

## CPP 28: Poster III

Organic Electronics and Photovoltaics (1-30), Hybrid and Perovskite Photovoltaics (31-41), Molecular Electronics and Excited State Properties (42-45), Interfaces and Thin Films (46-53), Electrical, Dielectrical and Optical Properties of Thin Films (54-56)

Time: Wednesday 11:30–13:30

Location: Poster C

CPP 28.1 Wed 11:30 Poster C

**Revealing the effect of solvent additive selectivity on formation kinetics in printed active layers for organic solar cells —**

•JINSHENG ZHANG<sup>1</sup> and PETER MÜLLER-BUSCHBAUM<sup>1,2</sup> — <sup>1</sup>TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — <sup>2</sup>TUM, MLZ, 85748 Garching, Germany

Solvent additives have received tremendous attention in organic solar cells as an effective way to optimize morphology and phase separation. However, most research primarily focuses on solvent additives with superior solvation for non-fullerene acceptors (NFA) over polymer donors, such as the 1-chloronaphthalen (1-CN), 1, 8-diiodooctane (1,8-DIO). Few researches are related to solvent additives characterized by better solubility for polymer donors than NFA. Furthermore, the impact of solvent additives is mainly investigated through spin coating rather than slot-die coating, which exhibits distinct kinetics in film formation. Hence, the influence of solvent additive selectivity on the kinetics of active layer formation in the printed active layer remains unknown. In this study, we use PBDB-T-2F as the donor and BTP-4F as the acceptor and introduce two distinct solvent additives\*one with superior solubility for PBDB-T-2F compared to BTP-4F, and the other with inferior solubility for PBDB-T-2F. The drying process of the slot-die coated active layers with different solvent additives is studied by in situ UV-vis absorption spectra and in situ grazing incidence wide angle X-Ray scattering (GIWAXS).

CPP 28.2 Wed 11:30 Poster C

**Organic Solar Cells for Space Application: Investigation of the Nanostructure and Degradation Effects Due to Mechanical Stress —**

•JAN DARSOW<sup>1</sup>, LUKAS V. SPANIER<sup>1</sup>, CHRISTIAN GSCHIEDLE<sup>2</sup>, and PETER MÜLLER-BUSCHBAUM<sup>1,3</sup> — <sup>1</sup>TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — <sup>2</sup>TUM School of Engineering and Design, Chair of Astronautics, 85748 Garching, Germany — <sup>3</sup>TUM, MLZ, 85748 Garching, Germany

Organic solar cells (OSCs) are emerging as a promising candidate as an energy source for space applications because of their high gravimetric power density and flexible nature. This would save fuel and space in a rocket flight. However, several challenges must be addressed for OSCs to fulfil their potential in space. Following a previous project that deployed OSCs in space on a suborbital rocket, this work aims to further investigate the degradation of OSCs due to the harsh conditions during space flights. Primarily the degradation due to intense mechanical stress will be investigated. OSCs are exposed to extreme accelerations and vibrations during rocket launch and re-entry. This will be simulated with a shaker stress test followed by an investigation of the OSCs changed structural and electronic properties. The examined OSCs are based on a BTP-4F and PTQ-2F bulk heterojunction (BHJ) and are fabricated on glass and flexible PET substrates. Another topic of this work is research on the effects of annealing the BHJ, which leads to a tuning of the absorption spectrum.

CPP 28.3 Wed 11:30 Poster C

**Setup for in Operando X-ray Scattering of Thin Film Solar Cells under Dynamic Temperature Variation —**

•SIMON ALEXANDER WEGENER<sup>1</sup> and PETER MÜLLER-BUSCHBAUM<sup>1,2</sup> — <sup>1</sup>TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — <sup>2</sup>MLZ, TUM, 85748 Garching, Germany

Thin film solar cells hold immense promise for space applications due to their lightweight and flexible nature, making them ideal for powering satellites and spacecraft. Understanding their performance under extreme conditions is pivotal for their successful deployment in space missions. This study introduces an experimental setup designed for operando grazing-incidence wide-angle X-ray scattering (GIWAXS) and grazing-incidence small-angle X-ray scattering (GISAXS) measurements on perovskite and organic thin film solar cells. The setup enables rapid temperature changes, simulating a wide range of operational environments. Crucially, the apparatus exposes solar cells to simulated sunlight of changeable intensity, facilitating measurements

under realistic light conditions. Furthermore, it allows modulation of complete day-night cycles, adjusting both, light intensity and temperature up to 130 degrees Celsius to replicate dynamic environmental fluctuations. This methodology offers a comprehensive approach for dynamically evaluating thin film solar cells, providing insights into their structural and functional characteristics under diverse environmental conditions.

CPP 28.4 Wed 11:30 Poster C

**Controlling spontaneous orientation polarization in exciplex-forming OLEDs —**

•ALBIN CAKAJ, LEA KOLB, ALEXANDER HOFMANN, and WOLFGANG BRÜTTING — Experimental Physics IV, Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

The resulting internal electrical field, due to spontaneous orientation polarization (SOP), affects the charge injection and accumulation behavior of organic light emitting diodes (OLEDs) significantly. While the community has just recently started to understand the formation process and its active control, it is still not completely clear if this effect is advantageous or detrimental in organic semiconductor devices [1]. In our studies, we investigated an exciplex-forming mixture of the polar species TPBi and the nonpolar molecule TCTA regarding their electrical and optical orientation as well as their properties as an emissive layer in OLEDs. By substrate temperature control the film polarization can be tuned over a broad range from 0 to 125 mV/nm, comparable to recent studies for single-molecule films [2]. But despite of the loose exciton binding, the photoluminescence spectra are not affected by changes in the degree of SOP. Investigations on mixed and bilayer devices hint to the conclusion that exciton quenching is almost not apparent in this material combination. This makes the investigated exciplex system possibly a good candidate as a co-host for efficient OLEDs. [1] A. Hofmann et al. Adv. Optical Mater. DOI:10.1002/adom.202101004 (2021) [2] A. Cakaj et al. ACS Appl. Mater. Interfaces, DOI:10.1021/acsmi.3c13049 (2023)

CPP 28.5 Wed 11:30 Poster C

**Thickness and Temperature-Dependent Charge Carrier Mobility of Non-fullerene Acceptors in Single-Carrier Electron-Only Devices —**

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The charge carrier mobility of organic semiconductors is crucial for high-efficiency organic solar cells. This study aims to investigate the charge carrier transport properties in disordered non-fullerene acceptors (NFAs), explicitly focusing on ITIC and its derivatives, namely, ITIC-4F and ITIC-4Cl. The charge carrier transport properties were investigated on single-carrier electron-only devices using the field-independent space-charge-limited-current (SCLC) method. To reveal the impact of order/disorder and halogenation, specifically fluorination or chlorination, thickness and temperature-dependent carrier mobilities were studied systematically. Furthermore, thermionic emission and Fowler-Nordheim tunneling models were applied to calculate the barrier heights at the metal/organic interfaces under forward and reverse bias conditions. Finally, different spectroscopic and microscopic techniques were used to further investigate the optical and morphological properties of the organic semiconductors.

