar energy for renewable electricity supply. For photovoltaics, such as organic solar cells (OSCs) and perovskite solar cells (PSCs), the light management is an essential issue for achieving higher efficiency and the utilization of plasmonic metal nanostructures has been demonstrated as a promising approach for enhancing light harvesting. In view of this point, to regulate the plasmonic spectral of gold nanoparticles (Au NPs) for maximizing the enhancement in light-absorption of active layer, we assembly the metal NPs onto the electron collecting layer to broaden absorption band of photoactive layer of OSCs and PSCs as well as enhance the device performance. To meet the optimal results, we put effort into the plasmonic structure regulation, since the size, density and morphology of the metallic NPs will influence the crystallinity of the photoactive film and charge transportation of the device. In addition, grazing incidence wide angle x-ray scattering (GIWAXS) is used to probe the crystalline structure of the polymer/perovskite active layers. Grazing incidence small angle x-ray and neutron scattering (GISAXS and GISANS) is used to study the quality of the interface in terms of contact area between the materials.

CPP 49.11 Tue 14:00 P1A

Time-Resolved Microwave Conductivity: Temperature Dependent Dielectric Constant and Charge Carrier Dynamics of Methylammonium Lead Iodide — ●PATRICK DÖRFLINGER, JULIAN HÖCKER, PHILIPP RIEDER, ANDREAS SPERLICH, and VLADIMIR DYAKONOV — Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg

Perovskite solar cells are one of the most promising new photovoltaic technologies with steadily rising efficiencies. To further improve their potential performance, it is essential to understand their optoelectronic properties as well as to develop novel, not yet established, perovskite materials. With Time-Resolved Microwave Conductivity (TRMC) the mobility and lifetime of photogenerated charge carriers in a perovskite layer, e.g. methylammonium lead iodide (CH₃NH₃PbI₃), can be determined in a non-contact way. Besides the well known data handling in TRMC, one crucial parameter exhibits a strong dependency with temperature. The dielectric constant is not yet experimentally reported in literature for any perovskite material at 9 GHz, the frequency at which TRMC is measured. Considering the behaviour of the dielectric constant of the perovskites and its variation with temperature, one

can estimate the temperature dependent mobility with better accuracy. We perform temperature dependent measurements for MAPbI₃ from different preparation routes and discuss the power-law behaviour of the mobility in the context of temperature dependence of dielectric constant and the phase transitions of these materials.

CPP 49.12 Tue 14:00 P1A

In-situ GISAXS and GIWAXS measurements during slot-die printing of perovskite thin-films — ●MANUEL A. SCHEEL¹, LENNART K. REB¹, RENJUN GUO¹, SEBASTIAN GROTT¹, VOLKER KÖRSTGENS¹, WEI CHEN¹, NIAN LI¹, MATTHIAS SCHWARTZKOPF², STEPHAN V. ROTH^{2,3}, and PETER MÜLLER-BUSCHBAUM¹ — ¹Technische Universität München, Physik Department, Lehrstuhl für Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching, Germany — ²DESY, Notkestr. 85, 22607 Hamburg — ³KTH, Department of Fibre and Polymer Technology, SE-100 44 Stockholm, Sweden

Organic-inorganic metal halide perovskite based solar cells (PSCs) are currently intensely researched for their potential as cheap and highly efficient next generation solar cells applicable for industrial scale production. In principle, industrial requirements can be met by roll-to-roll slot-die coating. Highly crystalline and uniform films with low defect concentrations are paramount in reaching high power conversion efficiencies in PSCs. In order to better understand morphology evolution and crystallization kinetics during printing deposition in-situ GISAXS and in-situ GIWAXS measurements were done on methyl ammonium lead iodide (MAPI) thin films also covering the wet film stage during the printing process. Printing was carried out at ambient conditions with a self-built slot-die coater equipped with a meniscus guiding blade and temperature controlled sample stage on glass/ITO/PEDOT:PSS.

CPP 49.13 Tue 14:00 P1A

In-situ Observation of Perovskite Formation Upon Deposition of Tin Iodide onto Formamidinium Iodide — ●JONAS GLASER, JONAS HORN, and DERCK SCHLETTWEIN — Justus Liebig University Gießen, Institute of Applied Physics

As lead-based organic-inorganic halide perovskite solar cells have emerged as promising technology for low-cost and highly efficient photovoltaics, issues such as upscaling the manufacturing process and the toxicity of lead are put into focus of interest. Substituting lead by tin, originated in the same main-group with similar properties, yielded solar cell devices with power conversion efficiencies close to 10 %. Usually, tin-based perovskites are prepared via spin-coating from a precursor solution containing formamidinium iodide (FAI) and tin iodide (SnI₂). A different approach consists in the interdiffusion method, which combines spin-coating of the organic part with subsequent physical vapor deposition of SnI₂ and final annealing [1]. In order to study the formation of the perovskite phase in detail, an experimental setup for in-situ optical characterization of formamidinium tin iodide (FASnI₃) has been established, in order to study the transformation of the organic base-layer into the target perovskite through stepwise evaporation of SnI₂ and/or annealing.

1. J. Xi, Z. Wu, B. Jiao, H. Dong, C. Ran, C. Piao, T. Lei, T.-B. Song, W. Ke, T. Yokoyama, X. Hou, M. G. Kanatzidis, *Adv. Mater.* **29**, 1606964 (2017).

CPP 49.14 Tue 14:00 P1A

Morphological effects of cesium incorporation in mixed organic mixed halide perovskites — LENNART KLAUS REB, ●MANUEL ANDREE SCHEEL, RENJUN GUO, and PETER MÜLLER-BUSCHBAUM — TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching, Germany

Sunlight is one of the most promising energy source towards a sustainable future power generation. In the emerging field of new-generation thin-film photovoltaics, perovskite solar cells recently surpassed a power conversion efficiency of 25 % and are therefore a promising complement or even alternative for the commercially established silicon-based solar cells. Especially the highly tunable chemical composition of the perovskite layer allows optimizing the hybrid crystal structure in a way to profit from its unique optoelectronic properties. The incorporation of the alkali metal cation cesium (Cs) into the perovskite lattice has been shown to be beneficial for properties of the perovskite layer by influencing the crystal size and orientation in thin-films. Understanding and controlling the bulk film morphology is therefore essential for highly stable and efficient perovskite solar cells. In this work, we apply statistically relevant grazing-incidence wide-angle X-ray scattering (GIWAXS) to investigate the effect of Cs incorporation on the film morphology. In particular, we investigate

the popular (FAPbI₃)₈₃(MAPbBr₃)₁₇ perovskite composition in thin-films with different Cs contents and discuss the influence of Cs on their bulk film morphology with focus on the crystallinity.

CPP 49.15 Tue 14:00 P1A

Influence of the optical microcavity effects on the emission and absorption of perovskite solar cells — ●JAKOB WOLANSKY, CHRISTIAN WOLFF, LORENA PERDIGÓN-TORO, and DIETER NEHER — University of Potsdam, Institute of Physics and Astronomy, Germany

Perovskite solar cells are thin-film devices with usual thicknesses of some hundred nanometres, comparable with the wavelength of absorption and emission of light. Therefore, microcavity effects can influence the device emission and absorption properties, and finally its photovoltaic response.

In this work several parameters of the device stack are varied (e.g. thickness of the perovskite and the transport layers) and their influence on the luminescence and absorption spectra are consequently investigated. This is complemented by a detailed study of the electroluminescence and external quantum efficiency and their correlation via the reciprocity relation by U. Rau[1]. Finally, angular dependent measurements are performed and compared to the results of optical modelling.