CPP 28.6 Wed 11:30 Poster C

**Optimization of Slot-Die Printed Organic Solar Cells —**

•CHRISTOPH G. LINDENMEIR<sup>1</sup>, MANUEL A. REUS<sup>1</sup>, SIMON WEGENER<sup>1</sup>, CHRISTOPHER R. EVERETT<sup>1</sup>, JULIAN E. HEGER<sup>1</sup>, SIGRID BERNSTROFF<sup>2</sup>, and PETER MÜLLER-BUSCHBAUM<sup>1,3</sup> — <sup>1</sup>TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — <sup>2</sup>Elettra, 34149 Basovizza, Trieste, Italy — <sup>3</sup>TUM, MLZ, 85748 Garching, Germany

In research, organic solar cells (OSCs) have received a lot of attention in recent years because of their low weight, non-toxicity, short

energy payback times and high efficiencies. OSCs are also particularly intriguing to the industry because of their easy solution-based manufacturing technique, which allows for thin and flexible solar cells. The OSCs can be manufactured with different deposition technologies such as printing and spin-coating due to the solution-based fabrication process. Slot-die printing is a very promising printing approach because it is fast, causes low waste and is easily upscalable. Here, we optimize the slot-die printing technique of OSCs under ambient and nitrogen conditions and compare their attributes to spin-coated OSCs. The OSCs are compared using measuring techniques such as spectroscopy and real-space imaging in combination with X-ray scattering.

CPP 28.7 Wed 11:30 Poster C

**Characterization of Differently Substituted Imidazo[1,5-a]quinoline Thin Films for Applications as OLED Emitters** — ●AARON PIEPER<sup>1</sup>, THOMAS OEL<sup>2</sup>, PASCAL SCHWEITZER<sup>1</sup>, CARINA RÖSSIGER<sup>2</sup>, RICHARD GÖTTLICH<sup>2</sup>, and DERCK SCHLETTWEIN<sup>1</sup> — <sup>1</sup>Institut für Angewandte Physik, Justus-Liebig-Universität Gießen — <sup>2</sup>Institut für Organische Chemie, Justus-Liebig-Universität Gießen

Imidazo-[1,5-a]-quinolines and -iso-quinolines are characterized by an emission in the blue range of the visible spectrum. This can be particularly interesting for applications as emitter molecules in OLEDs. We prepared thin films of differently substituted quinolines and iso-quinolines by physical vapor deposition in high vacuum. Their growth mode on technically relevant contact phases like poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT:PSS) and indium tin oxide (ITO) was studied by non-contact atomic force microscopy. Spectroscopic studies of these thin films were conducted to assess their luminescence and absorbance/excitation properties. First steps were taken to incorporate these materials into a simple OLED layer stack based on PEDOT:PSS as a hole injector and bathocuproine (BCP) as an electron transport layer.

CPP 28.8 Wed 11:30 Poster C

**Electroluminescence and Charge Transport Barriers in Blue OLED Based on Thin Films of 3 Phenyl-1-(quinoline-2-yl)imidazo[1,5-a]quinoline** — ●PASCAL SCHWEITZER<sup>1</sup>, CARINA RÖSSIGER<sup>2</sup>, ALPER YILMAZ<sup>1</sup>, GUSTAV NOLTE<sup>1</sup>, MARIUS ECKERT<sup>1</sup>, RICHARD GÖTTLICH<sup>2</sup>, and DERCK SCHLETTWEIN<sup>1</sup> — <sup>1</sup>Institut für Angewandte Physik, Justus-Liebig-Universität Gießen — <sup>2</sup>Institut für Organische Chemie, Justus-Liebig-Universität Gießen

3-Phenyl-1-(quinoline-2-yl)-imidazo-[1,5-a]-quinoline (PhCIC) is a promising organic emitter molecule for the possible application in blue organic light-emitting diodes (OLEDs). We prepared thin films by physical vapor deposition and studied their photoluminescence (PL) and electroluminescence (EL) to evaluate PhCIC as emitter. Poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT:PSS) served as back contact, poly(9-vinylcarbazole) (PVK) as hole injector, and bathocuproine (BCP) as electron injector contacted by Al. Emission by PVK in the same spectral range as that of PhCIC hindered a detailed discussion. This problem was solved by omitting PVK and the measured EL of PhCIC was in good agreement with PL of PhCIC in solution or as a thin film. To identify the contact responsible for the quite high onset voltage of 10-15 V that we found, film growth and electrical contact formation of PhCIC to PEDOT:PSS and BCP were studied *in situ* by Kelvin probe force microscopy (KPFM). We conclude that charge injection barriers significantly contribute to the onset voltage and possible steps to tune the alignment of transport levels will be discussed.

CPP 28.9 Wed 11:30 Poster C

**Film Growth and Work Function of 3-Phenyl-1-(quinoline-2-yl)imidazo[1,5-a]quinoline on Poly(3,4-ethylenedioxythiophene) polystyrene sulfonate and Injection Barriers in a Layered System with Bathocuproine** — ●GUSTAV NOLTE<sup>1</sup>, PASCAL SCHWEITZER<sup>1</sup>, CARINA RÖSSIGER<sup>2</sup>, RICHARD GÖTTLICH<sup>2</sup>, and DERCK SCHLETTWEIN<sup>1</sup> — <sup>1</sup>Institut für Angewandte Physik, Justus-Liebig-Universität Gießen — <sup>2</sup>Institut für Organische Chemie, Justus-Liebig-Universität Gießen

3-Phenyl-1-(quinoline-2-yl)-imidazo-[1,5-a]-quinoline (PhCIC) is an organic semiconductor which could be applicable in organic light emitting diodes (OLEDs) as a blue emitter. To assess the potential of its application we prepared thin films of PhCIC on poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT:PSS) by physical vapor deposition and investigated film growth and work function *in situ* by means of Kelvin probe force microscopy (KPFM). Similarly, the film growth of bathocuproine (BCP) on PhCIC was stud-

ied. On PEDOT:PSS, PhCIC showed a Stranski-Krastanov type film growth, with the formation of an interface dipole in the base layer and a notable difference in work function between base layer and islands. In contrast, BCP showed a rather homogeneous film growth on PhCIC, forming a space charge region. The alignment of energy levels in the layered system was inferred, showing a significant hole injection barrier from PEDOT:PSS to PhCIC and a smaller barrier for the injection of electrons from BCP to PhCIC.