[1] U. Rau, *Physical Review B* **76**, 085303 (2007)

CPP 49.16 Tue 14:00 P1A

Pathways towards 30% efficient single-junction perovskite solar cells — ●JONAS DIEKMANN¹, PIETRO CAPRIOGLIO¹, DANIEL ROTHHARDT¹, MALAVIKA ARVIND¹, THOMAS UNOLD², THOMAS KIRCHARTZ^{3,4}, DIETER NEHER¹, and MARTIN STOLTERFOHT¹ — ¹University of Potsdam — ²Helmholtz-Zentrum-Berlin — ³Forschungszentrum Jülich — ⁴University of Duisburg-Essen

Perovskite semiconductors have demonstrated outstanding external luminescence quantum yields, therefore potentially allowing power conversion efficiencies (PCE) close to the thermodynamic limits. In this work, we establish a simulation model that well describes efficient p-i-n type perovskite solar cells (PCE = 20%) and a range of different experiments helping to quantify the efficiency-limiting processes in state-of-the-art devices. Based on these results, we studied the role of important device and material parameters with a particular focus on chemical doping, carrier mobilities, energy level alignment and the built-in potential across all stack layers. We demonstrate that an efficiency regime of 30% can be unlocked by optimizing the built-in potential across the perovskite layer by using either highly doped thick transport layers (TLs) or ultrathin undoped TLs, e.g. self-assembled monolayers. Importantly, we only consider parameters that have been already demonstrated in recent literature, that is a bulk lifetime of 0.01 ms, interfacial recombination velocities of 100 cm/s, a perovskite bandgap of 1.47 eV and an EQE of 95%. A maximum efficiency of 31% is obtained for a bandgap of 1.4 eV using doped TLs.

CPP 49.17 Tue 14:00 P1A

Enhancing the Open-Circuit Voltage of Inverted Perovskite Solar Cells via Post Treatment Precursor Engineering — ●ZEKARIAS TEKLU, SHAHIDUL ALAM, STEFFI STUMPF, ULRICH S. SCHUBERT, and HARALD HOPPE — Friedrich Schiller University Jena, Germany

We develop a method of precursor engineering to prepare high-quality perovskite film and its stable PSC with enhanced Voc based on PbAc₂ and MAI. The precursor engineering process is done through simple post-treating on pure MAPbI₃ host film with (MABr, FABr and FAI)solutions resulted in the formation of mixed cation and or mixed anion of MAPbI₃-xBrx, FAxMA1-xPbI₃-xBrx, and FAxMA1-xPbI₃ perovskites respectively. This post treatment step leads to increased crystal grain dimension, compact and uniform morphology. The dipolar molecules of MABr, FABr, and FAI can simultaneously passivate both cationic and anionic defects of MAPbI₃ perovskite films and reduced the defects density, non-radiative recombination and electronic disorder, which are responsible for the Voc reduction. With the post engineering precursor modification, we have developed, the device Voc is enhanced markedly from 0.5 V to 1.08 V of average. The optimized device based on the FAxMA1-xPbI₃ obtained from the cation intermixing engineering of FAI on MAPbI₃ film shows a promising power conversion efficiency of 16%. As compared to conventional passivation approaches, by using anti-solvent engineering and fast crystallization, which are typically carried out at difficult and short time windows. Our post-treatment process can be easily done on the already crystallized perovskite film.

CPP 49.18 Tue 14:00 P1A

Role of Additives in Perovskite film formation for large area semi-transparent devices — ●GOPINATH PARAMASIVAM¹, JANARDAN DAGAR¹, FLORIAN MATHIES¹, CHANDRA SHAKHER PATHAK³, IRIS VISOLY-FISHER³, and EVA UNGER^{1,2} — ¹Helmholtz Zentrum Berlin, Germany — ²Lund University, Sweden — ³Ben Gurion University, Israel

Organic-Inorganic Hybrid perovskites have seen a profound interest over the last decennary. Perovskite solar cells (PSC) have reached a record power conversion efficiencies of over 25%. Its accessibility for large-area processing has seen applications in building-integrated photovoltaics. Perovskite Tandems have been realized to surpass the Shockley Quiesser Limit which limits the efficiency of the single-junction solar cells. Semitransparent solar cells make it a wider prospect for the PSCs to be witnessed in the tandem and building-integrated photovoltaics. Herein, we aim to present a detailed role of the additives in controlling the morphology of the films and in the chemical stability of the perovskite. We deployed various polymer hybrids into the perovskite precursor to improve the performance of the perovskites, where we see a change in the morphology with different polymers and performance is enhanced. We also intend to show our results on how the polymer additives tuned our inks for large area deposition through Slot die coating and Inkjet printing. We have achieved 16% power conversion efficiency on semitransparent devices in n-i-p architecture and 19% in opaque devices through spin coating.

CPP 49.19 Tue 14:00 P1A

Orders of Recombination in Perovskite Solar Cells — ●CHRISTIAN WOLFF¹, SEAN BOURELLE², SASCHA FELDMANN², FELIX DESCHLER^{2,3}, and DIETER NEHER¹ — ¹Institute für Physik und Astronomie, Universität Potsdam, Potsdam, Germany — ²Cavendish Laboratory, Department of Physics, University of Cambridge, Cambridge, UK. — ³Walter Schottky Institut, Technische Universität München, Garching, Germany

Understanding the mechanism and order of recombination in solar cells is of great importance to advance device performance. Pump-probe measurements on neat perovskite layers showed that the rate of recombination is in accordance with $dn/dt = -a \cdot n - b \cdot n \cdot (n + p_0) - c \cdot n^3$, which has been explained as the superposition of SRH, free-carrier, and Auger recombination. The situation in the full devices is more difficult, because charges recombine furthermore at surfaces, within other layers or across interfaces. Different measurements have been applied & reported, but thus far rendered an inconsistent picture of the dominant recombination orders and corresponding lifetimes. Combining multiple spectroscopic and electronic experiments, we provide a consistent picture of the dominating processes. We find that recombination under 1 sun illumination is dominated by a first-order process, while at higher intensities radiative recombination is prevailing. Therefore, the recombination in full devices can be well described by a simple rate equation, without the need to employ mixed-order processes. With this, we are able to reconstruct all device characteristics from dynamic variables.

CPP 49.20 Tue 14:00 P1A

Optical properties of electrons interacting with rotating molecules — ●VOLKER KARLE, AREG GHAZARYAN, and MIKHAIL LEMESHKO — Institute of Science and Technology Austria (IST Austria), Am Campus 1 3400 Klosterneuburg, Österreich

Recently solar panels based on halide perovskites have seen a tremendous increase in efficiency. However, the key mechanism responsible for this efficiency remains obscure [1]. In this project we theoretically investigate the interactions between electrons and molecules and calculate the resulting change in the absorption coefficient, which can be related to quantum efficiency. The main idea is based on the fact that rotating molecules can exchange angular momentum with the electrons [2]. Furthermore, electrons can decrease their ground-state energy by building up correlations with the molecules. This changes their absorption and mobility properties and could be used for tuning material properties.

[1] T. Chen, W.-L. Chen, B. J. Foley, J. Lee, J. P. Ruff, J. P. Ko, C. M. Brown, L. W. Harriger, D. Zhang, C. Park, and others, Proceedings of the National Academy of Sciences 114, 7519 (2017).