CPP 28.10 Wed 11:30 Poster C

**Transient electroluminescence and current studies on TADF-based OLEDs** — ●THOMAS FLEISCHMANN<sup>1</sup>, BJÖRN EWALD<sup>1</sup>, and JENS PFLAUM<sup>1,2</sup> — <sup>1</sup>University of Würzburg, Faculty of Physics and Astronomy, Experimental Physics VI, 97074 Würzburg — <sup>2</sup>CAE Bayern, 97074 Würzburg

The external quantum efficiency of Organic Light Emitting Diodes (OLEDs) is limited by long-living dark triplet states of conventional fluorophores. This restriction can be lifted by an efficient reverse intersystem crossing (RISC) process which converts non-emissive triplet states into emissive singlet states. This process is prominent in thermally activated delayed fluorescence (TADF) emitters, where the singlet-triplet energy splitting is on the order of thermal energy at room temperature. However, the utilization of TADF emitters comes at the expense of a delayed fluorescence at significantly lower decay rates and a high sensitivity of the photodynamics on the local emitter-host interactions. In this contribution, we analyze the transient behavior of TADF-based OLEDs by applying voltage pulses and recording the time-resolved electroluminescence and current. Comparing these time-resolved properties we conclude on capacitive effects in our OLEDs, e.g. induced by the Schottky-barriers at the contact interfaces, and the photodynamics of the molecular emitters.

CPP 28.11 Wed 11:30 Poster C

**P-type PbS CQDs ink for solar cells fabricated via slot-die coating.** — ●FARYAL TALIB<sup>1</sup>, HUAYING ZHONG<sup>1</sup>, and PETER MÜLLER-BUSCHBAUM<sup>1,2</sup> — <sup>1</sup>TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — <sup>2</sup>TUM, MLZ, 85748 Garching, Germany

PbS CQDs have demonstrated a greater power conversion efficiency (PCE) of over ~15% as it utilizes the infrared part of the solar spectrum, making them a compelling candidate for solar cell applications. CQD's ink for solar cells using slot-die coating stems from the potential to streamline the fabrication process and enhance the performance of PbS CQD solar cells. Utilizing the ink and slot-die coating can significantly reduce the need for repetitive layer deposition on the substrate, leading to a more scalable and efficient manufacturing process. This approach addresses the issue of material wastage associated with conventional (solid-state ligand exchange) methods. We are focused on electron-blocking layers (EBLs) of P-type PbS with appropriate ligands to optimize the solar cell's efficiency. The selection of suitable EBL materials with high conductivity, transparency, solution processability, and favorable stability presents a challenge for effective utilization in solar cells.

CPP 28.12 Wed 11:30 Poster C

**Calculation of inter-molecular transition rates depending on structural parameters with DFTB** — ●FABIAN TEICHERT<sup>1</sup>, ROBIN SILLIGMANN<sup>1</sup>, FLORIAN GÜNTHER<sup>2,3</sup>, and ANGELA THRÄNHARDT<sup>1</sup> — <sup>1</sup>Institute of Physics, Chemnitz University of Technology, Chemnitz, Germany — <sup>2</sup>Departamento de Física, Instituto de Geociências e Ciências Exatas, Universidade Estadual Paulista "Júlio de Mesquita Filho", Rio Claro, Brazil — <sup>3</sup>Instituto de Física de São Carlos, Universidade de São Paulo (USP), São Carlos, Brazil

We investigate the transition rates of electrons between two organic molecules, especially concerning thiophene and zinc porphyrine. For this, we calculate HOMO and LUMO states and energies, reorganization energies and Hamiltonian coupling matrices with DFTB using the software dftb+. Based on these results, the transition rates are computed using Marcus theory for charge transfer. We present result for two systems: (1) two thiophene molecules and (2) two zinc porphyrine molecules. We show reorganization energies, Hamiltonian coupling constants and transition rates dependent on the structural configuration. E.g. the thiophene molecules are shifted and rotated against each other. The final goal of our work is to obtain the statistical distribution of all the results due to the statistical fluctuation of the structure. This is suitable as input for subsequent Monte-Carlo hopping simulations, which can be used to describe the large-scale

transport of charges within organic materials for e.g. solar cell applications.

CPP 28.13 Wed 11:30 Poster C

**Light-Triggered Azobenzene-Bithiophene SAM as a Fullerene Trap** — DMITRY RYNDYK and OLGA GUSKOVA — IPF Dresden, Dresden, Germany

Optimizing the efficiency of organic photovoltaic devices may involve strategically utilizing well-defined monolayers containing azobenzene-bithiophene (Azo-BT) switches as electrode modifiers or buffer layers. These monolayers span the interface between the inorganic and organic components, allowing precise control over nanoscale morphology at the electrode. As demonstrated previously [1], cis- and trans-Azo-BT switches chemisorbed on the gold (111) surface exhibit varying geometrical, electronic, and charge transport properties. In this study, we investigate cis-, trans-, and mixed Azo-BT monolayers, with a particular focus on "nanotraps" - nanometer-sized nanopores formed in the monolayers - and their potential to capture C60. Our findings reveal that the photoswitchable "closed" and "open" configurations of Azo-BT nanotraps remain stable at room temperature under experimentally relevant surface densities [2]. We calculate the energies of C60 inside the open nanotraps, demonstrating that the minimum is located inside the pore close to the surface, indicating effective C60 capture. This conclusion is further supported by the Nudged Elastic Band method and Born-Oppenheimer MD calculations. All calculations were performed using the CP2K software (cp2k.org) with the PBE functional, Goedecker-Teter-Hutter pseudopotentials, in conjunction with the DFT-D2 method. [1] Savchenko V. et al. *Processes* 11 (2023) 2625. [2] Viero Y. et al. *J. Phys. Chem. C* 119 (2015) 21173.

CPP 28.14 Wed 11:30 Poster C

**Dipolar doping of organic semiconductors for photovoltaics** — PATRICK BUNK, HONGWON KIM, ALBIN CAKAJ, ALEXANDER HOFMANN, and WOLFGANG BRÜTTING — Experimental Physics IV, Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

Previous investigations in the field of organic LEDs showed an improvement in device performance through the doping of dipolar materials, which exhibit a buildup of a giant surface potential (GSP)[1]. However, to the best of our knowledge, dipolar doping has not yet been investigated in the context of organic photovoltaics. For this reason, we investigated prototypical small molecular electron acceptor and donor materials doped with 1,3-Bis[2-(4-tert-butylphenyl)-1,3,4-oxadiazol-5-yl]benzene (Oxd-7) in different ratios using Kelvin Probe (KP). Throughout all doped electron acceptor materials, the GSP was completely suppressed. The doped electron donor (29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32)copper(II) (CuPC) showed a partially suppressed GSP. To investigate the different phases of Oxd-7 in the host material, a Kelvin probe force microscope (KPFM) was used. Furthermore, X-ray diffraction (XRD) measurements led to a better understanding of the orientation of the molecules.

[1] Noguchi et al., *Adv. Optical Mater.* 2022, 10, 2201278, <https://doi.org/10.1002/adom.202201278>

CPP 28.15 Wed 11:30 Poster C

**Versatile Setup for Gas Phase Spectroscopy of Organic Molecules** — SEBASTIAN KAISER, SEBASTIAN SCHELLHAMMER, and SEBASTIAN REINEKE — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute for Applied Physics, Technische Universität Dresden

In order to gain a better insight into the optical properties and the associated electronic structure of organic semiconductors, it is reasonable to complement the often application-oriented investigations on thin films and solutions with further measurements. Spectroscopy of molecules in the gas phase could resolve vibronic substructures and attenuate ambient effects such as polarization also providing ideal reference data for material simulations. In this contribution, we present a new experimental setup for the spectroscopy of organic semiconductors in gas phase that aims at combining simplicity with efficiency and versatile applicability. The setup is evaluated by using Alq3, MADN, NPB, and TBPe. Sealed under vacuum in a glass ampoule, the materials are heated above the vaporization temperature using hot air. The transparent ampoule allows excitation and detection of emission from the molecules in gas phase with relative ease. However, we also find a strong temperature dependence of the emission spectra resulting from material decomposition, especially for NPB. This is accompanied by a visible discoloration of the cooled material after the measurement. As a first approach, the designed experimental setup is promising. Still,

to resolve excitonic substructures, further improvements are required, especially concerning temperature control.

CPP 28.16 Wed 11:30 Poster C

**Printed n-type PbS Quantum Dot ink towards solar cells** — MRINALINI CHATTERJEE<sup>1</sup>, HUAYING ZHONG<sup>1</sup>, and PETER MÜLLER-BUSCHBAUM<sup>1,2</sup> — <sup>1</sup>TUM School of Natural Sciences, Chair of Functional Materials, 85748 Garching, Germany — <sup>2</sup>TUM, MLZ, 85748 Garching, Germany

Colloidal Quantum dots (CQDs) have received growing attention in the past decades to produce next generation photovoltaic devices. The quantum confinement effect and size tunability of QDs have enabled customization of their electronic properties, leading to prospective increase in photo-conversion efficiency. Moreover, the solution processibility of QDs has facilitated the single step ink deposition, presenting a more efficient alternative to the conventional layer-by-layer spin-coating method. Despite this, a key challenge remains in realizing high quality, stable ink for active layer deposition for upscaling.

This work focuses on transitioning from conventional spin coating to scalable techniques (slot-die coating) for improved control of film morphology and thickness. To overcome challenges associated with the conventional solvent, Butylamine (BTA), we investigate the effect of alternative solvents including Propylene Carbonate (PC) and Formamide (FA) for the CQD ink, thus optimizing its stability. To do so, characterization techniques such as Fourier transform infrared spectroscopy (FTIR), X ray diffraction (XRD) are used for the chemical and structural analysis. Optical and morphological properties are studied by UV-vis spectroscopy, Scanning electron microscopy (SEM) respectively.

CPP 28.17 Wed 11:30 Poster C

**Investigation of structural order at the BF-DPB:BPYMPM donor-acceptor interface by scanning tunneling microscopy** — MILENA MERKEL<sup>1,2</sup>, PHILIPP WIESENER<sup>1,2</sup>, KOEN VANDEWAL<sup>3</sup>, and HARRY MÖNIG<sup>1,2</sup> — <sup>1</sup>Physikalisches Institut, Universität Münster, Wilhelm-Klemm-Strasse 10, Münster 48149, Germany — <sup>2</sup>Center for Nanotechnology (CeNTech), Heisenbergstrasse 11, Münster 48149, Germany — <sup>3</sup>Institute for Materials Research (IMO-IMOMECE), Hasselt University, Wetenschapspark 1, 3590 Diepenbeek, Belgium

The two molecules B2PYMPM and B4PYMPM serve as electron acceptors in both organic light-emitting diodes and organic solar cells. They differ only in the position of the nitrogen atoms in their lateral pyridine rings, which however leads to the formation of intermolecular hydrogen bonds and subsequent molecular stacking only in the case of B4PYMPM [1]. Paired with the electron donor BF-DPB, the increased structural order of the B4PYMPM molecules results in highly efficient free charge carrier generation [2].

To understand the differences in charge carrier dissociation between the two acceptors, we used a combined approach of scanning tunneling microscopy (STM) and X-ray photoelectron spectroscopy (XPS). Our STM data with intramolecular resolution comparatively provide insights into the nano-scale self-assembly and inherent intermolecular interactions, which are correlated with XPS core level spectra.

[1] Yokoyama et al., *Adv. Funct. Mater.*, 21, 1375-1382 (2011)

[2] Ullbrich et al., *Nat. Mater.*, 18, 459-464 (2019)

CPP 28.18 Wed 11:30 Poster C

**Study on morphology formation of sequential deposition printed organic solar cells** — LIXING LI<sup>1</sup> and PETER MÜLLER-BUSCHBAUM<sup>1,2</sup> — <sup>1</sup>TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — <sup>2</sup>TUM, MLZ, 85748 Garching, Germany

Layer-by-layer (LbL) organic solar cells (OSCs) exhibit advantages over bulk heterojunction (BHJ) structures due to their interleaved network of donor/acceptor materials and a p-i-n device configuration. The emergence of small-molecule non-fullerene materials has extended the lifetime of excitons, thus making LbL OSCs gain more and more attention. However, most research on LbL OSCs focuses on spin-coating preparation, which may not be applicable for future large-scale production. Our study explores the fabrication of LbL OSCs using printing techniques. PM6 and several different non-fullerene materials are utilized as donors and acceptors, respectively. We use in situ GIWAXS, GISAXS, and UV-vis absorption spectroscopy to investigate morphology formation.

CPP 28.19 Wed 11:30 Poster C

**OLED fabrication with a self-designed semi-automated va-**

**por deposition system** — ●MONA LÖTHER, AHMED MOHAMED, FELIX KÜBERT, JOHANNES LESER, VLADIMIR DYAKONOV, and ANDREAS SPERLICH — Experimental Physics 6, Julius-Maximilians-Universität Würzburg (JMU), 97074 Würzburg

A common method for producing organic light-emitting diodes (OLEDs) involves physical vapor deposition (PVD) of organic and metallic layers in ultra-high vacuum. We have devised a production process featuring a self-designed semi-automated PVD system with two chambers of similar structure - one for organic PVD and the other for metal PVD - connected by an airlock. Each chamber includes a substrate carrier, stepper motors, crystal oscillators for measuring layer thicknesses, rotary-linear motion feedthroughs, and magnetic sensors for precise substrate placement. The organic chamber houses six crucibles, including two pairs of co-evaporating crucibles, while the metal chamber houses two metal boats. The production steps are as follows: placing cleaned ITO-coated substrates in the first chamber, adjusting a mask, sequentially evaporating organics, transferring the substrate to the second chamber without exposure to ambient air, adjusting a different mask, and evaporating metals. A Python program coordinates essential operations such as temperature control, automated positioning of the substrates above the crucibles and metal boats, control of the evaporated layer thickness through shutter control, and data assimilation. The setup has been successfully tested in the fabrication of blue OLEDs based on  $\nu$ -DABNA.