[2] D. H. Fabini, T. A. Siaw, C. C. Stoumpos, G. Laurita, D. Olds, K. Page, J. G. Hu, M. G. Kanatzidis, S. Han, and R. Seshadri, Journal of the American Chemical Society 139, 16875 (2017).

CPP 49.21 Tue 14:00 P1A

Magneto-Optical Properties of magnetically-doped Per-

ovskite Semiconductors — ●TIMO NEUMANN^{1,2}, JONATHAN ZERHOCH², SASCHA FELDMANN¹, MARTIN BRANDT², and FELIX DESCHLER² — ¹Cavendish Laboratory, University of Cambridge, Cambridge, UK — ²Walter Schottky Institut, Technische Universität München, 85748 Garching, Germany

Dilute magnetic semiconductors (DMS) constitute a material class which combines semiconducting and magnetic properties by introducing magnetic impurities to an otherwise non-magnetic host semiconductor. Fully inorganic DMS have been known for decades and advanced material processing techniques have enabled control over various functionalities like spin injection and the control of magnetism by electric fields and currents. Due to their outstanding optoelectronic properties and high defect tolerance, organo-metal halide perovskites form an ideal system for efficient magnetic doping. We perform temperature and magnetic field dependent magnetometry to characterise the magnetic properties of magnetically-doped perovskite semiconductors and employ polarisation-dependent, low temperature magnetophotoluminescence measurements to reveal the coupling between localised magnetic impurities and optically excited charge carriers.

CPP 49.22 Tue 14:00 P1A

Stabilizer-assisted tin-lead perovskite solar cells for high efficiency and stability — ●RUI WANG, RENJUN GUO, and PETER MÜLLER-BUSCHBAUM — TU München, Physik-Department, Lehrstuhl für Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching, Germany

Lead-based perovskites have proven to exhibit high photovoltaic performance and power conversion efficiency of over 20%. FA-stabilized perovskites show high long-term stability and are thermally endurable where other perovskite devices do not continue to function and lose their perovskite phase. Important is to further improve perovskite-based solar cells as a goal by reducing or removing the use of the heavy metal lead. To stabilize more the perovskite solar cell, PEA (phenethylammonium) is mixed with FA to achieve better stability. Thus, we systematically investigate the performance of FA(1-x)PEAI(x)Pb(1-x)Sn(x)I₃ mixed metal halide perovskites. Adding Sn leads to the stabilization of the black perovskite phase and the low formation temperature of 100°C is sufficient to reach of the formation of the perovskite phase. The efficiency we aimed at is over 10% with Sn content of x=0.5, 0.8, 0.3. The higher amount of Sn is expected to not enhance device performance.

CPP 49.23 Tue 14:00 P1A

GI/T-XPCS for slot-die coated perovskite thin films — ●CHRISTOPHER GREVE¹, MICHAEL BUCHHORN¹, DINESH KUMAR², ALEXANDER HEXEMER², LUTZ WIEGART³, and EVA M. HERZIG¹ — ¹Dynamik und Strukturbildung - Herzig Group, Universität Bayreuth, Universitätsstraße 30, 95447 Bayreuth, Germany — ²Advanced Light Source, Lawrence Berkeley National Lab, 1 Cyclotron Road, Berkeley Ca 94720, USA — ³NLSII, Brookhaven National Lab, Brookhaven Avenue, Upton NY, USA

X-Ray Correlation Spectroscopy (XPCS) is a useful tool to investigate the dynamics and the morphology of hard and soft condensed matter. Via XPCS, it is possible to probe length scales < 100nm and time scales >10-4s. To obtain information about the underlying dynamics, the correlations of the scattered intensity (speckles) in a time series are investigated. We use XPCS to investigate slot-die coated thin films in situ in grating incident (GI) and grating incident transmission (GT) geometry to gain insights in the underlying processes of thin film formation. For printing, an up-scalable printer setup is used and as a system methylammonium lead iodide (MAPI) is featured. MAPI is known for its solar cells applications, but the underlying processes of thin film formation are poorly understood. XPCS offers the possibility to investigate the dynamics in the evolving MAPI thin film. In our approach the optimized GT geometry allows to model the data in the born approximation, thus to ignore multiple scattering events from the thin film and the need to consider their impact on extracted dynamics.

CPP 49.24 Tue 14:00 P1A

The effect of surfactant doping on the crystallization kinetics and stability of perovskite solar cells — ●YUQIN ZOU and PETER MÜLLER-BUSCHBAUM — TU München, Physik-Department, Lehrstuhl für Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching, Germany

Perovskite solar cells (PSCs) have gained high attention within the last years. They have achieved a remarkable development due to their ex-

cellent optical properties and the power conversion efficiency of PSCs has meanwhile crossed the 25% border. However, the efficiency, hysteresis and stability of PSCs are still the main obstacles to their commercial application. The existing challenges are largely attributed to the presence of defect states. Tailoring functional ligands to passivate the defects in perovskite films and interfacial traps is an effective way to improve the performance of PSCs. In the present study, a small amount of surfactants (SDBS) is introduced to modify the perovskite interface, so that a high efficiency and stability of the PSCs can be obtained by crystallization control and defect passivation. The crystal structure, phase and orientation are studied with grazing incidence wide angle X-ray scattering (GIWAXS).

CPP 49.25 Tue 14:00 P1A

Electrical transport through DNA templated metallic nanowires and ds-DNA. — ●ARCHA JAIN^{1,2}, TÜRKAN BAYRAK¹, JINGJING YE³, BILAL KHAN¹, RALF SEIDEL³, ARTUR ERBE¹, and STEFAN SCHULZ² — ¹Institute of Ion Beam Physics and Materials Research, HZDR, 01328 Dresden, Germany — ²Technische Universität Chemnitz, 09107 Chemnitz, Germany — ³Peter Debye Institute for Soft Matter Physics, Universität Leipzig, 04103 Leipzig, Germany

Here we investigate self-assembled devices using DNA as excellent constructive and self-organizing material for nanoelectronics. So-called DNA origamis have been used as molds to build metallic nanowires in any shape and size, in contact with double stranded (ds) DNA segments. The combination with electron beam lithography as top down process allows for attaching metallic wires to the DNA origamis of smallest dimensions.

We investigate the charge transport through self-assembled, DNA templated metallic nanowire- ds-DNA- metallic nanowire structures. The ds-DNA structures between the Au nanowires are about 15 nm long (~30bp). We characterize the charge transport through these structures by current-voltage measurements. This electrical measurement through ds-DNA demonstrate the feasibility to use DNA for electron transport in nanodevices (Molecular electronics) and also increase the potential to use this bio- molecule for future applications.

CPP 49.26 Tue 14:00 P1A

Energy transfer mechanism in fluorescent carbon nanoparticle/dye composite — ●SUMESH SOFIN R. G¹, ABEY ISSAC¹, MALIK R. S. AL NAABI¹, MYO T. ZAR MYINT¹, HTET H. KYAW², and OSAMA K. ABOU-ZIED³ — ¹Department of Physics, College of Science, Sultan Qaboos University, Al Khoud, Muscat, Sultanate of Oman. — ²Nano Chair, College of Science, Sultan Qaboos University, Al Khoud, Muscat, Sultanate of Oman. — ³Department of Chemistry, College of Science, Sultan Qaboos University, Al Khoud, Muscat, Sultanate of Oman.

The photoluminescence of carbon nanoparticles (CNPs) is fascinating due to its application potential though the PL mechanism is not completely understood. Energy transfer between fluorophores and CNPs is also an important aspect in the field of green energy harvesting. In this work, we studied the energy transfer process between CNPs Rhodamine 6G dye molecules. CNPs were prepared using microwave assisted green synthesis method. The prepared particles were characterized using various tools to understand the structure and morphology. UV-Vis absorption/emission spectroscopy and time-resolved fluorescence decay measurements were done on particles and particle/dye composites. The results were analysed using Stern-Volmer quenching and Fluorescence resonance energy transfer models. Deconvolution analysis were performed on all the emission peaks to get in-depth details of energy transfer mechanism. Quantum yield and molar extinction coefficient of CNPs were estimated in this work. These studies may shine some light on the emission mechanism of CNPs.

CPP 49.27 Tue 14:00 P1A

What is the role of planarity and flexibility for aggregation in organic semiconductor materials? — ●STEFAN WEDLER¹, AXEL BOURDICK², STAVROS ATHANASOPOULOS³, STEPHAN GEKLE², FABIAN PANZER¹, CAITLIN McDOWELL⁴, GUILLERMO C. BAZAN⁴, and ANNA KÖHLER^{1,5} — ¹Soft Matter Optoelectronics, U Bayreuth — ²Biofluid Simulation and Modeling, U Bayreuth — ³Universidad Carlos III de Madrid — ⁴Center for Polymers and Organic Solids, UC Santa Barbara — ⁵BIMF, U Bayreuth

Planarity and flexibility play an important role for the aggregation process in organic semiconductors. Stiff and planar molecules seem to aggregate more easily. However, it is not clear whether these factors are a prerequisite or just a side effect of aggregation. We have inves-

tigated their influence on the aggregation properties using two similar conjugated molecules, with benzothiadiazole donor moieties and thiophene acceptor units. They differ only by their central unit, where a bithiophene unit either allows for flexible twists (TT), or where it is bridged to provide a rigid planar connection (CT). Temperature dependent absorption and luminescence spectroscopy in solution shows that both molecules can readily form aggregates. However, CT exhibits only weak aggregation signatures. MD simulations and DFT calculations reveal that although TT planarizes upon aggregation, its flexibility prevents the formation of excimer-like states, which seems to be the case for CT.

CPP 49.28 Tue 14:00 P1A

Photophysics of Pentacene Blends with Weakly Interacting Spacer Molecules — ●FREDERIK UNGER, CLEMENS ZEISER, and KATHARINA BROCH — Institute of Applied Physics, University of Tübingen, Germany

One of the main interests in pentacene (PEN) arises from its ability to undergo singlet fission (SF), a process where absorption of a single photon results in the generation of two triplet excitons [1]. Although being used as a prototypical model system, the details of the SF mechanism in PEN are still not fully understood. It is therefore crucial to understand and enable controlled tuning of the absorption behavior of PEN.

We mixed PEN with weakly interacting spacer molecules ([5]-phenacene [2] and [6]-phenacene) and investigated the PEN Davydov splitting as function of mixing ratio. Subsequent exciton behavior was investigated by temperature dependent photoluminescence spectroscopy. The comparison of the two systems is of special interest as the chemical and physical properties for both spacer molecules are similar, except for the difference in molecule length.

[1] Smith, M. B., and Michl, J., Chemical Reviews 110 (2010), [2] Dieterle, J., et al., J. Phys. Chem. C (2015).

CPP 49.29 Tue 14:00 P1A

Directly probing the singlet-triplet dynamics in organic semiconductors by high intensity step-function photoexcitation — ●JONAS GEHRIG¹, ULRICH MÜLLER¹, LENA ROOS², ANKE KRUEGER², and JENS PFLAUM^{1,3} — ¹Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — ²Institute of Organic Chemistry, Julius Maximilian University of Würzburg, 97074 Würzburg — ³ZAE Bayern, 97074 Würzburg

The excitonic singlet-triplet dynamics of organic semiconductors play a crucial role for their efficient implementation in opto-electronic devices. We present a compact setup to probe the relevant time-dependent processes like inter-system crossing, singlet fission (SF) or thermally activated delayed fluorescence (TADF). Unlike single molecule spectroscopy or pump-probe techniques, we utilize step-function photoexcitation at high excitation intensities in combination with time correlated single photon counting. Applying this technique to neat single crystals of tetracene (Tc) and its 2,2'-ditetracene dimer (DTc) we observed a sub-ns SF in Tc while this process is efficiently suppressed in DTc. X-ray diffraction analysis in combination with theoretical coupled-cluster calculations attribute this striking difference to the respective crystal structure being slightly modified by the covalent linking at the DTc 2,2'-position. On the molecular level, represented by doped anthracene single crystals, the fluorescent properties of Tc and DTc are almost identical and the absence of SF in both host-guest-systems emphasizes the role of inter- rather than intramolecular interactions for this non-radiative decay process.

CPP 49.30 Tue 14:00 P1A

Theoretical study of p-type double-doping in a conjugated polymer — ●THOMAS BATHE¹, CHUAN-DING DONG¹, and STEFAN SCHUMACHER^{1,2} — ¹Department of Physics and Center for Optoelectronics and Photonics Paderborn (CeOPP), Paderborn University, Warburger Strasse 100, 33098 Paderborn, Germany — ²College of Optical Sciences, University of Arizona, Tucson, AZ 85721, USA

Efficient molecular doping is essential for achieving the charge carrier densities needed for applications of conjugated polymers in electronic devices. Recent studies [1] have demonstrated the possibility to induce two charges in a conjugated polymer blend for each individual small dopant molecule. Dopants with sufficiently high electron affinity have to be used and those were shown to form di-anions upon successful transfer of two charges, increasing the efficiency of molecular p-type doping without increasing the concentration of doping molecules. Here, the formation of di-anions in charge-transfer complexes is stud-

ied theoretically. A single dopant molecule (CN6-CP and F6TCNNQ, respectively) is investigated in the vicinity of two conjugated oligomers based on density functional theory calculations [2]. For certain configurations, double-doping is indeed found and evidenced by an integer charge transfer from both oligomers onto the dopant molecule, leading to di-anion formation for the dopant molecule. Signatures of double doping are also found in the calculated optical and vibrational spectra.

- [1] Kiefer et al., *Nature Materials* 18, 149-155 (2019).
 [2] Dong, Schumacher, *ChemRxiv* (2019).

CPP 49.31 Tue 14:00 P1A

Adsorption of the photochromic diarylethene CMTE on a diamond surface — ●FABIAN BAUCH¹, CHUAN-DING DONG¹, CHRISTIAN WIEBELER², CEDRIK MEIER¹, and STEFAN SCHUMACHER¹ — ¹Department Physik, Universität Paderborn, Deutschland. — ²Institut für Analytische Chemie, Universität Leipzig, Deutschland.

Photochromic materials bear great potential for electronic devices such as optical switches and optical memories due to their reversible photoisomerization mechanism [1]. The photochromic *cis*-1,2-dicyano-1,2-bis(2,4,5-trimethyl-3-thienyl)ethene (CMTE) exhibits particularly high fatigue resistance and thermal stability [2]. In particular, the CMTE undergoes a pericyclic cyclization reaction upon irradiation with UV light while visible light triggers the cycloreversion reaction [2]. In realistic applications the molecular material or molecule would typically reside on or be bound to a substrate surface. To investigate the influence of such a surface on the structural and electronics properties of the molecular photoswitch, here we perform detailed density functional theory (DFT) calculations for CMTE in free gas-phase and adsorbed on different diamond surfaces saturated with hydrogen. We also calculate the optical absorption of CMTE in a single-particle approach for different molecule orientations on the surfaces. We find that the electronic and optical properties of CMTE are very similar to the gas-phase results for the case, when the molecule is only physisorbed on the surface but not chemically bound.