CPP 28.20 Wed 11:30 Poster C

**Temperature-dependent characterization of TADF OLEDs** — ●FELIX KÜBERT, AHMED MOHAMED, JOHANNES LESER, MONA LÖTHER, VLADIMIR DYAKONOV, and ANDREAS SPERLICH — Experimental Physics 6, Julius-Maximilians-Universität Würzburg, 97074 Würzburg, Germany

When injecting charge carriers into the active layer of an OLED, the electrons recombine in  $S_1$  Singlet and  $T_1$  Triplet states at a 1:3 ratio. Third-generation OLEDs, to achieve fluorescence, use the surrounding thermal energy to lift the electrons from the  $T_1$  state up into the  $S_1$  state, where they can then emit fluorescence; so-called Thermally Activated Delayed Fluorescence (TADF). In this study, OLEDs based on  $\nu$ -DABNA as emitter material will be characterized in a continuous flow optical cryostat in a wide temperature range. For lower temperatures, the thermal energy in the OLEDs is insufficient for the TADF process, resulting in phosphorescence instead of fluorescence. Meanwhile, charge transport by hopping is also temperature-dependent and needs to be considered. Temperature-dependent measurements on OLEDs will therefore shed more light on the TADF process and further the optimization of OLEDs.

CPP 28.21 Wed 11:30 Poster C

**Design and fabrication of blue TADF OLEDs based on  $\nu$ -DABNA emitter** — ●AHMED MOHAMED, MONA LÖTHER, FELIX KÜBERT, JOHANNES LESER, VLADIMIR DYAKONOV, and ANDREAS SPERLICH — Experimental Physics 6, Julius-Maximilians-Universität Würzburg, 97074 Würzburg, Germany

Fabrication of efficient blue organic light emitting diodes (OLEDs) is the key challenge for OLED displays. The 2<sup>nd</sup> generation blue Phosphorescence OLEDs (PHOLED) still show low stability and have the requirements of heavy metals. Thermally activated delayed fluorescence (TADF) is considered a promising alternative of the PHOLED due to the 100% internal quantum efficiency. This study includes the design of a blue TADF OLED with the following structure [Glass/ITO/NPD /TCTA /mCP /mCBP: $\nu$ -DABNA /TSPO1 /LiF/Al]. The device was fabricated using a self-built semi-automated thermal evaporation machine with 6 sources in the organic chamber and 2 sources in the metal chamber. The thickness and surface roughness of all the organic and metallic layers were characterized using a thickness profilometer (DEKTAK) and atomic force microscope (AFM). The tooling factors of the quartz crystal monitors was calibrated by measuring the actual thickness of each layer separately. OLED efficiency is characterized by measuring the current-voltage-luminance (IVL), the current efficiency (cd/A), and emission spectra. Long-term stability of OLEDs were investigated. Optimization of layers thickness and surface roughness leads to further improvements on the stability and efficiency of OLEDs.

CPP 28.22 Wed 11:30 Poster C

**In-situ tracking the evolution of morphology and optical properties of thin films during spraying and annealing for organic solar cells** — ●SHUXIAN XIONG<sup>1,2</sup>, BENEDIKT SOCHOR<sup>1</sup>, CON-

STANTIN HARDER<sup>1,2</sup>, PETER MÜLLER-BUSCHBAUM<sup>2,4</sup>, and STEPHAN V. ROTH<sup>1,3</sup> — <sup>1</sup>DESY, 22607 Hamburg, Germany — <sup>2</sup>TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — <sup>3</sup>KTH Royal Institute of Technology, 10044 Stockholm, Sweden — <sup>4</sup>MLZ, TUM, Garching, Germany

Due to the rapid film formation during spraying, typically over tens of seconds, the resultant morphology is a delicate balance between multiple kinetic processes: solvent evaporation, diffusion of the constituents, phase separation, and ordering. The morphology is strongly rate-dependent, and real-time monitoring is necessary to follow the structural evolution with sufficient time resolution so that the properties of the film can be tailored. Based on the ultrasonic spray deposition technique (a scalable large-area deposition technique), using in-situ grazing incidence small/wide-angle x-ray scattering combined with in-situ annealing, this study pioneered the investigation of the morphology formation process from the liquid state to the final dry film under different spraying conditions. An in-depth understanding of the structural evolution during the non-equilibrium process helps to find the suitable processing parameters to produce thin films with well-performed photovoltaic properties in order to establish the relationship between spray processing control and tailored structures and the performance of polymer solar cell devices.

CPP 28.23 Wed 11:30 Poster C

**Detecting photogenerated charge carriers using triplet excitons of NFA-based solar-cell-acceptors using spin-sensitive spectroscopy** — ●MICHAEL BULGAKOV<sup>1</sup>, ANASTASIA KULTAEVA<sup>1</sup>, SHAHIDUL ALAM<sup>2</sup>, VLADIMIR DYAKONOV<sup>1</sup>, and ANDREAS SPERLICH<sup>1</sup> — <sup>1</sup>Experimental Physics 6, Julius-Maximilians-Universität Würzburg, 97074 Würzburg, Germany — <sup>2</sup>King Abdullah University of Science and Technology, Thuwal 23955-6900, Kingdom of Saudi Arabia

Since non-fullerene acceptors (NFAs) have outperformed their fullerene-based counterparts, there has been a concentrated effort in research to further enhance their performance as acceptor materials in organic solar cells. Contrary to fullerenes, where the C60-molecules provide little possibility for variation, NFAs offer a rich playground for adjusting chain lengths, incorporating functional side chains and further modifications on a molecular level. In this study, we examine five novel and promising materials that came out of this variation process. Using Electron Spin Resonance (ESR) and Optically Detected Magnetic Resonance (ODMR) techniques we detect and analyze charge carrier production and triplet-state recombination processes. The insights obtained from this investigation will offer valuable guidance for further optimizing the functionality of NFAs, paving the way to surpass the 20% performance threshold.

CPP 28.24 Wed 11:30 Poster C

**Structure prediction of low-dimensional molecular systems** — ●ALEXEY GUDOVANNY<sup>1</sup>, MARTIN PFEIFFER<sup>2</sup>, JULIA M. SCHÄFER<sup>2</sup>, DIRK HILDEBRANDT<sup>2</sup>, and FRANK ORTMANN<sup>1</sup> — <sup>1</sup>School of Natural Sciences, Technical University of Munich, Garching, Germany — <sup>2</sup>Heliatek GmbH, 01139, Dresden, Germany

An increasing number of different structural morphologies realized in organic semiconductor devices became a big challenge for the correct computational modelling of such systems. Methods based on crystal structure prediction became a popular and effective tool for predicting observable crystals used in semiconductors. However, this methodology, like most of its available software implementations, only works with homogeneous 3D systems, which makes modelling modified systems difficult. In this situation, the prediction of low-dimensional molecular systems, i.e., the molecular layer, expands our possibilities for the simulation of different interfaces and morphologies and their mixtures. Here we present an efficient and reliable workflow for the structure prediction of molecular layers, based on a multiscale approach for the structural search of the most thermodynamically stable candidates. Also, we implemented and benchmarked different structure sampling methods and determined the most effective ones. Predictions made were applied to the modelling of various semiconductor systems.

CPP 28.25 Wed 11:30 Poster C

**Organic photodiodes for biomedical applications at low light intensities** — ●RABIUL ISLAM<sup>1</sup>, SIDDHARTHA SAGGAR<sup>1</sup>, MICHAEL MERTIG<sup>1,2</sup>, and CAROLINE MURAWSKI<sup>1,2</sup> — <sup>1</sup>Kurt-Schwabe-Institut für Mess- und Sensortechnik Meinsberg e.V., Kurt-Schwabe-Str. 4, 04736 Waldheim, Germany — <sup>2</sup>Technische Universität Dresden,

Physikalische Chemie, 01062 Dresden, Germany

We designed organic photodiodes (OPDs) for wearable and implantable optical sensors that are implemented, e.g., in pulse monitoring or fluorescence imaging. Currently, biomedical sensing devices mostly rely on stiff and bulky inorganic semiconductor components and often require additional color filters. In contrast, OPDs enable light detection at higher absorption coefficients and with new form factors being ultra-thin and potentially flexible. Designing organic molecules enables inherent color filtering and device fabrication requires comparably low thermal budgets. All these characteristics make OPDs an ideal candidate for biomedical applications. To detect the often weak intensity signals, OPDs need to possess low dark currents and low noise. In this study, we fabricated solution-based OPDs using P3HT donor and PC71BM acceptor to demonstrate OPDs with reduced dark current, high linear dynamic range, and excellent detection of light intensities as low as 2 pW. Our fabricated OPDs can be used for photoplethysmography to detect the human pulse rate from a fingertip under illumination with white light. Our future research now aims at incorporating the OPDs into functional devices for monitoring neuronal activities by reading fluorescent signals.

CPP 28.26 Wed 11:30 Poster C

**Aligning molecular backbones in thin films of organic semiconductors by meniscus guided coating methods** — ●ROBIN M. TEICHGREBER<sup>1</sup>, CHRISTOPHER R. MCNEILL<sup>2</sup>, and EVA M. HERZIG<sup>1</sup> — <sup>1</sup>Dynamik und Strukturbildung - Herzig Group, Universität Bayreuth, Universitätsstr. 30, 95447 Bayreuth, Germany — <sup>2</sup>Material Science and Engineering, Monash University, 20 Research Way, Clayton, Australia

The performance of organic solar cells depends crucially on the ability of the generated excitons to diffuse to the donor/acceptor interfaces and to be dissociated there [1]. The exciton transport in the material depends strongly on the morphology of the film, including the orientation of the molecules. The orientation of the molecules is particularly important in highly anisotropic materials. While in previous studies [2][3] the focus was placed primarily on the orientation of the molecules relative to the substrate ("face-on" or "edge-on"), less attention was paid to the role of the orientation of the long axis of the molecules. Investigating the influence of molecular orientation on exciton transport requires samples that exhibit a high degree of alignment. We systematically study such samples using meniscus guided blade coating to gain a fundamental understanding of the physical processes that lead to the alignment of the molecular backbones. We employ methods based on optical spectroscopy and X-ray scattering to characterize the films. [1] Blom, P. W. M. et al. (2007). *Advanced Materials*. 19, 1551-1566 [2] Rand, B. P. et al. (2012). *Advanced Functional Materials*. 22, 2987-2995 [3] Ran, N. A. et al. (2017). *Nature Communication*. 8, 79

CPP 28.27 Wed 11:30 Poster C

**Analytical drift-diffusion model for steady-state drain currents in organic electro-chemical transistors** — ●ANDRES UNIGARRO<sup>1</sup> and FLORIAN GÜNTHER<sup>2</sup> — <sup>1</sup>Institut für Physik, Technische Universität Chemnitz, Germany — <sup>2</sup>Instituto de Geociências e Ciências Exatas, Universidade Estadual Paulista, Rio Claro, Brazil

Among the different devices developed in the field of organic electronics, organic electrochemical transistors (OECTs) have emerged as potential transducers in applications that require the conversion of ion fluxes to electronic current. For the rational optimization and understanding of the fundamentals of OECTs and OECT-based applications, however, it is essential to have theoretical models capable to predict and recreate the experimental data. The existing models used to describe the OECT functions discussed during the past decade mostly originate from Ohm's law, where the ion flux from the electrolyte into the semiconducting layer takes place only due to an electrical field. But ion migration also occurs upon diffusion. In this work we present an approach to model the ion concentration profile under steady-state conditions based on drift-diffusion principles. This allows to formulate an analytical expression of the source-drain current as a function of gate and drain voltages but also of material parameters like the salt concentration. We show that this allows expressing the volumetric capacitance (a parameter that determines the figure of merit for OECTs) as a function of these material parameters. We furthermore present adjustments of experimental data and comparisons to other OECT models.

CPP 28.28 Wed 11:30 Poster C

**Illuminating the dark side of triplet states** — ●MOHAMMAD

SAEED SHADABROO<sup>1</sup>, DIETER NEHER<sup>2</sup>, and SAFA SHOAE<sup>1,3</sup> — <sup>1</sup>Optoelectronics of Disordered Semiconductors, Institute of Physics and Astronomy, University of Potsdam, Potsdam-Golm, Germany — <sup>2</sup>Physics and Optoelectronics of Soft Matter, Institute of Physics and Astronomy, University of Potsdam, Potsdam-Golm, Germany — <sup>3</sup>Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., 10117 Berlin, Germany

Optimization of the energy levels at the donor\*acceptor interface of organic solar cells has driven their efficiencies to above 19%. However, further improvements towards efficiencies comparable with inorganic solar cells remain challenging because of high recombination losses, mediated by the lowest-energy (singlet and triplet) CT states, which empirically limit the open-circuit voltage (VOC). Using o-IDTBR blended with PM6, we achieve 1.16 V, associated with the achievement of remarkably low non-radiative recombination loss of 160 meV, despite the presence of triplets. In employing the present system as a model example, we elucidate the circumstance wherein, if the triplet lifetime surpasses that of the charge-transfer (CT) decay, the dissociation of triplet excitons to the CT state emerges as a feasible occurrence. This, in turn, serves to reduce the occurrence of an additional loss channel emanating from the T1 state. To shed light on these issues, here, an integrated approach that combines photophysics with device physics is employed in order to establish the relationships among non-radiative recombination losses mediated by the lowest states.