[1] M. Irie and M. Mohri. *J. Org. Chem.* 1988, 53, 4, 803-808. [2] C. Wiebeler, C. Bader. et.al. *Phys.Chem.Chem.Phys.*, 2014, 16, 1453.

CPP 49.32 Tue 14:00 P1A

Light-Induced Electron Transfer in the MOF-Based Noble-Metal-Free Photocatalyst Ni/CdS@MIL-101 as Studied with Fluorescence Lifetime Imaging Microscopy (FD-FLIM) — SEBASTIAN FEULNER¹, ●LOTHAR KADOR¹, MARA KLARNER², and RHETT KEMPE² — ¹University of Bayreuth, Institute of Physics, 95440 Bayreuth, Germany — ²University of Bayreuth, Institute of Inorganic Chemistry, 95440 Bayreuth, Germany

Particles of the semiconductor CdS on size-optimized metal-organic framework (MOF) crystallites act as a photo-catalyst for the H₂ liberation from amines. This acceptorless process is of great interest, since imine derivatives serve as intermediates to synthesize aromatic N-heterocycles which are highly desirable products for the fine chemical industry. The catalytic activity is strongly enhanced when co-catalytic Ni nanoparticles are present. We demonstrate that the photoluminescence lifetime of the CdS is shortened in the presence of Ni nanoparticles, so the improved catalytic activity can be related to electron transfer from the conduction band of the CdS to the Ni. The effect of Ni was found to be stronger than that of the noble metals Pt and Pd. The experiments were performed with a custom-built fluorescence lifetime imaging microscope operating in the frequency domain (FD-FLIM). It is based on a diode laser at 488 nm which was amplitude-modulated in the range 110 - 160 MHz. The data are evaluated with the polar-plot (or Cole-Cole plot) technique.

CPP 49.33 Tue 14:00 P1A

A new sample for coherent multidimensional spectroscopy: Preparation of molecules on cold rare gas clusters — ●ELENA LEISSLER, LUKAS BRUDER, ULRICH BANGERT, MARCEL BINZ, FRIEDEMANN LANDMESSER, DANIEL UHL, and FRANK STIENKEMEIER — Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg, Germany

The recent advances of coherent multidimensional spectroscopy towards the gas phase made new samples accessible, featuring low internal temperatures and minimal environmental perturbation [1]. In particular, matrix isolation on rare gas clusters is of interest, as it provides a high degree of control over molecule-molecule and molecule-solvent interactions. Doping the rare gas clusters with variable numbers of different molecules directly dictates the interaction strength. Here we present a cluster beam apparatus with a highly flexible doping unit.

The unit features high dopant densities and the possibility to simultaneously dope with various molecules out of the gas and solid phase.

[1] Lukas Bruder et al, *J. Phys. B: At. Mol. Opt. Phys.* 52 183501 (2019).

CPP 49.34 Tue 14:00 P1A

Recent advances in materials and modelling of organic electrochemical transistors — ●FLORIAN GÜNTHER, RENAN COLUCCI, HENRIQUE F. P. BARBOSA, GERMÁN GÓMEZ, PRISCILA CAVASSIN, and GREGÓRIO C. FARIA — Instituto de Física de São Carlos, Universidade de São Paulo, São Carlos, Brazil

Organic electrochemical transistors (OECTs) have been successfully used as a transducer in applications requiring conversion of ion fluxes to electronic current. To fully understand and optimize them, it is mandatory to develop in-depth theoretical predictions of experimental data that fits both modes of operation: depletion and accumulation. Moreover, it is imperative to count with a vast palette of semiconducting polymers that can be efficiently used as active layers in electrochemical devices. Here, we present a universal method and accompanying guidelines for fabricating OECTs using water-insoluble hydrophobic semiconducting polymers. By taking advantage of the interactions of semiconducting polymers in certain organic solvents and the formation of a stable liquid-liquid interface between such solvents and water, we fabricated accumulation mode OECTs with high transconductance and enhanced stability. Additionally, we present an extension of the well-known Bernard-Malliaras model for the steady-state response of OECTs to describe electrical responses of accumulation mode OECT. We have fit output-curves of accumulation mode OECT, fabricated with the universal method previously mentioned. In all cases we got good agreements between experimental data and theoretical fittings.

CPP 49.35 Tue 14:00 P1A

Modelling of anharmonic properties and thermal conductivity in organic semiconductors — ●FABIAN HAUPTMANN¹, SANDRO WIESER¹, TOMAS KAMENCEK¹, NATALIA BEDOYA-MARTINEZ², ROCHUS SCHMID³, JOHANNES PETER DÜRHOFT³, and EGBERT ZOJER¹ — ¹Institute for Solid State Physics, Graz University of Technology, NAWI Graz, Petersgasse 16, 8010 Graz, Austria — ²Materials Center Leoben, Roseggerstraße 12, 8700 Leoben, Austria — ³Computational Materials Chemistry group, Ruhr-Universität Bochum, Universitätsstraße 150, Bochum 44801, Germany

Thermal transport is important for most practical applications of functional materials. In (opto)electronic devices, it is typically desirable that materials dissipate heat as efficiently as possible. Conversely, for special purposes, like thermoelectric energy conversion, a low thermal conductivity is crucial. Organic semiconductors (OSC) are particularly relevant for optoelectronic applications, which is exemplified by their commercially successful use in displays for many devices. Moreover, OSCs have also been explored as promising candidates for thermoelectric applications. A central aspect for understanding thermal transport in OSCs is to realize, how the thermal conductivity and the structure of an OSC material are interrelated. In this work we parametrize advanced, system-specific force fields analogous to MOF-FF for a range of different acene-based OSC materials, to study their thermal expansion and thermal transport properties by using MD simulations. Our results, where available, are compared to experimental data.

CPP 49.36 Tue 14:00 P1A

Influence of morphology on the work function reduction by polyethylenimine — SUJITKUMAR BONTAPALLE^{1,2}, ●ANDREAS OPITZ², RAPHAEL SCHLESINGER², SETH R. MARDER³, SUSY VARUGHESE¹, and NORBERT KOCH^{2,4} — ¹Department of Chemical Engineering, Indian Institute of Technology Madras, Chennai, India — ²Department of Physics and IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin, Germany — ³School of Chemistry and Biochemistry and Center for Organic Photonics and Electronics (COPE), Georgia Institute of Technology Atlanta, Atlanta, USA — ⁴Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany

Polyethylenimine (PEI) layers are used to reduce the work function of electrode materials and are frequently applied to organic or perovskite opto-electronic devices. Intermixing of PEI from water-based solution with the conductive polymer poly(3,4-ethylenedioxythiophene):polystyrene sulfonate mixture can be avoided by the usage of anhydrous butanol as solvent for PEI. This preserves also the transparency of the polymer mixture. Heating of inhomogeneous PEI films in ultra-high vacuum ensures the removal of residual solvent and the homogeneous coverage. Thus, the work function of

PEI film is reduced to about 1.65 eV below the original substrate work function, which gives 2.3 eV as lowest observed value for zinc oxide.