CPP 28.29 Wed 11:30 Poster C

**Spark Discharge Doping - Unprecedented Aggregation Control in P3HT Solutions, Films and Blends** — ●FABIAN ELLER and EVA M. HERZIG — Dynamik und Strukturbildung - Herzig Group, Universität Bayreuth, Universitätsstr. 30, 95447 Bayreuth, Germany

We introduce a novel solution treatment utilizing spark discharges to enable a highly controlled aggregation of poly(3-hexylthiophene) (P3HT) in solution.[1] By choosing appropriate parameters of this current-induced doping treatment we demonstrate the fine tunability of the aggregate fraction and the quality of the polymer backbone order over exceptionally broad ranges.

When films are processed from highly ordered solutions, the high aggregate quality transfers to the films, which enables a strongly increased hole mobility. The aggregation control of the film formation is especially relevant to overcome the aggregation suppression in highly miscible blends, e.g. with Y-series non-fullerene acceptors (NFAs).

[1] F. Eller et al, *Small*. 19, 2207537, 1613-6810 (2023).

CPP 28.30 Wed 11:30 Poster C

**A Theoretical Study of the Optoelectronic Properties of WBDT Covalent Organic Frameworks** — ●LAURA FUCHS and FRANK ORTMANN — TUM School of Natural Sciences, Department of Chemistry, Lichtenbergstr. 4, 85748 Garching b. München

Covalent-organic frameworks (COFs) are intriguing materials for optoelectronic applications due to their high tunability of electronic and physical properties. One such example is the electron rich 2D imine-linked WBDT, composed of a Wurster-type motif with N,N,N\*,N\*-tetraphenyl-1,4-phenylenediamine (W) and benzodithiophene dialdehyde (BDT). Using density-functional theory, we investigate the structure, electronic band structure and density of states of the COF. Additionally, we study electronic transitions and optical properties based on its molecular fragments, focusing on the influence of a careful fragment selection.

CPP 28.31 Wed 11:30 Poster C

**Influence of Particle Size on the Formation of Solid Solutions Between MAPbI3 and MAPbBr3** — ●TOBIAS SIEGERT<sup>1</sup>, FATEMEH HADDADI BARZOKI<sup>2</sup>, MARKUS GRIESBACH<sup>1</sup>, CHRISTOPHER GREVE<sup>3</sup>, RALF MOOS<sup>4</sup>, EVA M. HERZIG<sup>3</sup>, ANNA KÖHLER<sup>1</sup>, and HELEN GRÜNINGER<sup>2,5</sup> — <sup>1</sup>Soft Matter Optoelectronics — <sup>2</sup>Inorganic Chemistry III — <sup>3</sup>Herzig Group - Dynamics and Structure Formation — <sup>4</sup>Department of Functional Materials — <sup>5</sup>Bavarian Center for Battery Technology (BayBatt), all University of Bayreuth, 95447 Bayreuth, Germany

Mixed halide perovskites, e.g., MAPbI3-xBrx, have emerged as promising candidates to be used as wide-bandgap absorbing layers in tandem solar cell applications due to their tunability of bandgap energy. However, pronounced halide migration, which leads to a severe drop in performance, is still hindering a commercialization. To analyze the halide kinetics, we investigate the thermally driven formation of a solid solution, i.e., halide mixing, between MAPbI3 and MAPbBr3 as a function

of the morphology of the perovskite powder. Here, the surface to bulk ratio of the parent powder particles is varied by systematically changing particle sizes.

CPP 28.32 Wed 11:30 Poster C

**Influence of unipolar charge carrier injection on lead-halide perovskite nanocrystals** — ●ROSHINI JAYABALAN<sup>1</sup>, WOLFGANG BRÜTTING<sup>1</sup>, THERESA HETTINGER<sup>2</sup>, MARCUS SCHEELE<sup>2</sup>, and YUTAKA NOGUCHI<sup>3</sup> — <sup>1</sup>Universität Augsburg, 86135 Augsburg, Germany — <sup>2</sup>Universität Tübingen, 72076 Tübingen, Germany — <sup>3</sup>School of Science and Technology, Meiji University, 214-8571 Kanagawa, Japan

The study on lead halide perovskite nanocrystals (LHP NCs), despite their recent existence, has seen a substantial progress in the research community. Similar to their bulk counterpart, their optical and electrical properties extend to the NCs, with additional advantages including band-gap tuning by size and near unity quantum yield, rendering them as potential emitter material in quantum dot light emitting diodes. With their significantly increased surface area, passivation of surface with appropriate ligands is crucial. While advances in stability and optical properties are outstanding, the electrical accessibility of NCs has gained less attention so far. Efficient electroluminescence relies on a thorough comprehension of the injection of charge carriers into the emitting material. Herein this study, we employ a metal-insulator-semiconductor device structure, with charge selective transport layers to ensure unipolar charge injection (electrons/holes) into the NCs. Finally, we have developed a technique, namely, the displacement current measurement (DCM) using these devices to understand the electronic properties of LHP NCs films in detail. Trapped charges, injection voltage are identified and carrier specific trends with respect to stability are determined.

CPP 28.33 Wed 11:30 Poster C

**Fabrication and Characterisation of Cesium-Formamidinium Lead Iodide Perovskite Nanocrystal Layers** — ●THOMAS BAIER<sup>1</sup>, GUANJIU PAN<sup>1</sup>, ALTANTULGA BUYAN-ARIVJIKH<sup>1</sup>, JINSHENG ZHANG<sup>1</sup>, YANAN LI<sup>1</sup>, MATTHIAS SCHWARTZKOPF<sup>2</sup>, SARATHAL KOYLOTH VAYALIL<sup>2</sup>, and PETER MÜLLER-BUSCHBAUM<sup>1,3</sup> — <sup>1</sup>TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — <sup>2</sup>DESY, 22607 Hamburg, Germany — <sup>3</sup>MLZ, TUM, 85748 Garching, Germany

Perovskite quantum nanocrystal solar cells are very promising in contributing to the renewable energy mix of the future being used as active layer within solar cells due to the quantum confinement, which occurs at crystals size below the Bohr radius. They provide high power conversion efficiencies, high photoluminescence quantum yield (PLQY), a narrow PL peak, and are stable in comparison to bulk perovskite. Furthermore, the range of usable X halides (I-, Br-, Cl-) and A cations (FA+, MA+, Cs+) enables fine control of the bandgap over the whole visible spectrum of the ABX<sub>3</sub> perovskite structure.

Cesium-formamidinium lead iodide perovskite nanocrystal layers have been prepared using different washing processes between several deposition steps, as well as changing the ratio between cesium lead iodide and formamidinium lead iodide perovskite nanocrystals. Therefore different measurement (PL, UV-Vis, microscopy, and SEM) and deposition techniques (spin-coating, and slot-die coating) were used to obtain the optoelectronic properties of the final film.