CPP 49.37 Tue 14:00 P1A

Influence of Morphology on the Density of Charge-Transfer States in Organic Donor/Acceptor Blends — ●ANNA-LENA HOFMANN¹, THOMAS ZECHEL¹, THERESA LINDERL¹, ALEXANDER HOFMANN¹, TOMOYA SATO³, KOHEI SHIMIZU², HISAO ISHII³, and WOLFGANG BRÜTTING¹ — ¹Institute of Physics, University of Augsburg, 86159 Augsburg — ²Graduate School of Science and Engineering, Chiba University, Chiba, Japan — ³Center for Frontier Science, Chiba University, Chiba, Japan

Charge-transfer (CT) states are considered as precursors for charge generation and their energy (E_{CT}) as the upper limit for the open-circuit voltage (V_{OC}) in organic donor/acceptor (D/A) solar cells. In this study the morphological influence of using a crystalline donor diindoperylene (DIP) versus an amorphous donor tetraphenylidibenzoperiflanthene (DBP) with almost identical ionization energy is investigated. As acceptor material the widely used fullerene C₆₀ is used. Reduced electroluminescence (EL) and reduced external quantum efficiency (EQE) spectra in the visible and near infrared spectrum are used to determine E_{CT} and the character of the CT density of states (CT DOS). This is then related to the morphology of the different D/A systems. In this context we try to verify the necessity of static disorder in the description of CT emission and absorption spectra of small molecule solar cells. Remarkably, the more crystalline donor DIP shows a significant contribution of static disorder, whereas for the amorphous DBP a description without static disorder solely based on Marcus theory is sufficient.

CPP 49.38 Tue 14:00 P1A

Effect of thiophene- and benzothiadiazole-based non-fullerene acceptors in organic solar cells — ●JANNIS KLOTZ, HANNAH LINDL, STEFANIE DIETZ, MARIA KOTOVA, ANDREAS SPERLICH, and VLADIMIR DYAKONOV — Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg

Organic bulk heterojunction solar cells based on small molecule non-fullerene acceptors (NFA) received a lot of attention in the past few years due to a rapid increase in the device efficiencies up to 16%. This breakthrough, being highly promising, was mostly driven by empirical material engineering rather than by device-physics design. In this work we compare the already well established thiophene-based acceptor molecule ITIC and a novel benzothiadiazole-based acceptor molecule Y6. We studied optical and electrical properties of pure materials and blends as well as working devices. The acceptor ITIC was combined with the donor polymer PBDB-T and Y6 with a fluorinated version of PBDB-T: PM6. The redshifted and increased absorption of the PM6:Y6 blend in comparison to PBDB-T: ITIC lead to substantially increased short circuit currents and thus to higher device efficiencies. Nevertheless, fluorinated materials have shown to have limited solubility and faster device degradation. We investigated device preparation and degradation of both to evaluate their prospects for organic solar cells.

CPP 49.39 Tue 14:00 P1A

The mechanism of doping low band gap polymers with a Lewis acid — ●SIMON BIBERGER^{1,2}, VIKTOR BRUS², DAVID CAO², BRETT YURASH², DIRK LEIFERT^{2,3}, THUC-QUYEN NGUYEN², and ANNA KÖHLER¹ — ¹Softmatter Optoelectronics (EP2), University of Bayreuth, Germany — ²Center for Polymers and Organic Solids, UCSB, Santa Barbara, USA — ³Organisch-Chemisches Institut, Westfälische Wilhelms-Universität, Münster, Germany

To p-dope organic semiconductors F4TCNQ is commonly used. This doping mechanism relies on the electron transfer from the HOMO of the semiconductor to the LUMO of the dopant. This occurs by a match of those energy levels. For a solution-processed semiconductor this approach suffers from the differential solubility of the dopant, the charge-transfer complex and of the polymer what ultimately limits the processability of the doped semiconductor. In this study we use electrophilic Lewis acids to p-dope conjugated polymers. Work by Zalar et al. (Adv. Mat. 2014, 26, 727-727) showed an increased mobility after addition of Lewis acid. Yet the mechanism behind this doping approach is still elusive. To understand this approach we systematically investigate the effect of structural and electronic factors by varying, e.g., the donor and acceptor strength of the polymer. Optical and electrical characterization, using, e.g., optical spectroscopy and EPR, were performed to understand the influence of the adduct formation

on the properties of the polymer.

CPP 49.40 Tue 14:00 P1A

Ground-state charge transfer and influence on charge carrier transport in organic donor-acceptor mixtures — HONGWON KIM, MARIUS GEBHARDT, DOMENIK VÖGEL, and ●WOLFGANG BRÜTTING — Experimental Physics IV, Institute of Physics, University of Augsburg, Augsburg Germany

In organic semiconductors, charge transfer states form at interfaces of electron accepting and donating molecules resulting in a partial or full transfer of electrical charges. This charge transfer doping is crucial to generate excess charges in (opto-)electronic devices. We have investigated charge transfer states and charge transport properties of organic semiconductor mixtures consisting of electron donating molecules, DIP, 6T, DBTTF, and DBP, doped by a strong acceptor, F6TCNNQ. Charge transfer effects are observed by optical absorption spectroscopy and electrical transport properties are characterized depending on field and temperature by current-voltage measurements and impedance spectroscopy. In this way, it is possible to distinguish between integer charge transfer states and charge transfer complex formation, and to explain high electrical conductivity at a certain doping concentration with morphology and derived design rules for efficient charge transfer.

CPP 49.41 Tue 14:00 P1A

Influence of solvent on the morphology and optical properties of printed active layers based on PBDB-T-SF:IT-4F for application in organic solar cells — ●DANIEL MAXIMILIAN STEGER, KERSTIN SABRINA WIENHOLD, and PETER MÜLLER-BUSCHBAUM — Technische Universität München, Physik-Department, Lehrstuhl für Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching, Germany

The morphology of the active layer of polymer-based organic solar cells (OSCs) greatly influences their efficiency. Therefore factors determining the structure such as the used solvents are highly relevant in current research. The active layer consist of a blend of the polymer donor material PBDB-T-SF and the non-fullerene small molecule acceptor material IT4F. In this work the active layer is, in contrast to most other studies, produced via thin film printing, as this technique is a very promising approach to increase the scalability of solar cell production. The influence of the solvent on the morphology is investigated by observing the optical properties via UV/VIS- and fluorescence spectroscopy, the surface structure via atomic force microscopy (AFM) and studying the inner morphology by using scattering methods such as grazing incidence wide angle x-ray scattering (GIWAXS) and grazing incidence small angle x-ray scattering (GISAXS).

CPP 49.42 Tue 14:00 P1A

Influence of printing temperature on the efficiency of organic solar cells — ●LINUS FIDELIS HUBER, KERSTIN SABRINA WIENHOLD, and PETER MÜLLER-BUSCHBAUM — Technische Universität München, Physik-Department, Lehrstuhl für Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching, Germany

Solar cells have been a prominent and successful concept for eco-friendly energy conversion for a long time, but in search for better efficiencies and cheaper production costs, new materials and production techniques need to be explored. Printable-thin-film solar cells could lower production-cost by means of a high scale-up potential and an easier production process. They can also yield high efficiencies, are of lighter weight, flexible and semitransparent. This suggests a wide variety of possible applications, where silicon-solar cells seem to be less applicable. Printing temperature is an important parameter and varying it, could lead to better efficiencies and a broader understanding of the polymers dependence on temperature. We focus on novel low band gap polymers in combination with non-fullerene acceptor molecules. Four different printing temperatures are studied and evaluated using UV-Vis, photoluminescence, AFM and GISAXS measurements.

CPP 49.43 Tue 14:00 P1A

Studying aggregation behavior of Conjugated Polyelectrolytes as a function of molecular weight for Poly(3-hexylthiophen-2,5-diyl) (P3HT) and Poly(6-(thiophene-3-yl)hexane-1-sulfonate) (PTHS) — ●SANWARDHINI PANTAWANE and STEPHAN GEKLE — Biofluid Simulation and Modeling, Theoretische Physik VI, Universität Bayreuth, Bayreuth, Germany

Aggregation of π conjugated polymers like Poly(3-hexylthiophen-2,5-

diyl) (P3HT) and the improved P3HT substitute - Poly(6-(thiophene-3-yl)hexane-1-sulfonate) (PTHS) is important for their performance in optoelectronic devices. It is experimentally observed that the red shift in the UV-vis spectra with increasing molecular weight is much stronger for PTHS than for P3HT, even though both molecules are structurally very similar. To understand this, we prepared different polymer chains of P3HT and PTHS starting with 13 monomers each, as was done in the experimental studies, and carry out molecular dynamics simulation in water and sodium ions, to correlate the fluorescence spectra with difference in the aggregation conformation as a function of the polymer's molecular weight. We perform free energy calculations to pull the end rings of the polymer towards each other and investigate their potential of mean force (PMF). This study gives us an insight about the folding probability of the P3HT and PTHS chains with varying lengths.

CPP 49.44 Tue 14:00 P1A

Impact of Mixing on Coupling of Transition Dipole Moments in Pentacene: Dinaphtho[2,3-b:2',3'-f]thieno[3,2-b]thiophene — ●ARNE MORLOK¹, CLEMENS ZEISER¹, DANIEL LEPPLE¹, GUILLAUME SCHWEICHER², YVES GEERT³, and KATHARINA BROCH¹ — ¹Universität Tübingen, Institut für Angewandte Physik, Auf der Morgenstelle 10, 72076 Tübingen, Germany — ²University of Cambridge, Cavendish Laboratory, JJ Thompson Avenue 19, CB3 0HE Cambridge, UK — ³Université Libre de Bruxelles, Chemistry Departement, Avenue Franklin Roosevelt 50, 1050 Bruxelles, Belgium

The coupling of transition dipole moments (TDMs) strongly affects the optical properties of organic semiconductors (OSCs), for instance in H- or J-type coupling or Davydov-splitting [1]. Despite changes in the unit cell parameters, in blends of pentacene (PEN) with the H-aggregate diindenoperylene (DIP) no significant changes in the H-type coupling have been observed, which is consistent with the orientation of the TDMs [2]. For J-aggregates however, the impact of mixing and the corresponding increase in intermolecular distances will be more pronounced but has so far not been discussed in detail in the literature.

Here, we report the optical properties of dinaphtho[2,3-b:2',3'-f]thieno[3,2-b]thiophene, which shows the optical properties of a J-aggregate, in blends with PEN. We observe strong changes in the intensity of absorption peaks, which can be directly related to the increase in the lattice spacing and the reduced coupling of TDMs.

[1] F. C. Spano, Acc. Chem. Res. 43 (2010)

[2] K. Broch et al., J. Phys. Chem. C 117 (2013)

CPP 49.45 Tue 14:00 P1A

Der Einfluss von Elektrophorese auf die aktive Schicht organischer Solarzellen — ●FABIAN ELLER, STEPHAN PRÖLLER and EVA M. HERZIG — Dynamik und Strukturbildung - Herzig Group, Universität Bayreuth, Universitätsstr. 30, 95447 Bayreuth

Slot-die coating bietet die Möglichkeit, organische Dünnschicht solarzellen effizient mit industriennahen Methoden herzustellen. Um einen hohen Wirkungsgrad zu erreichen, ist eine optimale Nanostrukturierung des Dünnschichtfilms notwendig. Wir haben gezeigt, dass die Morphologie des gedruckten Filmes mit einem elektrischen Feld während des Druckprozesses beeinflusst werden kann [1].

Um den Effekt eines elektrischen Feldes auszunutzen, charakterisieren wir systematisch die elektro-phoretischen Mobilitäten von halbleitenden Materialien für die Nutzung in OPV Systemen. Die Abhängigkeit von diversen externen Parametern und der Lösungsherstellung erlaubt es uns, die Mobilitäten gezielt einzustellen.

Unser Ziel ist es die Morphologie und damit den Wirkungsgrad von gedruckten Solarzellen in unterschiedlichen Materialsystemen durch Anlegen eines elektrischen Feldes zu steuern.

[1] paper, submitted

CPP 49.46 Tue 14:00 P1A

Donor-Acceptor Polymers with PDMS-Ur based cross-linkers: A Novel Hybrid Material for Stretchable Semiconductor Applications — ●FLORIAN GÜNTHER¹, UBIRAJARA P. RODRIGUES-FILHO², and ROBERTO M. FARIA¹ — ¹Instituto de Física de São Carlos, Universidade de São Paulo, São Carlos, Brazil — ²Instituto de Química de São Carlos, Universidade de São Paulo, São Carlos, Brazil

The visions that we have for our future, especially the expectations we have on electronic devices, require the invention of new materials. In the past decades, organic semiconducting materials have been intensively studied since they show some advantages over bulk semiconductors. E.g., they offer the possibility to fabricate flexible devices. So far,

however, flexibility has mainly been studied in terms of bendable and twistable thin films. The next stage on the road map towards higher functionality is therefore to focus on stretchability. Our work aims at combining the semiconducting properties of donor-acceptor polymers, especially those based on dithienyl-diketopyrrolopyrrole (TDPP), with the flexible properties of polydimethylsiloxane (PDMS). More specific, the TDPP-based DA backbones shall be crosslinked via PDMS by forming urethane (Ur) bonds between these two compounds. For this, the so-called Figovsky reaction can be used. The urethane bonds promise a higher chemically and mechanically stability due to additional hydrogen bonds. In this presentation, we are going to show our synthesis and fabrication strategies as well as our results on the semiconducting properties obtained so far.

CPP 49.47 Tue 14:00 P1A

Direct measurement of charge recombination losses in organic solar cells by transientspectroscopy — ●FLORIAN GÜNTHER, DANIEL R. B. AMORIM, ROBERTO M. FARIA, and PAULO B. MIRANDA — Instituto de Física de São Carlos, Universidade de São Paulo, São Carlos, Brazil

Research on organic solar cells has increased significantly in the past decade, covering both applied and basic aspects. Improvements in their performances depend on a deep knowledge about the photophysical and electronic processes that occur in the materials. The dynamics of charge recombination within operating devices is one important issue being relevant for determining the charge recombination losses and the overall device efficiency. In our work, we directly probe the dynamics of charge recombination and extraction in organic solar cells by combining transient photoinduced absorption spectroscopy (TAS) with transient photocurrent (TPC) measurements in the ns to ms time range after excitation of the device by a short laser pulse. TAS probes the dynamics of the charge density inside the organic active layer of the solar cell, while TPC measures the rate of charge extraction from the device. Comparing both measurements it is possible to determine how much photogenerated charge is lost within the active layer due to charge recombination, a major loss mechanism that limits the overall device efficiency. Using this technique, we have probed high-quality solar cells based on porphyrinderivatives and also traditional polymer-based (P3HT:PCBM) solar cells.

CPP 49.48 Tue 14:00 P1A

Improvement of hole transport layer selectivity for polymer solar cells — ●AURELIEN SOKENG DJOUMESSI^{1,2}, JOSE PRINCE MADALAIMUTHU^{1,2}, SHAHIDUL ALAM^{1,2}, ULRICH S. SCHUBERT^{1,2}, and HARALD HOPPE^{1,2} — ¹Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich Schiller University Jena, Germany — ²Laboratory of Organic and Macromolecular Chemistry (IOMC), Friedrich Schiller University Jena, Germany

Since the device performance and stability strongly depend on the interfacial layers, the hole transport layer (HTL) is one of the crucial parameters of polymer solar cells. Specifically interesting for charge extraction is the selectivity of the HTL. Furthermore unfavorable interactions with electrodes or the photoactive layer should be screened. We investigated organic solar cells in conventional architecture by varying the HTL systematically between PEDOT:PSS and a sol-gel derived metal oxide. The impact of modified HTL in the solar cells were investigated by different optical and electrical characterizations. In order to observe the effect on the recombination mechanism of the solar cells, light intensity-dependent current-voltage (LID-IV) measurements and analysis of IV-characteristics were performed.

CPP 49.49 Tue 14:00 P1A

Qualification of Thieno-Quinoxaline Based Polymers for Application in Non-Fullerene Organic Solar Cells — ●MD MOJIBUL ISLAM^{1,2}, SHAHIDUL ALAM^{1,2}, CHRISTOS L. CHOCHOS^{4,5}, ULRICH S. SCHUBERT^{1,2,3}, and HARALD HOPPE^{1,2} — ¹Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich Schiller University Jena, Jena, Germany — ²Laboratory of Organic and Macromolecular Chemistry (IOMC), Friedrich Schiller University Jena, 07743 Jena, Germany — ³Jena Center for Soft Matter (JCSM), Friedrich Schiller University Jena, Jena, Germany — ⁴Institute of Chemical Biology, National Hellenic Research Foundation, Athens, Greece. — ⁵Advent Technologies SA, Patra, Greece

Next-generation organic solar cells should not only be improved in performance but also should be environment-friendly throughout the production process. The processing of polymer-based solar cells with green solvents are highly desirable to make environmental friendly so-

lar cells. In this study, we present bulk heterojunction polymer solar cells based on the thieno-quinoxaline based polymers blended with non-fullerene acceptor (NFA) in the non-halogenated solvent. Solar cells were prepared in conventional and inverted architecture, in order to investigate the material properties various spectroscopic measurements were performed in the pristine and blend films, as well as in the solutions. Finally, photovoltaic performances were investigated by different opto-electrical characterizations.

CPP 49.50 Tue 14:00 P1A

Re-evaluation of the IV-Curve — ●RICO MEITZNER^{1,2}, SHAHIDUL ALAM^{1,2}, AMAN ANAND^{1,2}, ULRICH S. SCHUBERT^{1,2} und HARALD HOPPE^{1,2} — ¹Center for Energy and Environmental Chemistry, Friedrich-Schiller-Universität Jena, 07743 Jena — ²Institute for Organische und Makromolekulare Chemie (IOMC), Friedrich-Schiller Universität, 07743 Jena

The most basic measurement performed on solar cells is an IV-characterization. Most commonly the basic solar cell parameters, like open circuit voltage, short circuit current density, fill factor and power conversion efficiency are extracted from these measurements. From further analysis of these curves, we found that they could actually reveal more than meets the eye normally. We want to present a new method to analyze these curves and how it could help getting a better view on what to look into with more depth for these devices.

CPP 49.51 Tue 14:00 P1A

IR Spectroscopic Investigation on Immobilization of organic dopants — ●RAINER BÄUERLE^{1,2,3}, PATRICK REISER^{1,4}, FRANK SIMON BENNECKENDORF^{1,3,4}, MARC-MICHAEL BARF^{1,5}, SEBASTIAN BECK^{1,2}, ANNEMARIE PUCCI^{1,2}, UWE H. F. BUNZ^{1,3}, and WOLFGANG KOWALSKY^{1,5} — ¹InnovationLab, Heidelberg — ²Kirchhoff Institute for Physics, University of Heidelberg — ³Organisch-Chemisches Institut, University of Heidelberg — ⁴Materials Science Department, Surface Science Division, TU Darmstadt — ⁵Institute for High-Frequency Technology, TU Braunschweig

One challenge in doping of organic semiconductors lies in the unstable spatial distribution of dopants. The simple intermixing of dopants to a matrix semiconductor makes them subject to diffusion and drift. With a universal anchor group that covalently binds to most semiconductors this problem can be overcome. We investigate the influence of an azide group as such anchor in a semiconductor thin film on the diffusion of dopants via infrared spectroscopy.

A derivate of the literature known n-dopant DMBI without anchor leaves a film of PCBM under UHV conditions undoped in time. The same dopant anchored via an azide group remains in the film after days in UHV proofing a successful suppression of diffusion. During UV activation of the anchor only the azide absorption band vanishes indicating no major disintegration of both dopant and matrix. Unaltered electric properties make this approach feasible for use in organic devices. The universal use is demonstrated by successfully anchoring in the n-type small molecule PCBM and in the p-type polymer P3HT.

CPP 49.52 Tue 14:00 P1A

Efficiency loss channel determination in colloidal InP-based quantum dot light emitting diodes — ●MANUEL ENGELMAYER¹, YOHAN KIM², ANDRÉ GESSNER², and WOLFGANG BRÜTTING¹ — ¹Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — ²Fraunhofer Institute for Applied Polymer Research IAP, 14476 Potsdam, Germany

Colloidal quantum dot light emitting diodes have gained huge interest in both academia and industry over the course of the last years. In order to enable high luminances at low voltages with a reasonable energy consumption, the origin of efficiency losses must be clarified and then suppressed. CdSe-based literature shows two major possible loss channels, one being current dependent Auger quenching and the other being field-induced quenching. Unfortunately, purely electrical characterisation is not able to fully specify the respective contributions to the overall efficiency loss.

To gain deeper insights into the loss mechanisms of such quantum dot light emitting diodes, we built an experimental setup for combined electro- and photoluminescent excitation of quantum dots, which allows to simultaneously monitor the electrical and optical device efficiency. By comparing these with the photoluminescent quantum efficiency at an applied reverse bias, we are able to separate the superimposed effects of Auger and field-dependent efficiency loss.

First results for InP-based core-shell quantum dot light emitting diodes point towards Auger recombination being the dominant efficiency loss mechanism.

CPP 49.53 Tue 14:00 P1A

Charge Transfer at the Interface of Dye-sensitized Solar Cells with Mg_xZnO_{1-x} — ●NICO HOFEDITZ¹, ANDREAS RINGLEB², DERCK SCHLETTWEIN², and WOLFRAM HEIMBRODT¹ — ¹Department of Physics and Material Sciences Center, Philipps-University Marburg, Renthof 5, 35032 Marburg, Germany — ²Institute of Applied Physics, Justus-Liebig-University Gießen, Heinrich-Buff-Ring 16, 35392 Giessen, Germany

Dye-sensitized solar cells containing the indoline dye D149 have been prepared with an iodide/triiodide electrolyte. The mesoporous photoanode has been prepared from ZnO with different concentrations of Mg. Hereby the effect of Mg-doping on cell performance can be studied.

An important process in high efficient dye-sensitized solar cells is an optimized electron transfer, i.e., the electron injection yield from the dye into the conduction band of the (Mg_x)ZnO_{1-x} at the organic-inorganic interface.

The desired effect of the Mg-doping is an increased open-circuit voltage of the cell through a change in the energy level alignment of the anode. Since this has an effect on the charge injection characteristics, we use time-resolved photoluminescence spectroscopy to study this process in detail.