CPP 28.34 Wed 11:30 Poster C

**In situ Grazing-Incidence Small-Angle X-ray Scattering Observation of TiO<sub>x</sub> Sputter Deposition on SnO<sub>2</sub> Layer for Perovskite Solar Cells Application** — ●XIONGZHUO JIANG<sup>1</sup>, ZHUIJUN XU<sup>1</sup>, GUANJIU PAN<sup>1</sup>, YUSUF BULUT<sup>2</sup>, KRISTIAN RECK<sup>3</sup>, THOMAS STRUNSKUS<sup>3</sup>, FRANZ FAUPEL<sup>3</sup>, STEPHAN V. ROTH<sup>2</sup>, and PETER MÜLLER-BUSCHBAUM<sup>1,4</sup> — <sup>1</sup>TUM School of Natural Science, Chair for Functional Materials, 85748 Garching, Germany — <sup>2</sup>Deutsches Elektronen-Synchrotron (DESY), 22607 Hamburg, Germany — <sup>3</sup>Lehrstuhl für Materialverbunde, Institut für Materialwissenschaft, Christian Albrechts-Universität zu Kiel, 24143 Kiel, Germany — <sup>4</sup>TUM, MLZ, 85748 Garching, Germany

It is crucial to suppress the non-radiation recombination in the hole-blocking layer (HBL) and at the interface between the HBL and active layer for performance improvement. We deposited a TiO<sub>x</sub> thin layer atop the SnO<sub>2</sub> layer via sputter deposition at room temperature as an interface modification layer. The structure evolution of TiO<sub>x</sub> during sputter deposition is investigated via in situ grazing-incidence small-angle X-ray scattering. The HBL, combined with the TiO<sub>x</sub> interface modification layer, shows a suitable transmittance, smoother

surface roughness, and fewer surface defects, thus resulting in lower trap-assisted recombination at the interface between the HBL and the active layer. With this SnO<sub>2</sub>/TiO<sub>x</sub> functional bilayer, the perovskite solar cells exhibit higher power conversion efficiencies than the unmodified SnO<sub>2</sub> monolayer devices.

CPP 28.35 Wed 11:30 Poster C

**Enhanced Air Stability of Tin Based Perovskite Solar Cells with Quercetin** — ●XIAOJING CI<sup>1</sup> and PETER MÜLLER-BUSCHBAUM<sup>1,2</sup> — <sup>1</sup>TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — <sup>2</sup>TUM, MLZ, 85748 Garching, Germany

As the most essential alternative materials for eco-friendly perovskite solar cells (PSCs), tin-based perovskites have achieved an efficiency of 14.81 %, which is far less than 25.7 % of lead-based champion devices. The main reason is that it is easy to oxidize Sn<sup>2+</sup> to Sn<sup>4+</sup> in the presence of oxygen and water due to the low stability of the Sn<sup>2+</sup> state. The oxidation of Sn<sup>2+</sup> will form vacancies in the perovskite structure, leading to p-type self-doping and introducing additional defect states. These defects can enhance the device's leakage current and charge carrier recombination, limit the increase of open circuit voltage, and thus reduce the solar cell efficiency. Here, we introduce quercetin, a phenolic derivative with antioxidation properties extracted from plants, as the additive to reduce the existence of Sn<sup>4+</sup> and prevent the FASnI<sub>3</sub> film from degradation. We use grazing-incidence wide-angle X-ray scattering (GIWAXS) to gain insights into the detailed steps of growth and degradation progress of the active layer. Thereby, GIWAXS offers a way to gain information about the time evolution during the crucial steps of interface formation.

CPP 28.36 Wed 11:30 Poster C

**Tuning band gap of double perovskite by anion exchange** — ●ZHAONAN JIN<sup>1</sup> and PETER MÜLLER-BUSCHBAUM<sup>1,2</sup> — <sup>1</sup>TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — <sup>2</sup>TUM, MLZ, 85748 Garching, Germany

Double perovskite is a relatively new kind of lead-free perovskite that possesses low toxicity, long charge carrier lifetime and small effective charge carrier mass. It is considered as a promising photovoltaic material. Bismuth-based double perovskites have received considerable attention in recent years, and among them, Cs<sub>2</sub>AgBiX<sub>6</sub> (X = Cl, Br, I) has displayed the most promising potential for photovoltaic applications due to the suitable band gap. Some researchers studied thermoelectric properties of double halide perovskite Cs<sub>2</sub>AgBiI<sub>6</sub> and proved that it is an excellent candidate for thermoelectric applications. Increasing the content of iodide ions in Cs<sub>2</sub>AgBiX<sub>6</sub> can effectively narrow the band gap. In this work, the iodide ions will be introduced to Cs<sub>2</sub>AgBiBr<sub>6</sub> by adding TMSI when spin-coating. It is reported that no more anion exchange happened with more TMSI. Therefore, Cs<sub>2</sub>AgBi(BrxI<sub>1-x</sub>)<sub>6</sub> perovskite solar cells will be fabricated by solution method. The anion exchange process is studied in this work. Morphology, device characterizations techniques like XRD, SEM, J-V curves, EQE spectra etc. are taken to help optimize the morphology of thin films and PCE of solar cells. In-operando studies are taken to identify morphology changes during device operation.

CPP 28.37 Wed 11:30 Poster C

**Effect of Additives on Dion-Jacobson Two-Dimensional Perovskite Solar Cells** — ●KIN LONG FONG<sup>1</sup>, KUN SUN<sup>1</sup>, and PETER MÜLLER-BUSCHBAUM<sup>1,2</sup> — <sup>1</sup>TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — <sup>2</sup>TUM, MLZ, 85748 Garching, Germany

Solar cells based on two-dimensional (2D) perovskite materials have received more attention in recent years due to their stability compared to their three-dimensional counterparts. However, their power conversion efficiencies (PCEs) are still lagging behind, posing a major challenge before their commercialization. In this work, we study the effects of additives, namely MA<sub>2</sub>PbCl<sub>2</sub>, and a mixture of MA<sub>2</sub>Cl and PbCl<sub>2</sub>, on the structures of Dion-Jacobson (DJ) 2D perovskite films fabricated with 1,4-phenylenedimethan ammonium (PDMA) spacer molecules. Solar cells made with these films are also investigated, and their efficiencies are presented. This research aims to enhance our understanding of the impact of different additives on the PCEs of solar cells based on PDMA spacers.

CPP 28.38 Wed 11:30 Poster C

**Exploring the potential of lead halide perovskite as materials with high Stokes shift for photovoltaic applications**

— ●ELSHAIMAA DARWISH, JACK ELIA, ANDRES OSVET, MIROSLAW BATENBATEWSCHUK, and CHRISTOPH BRABEC — i-MEET Institute Materials for Electronics and Energy Technology, Erlangen

Lead halide perovskites has been attracting a lot of research interest over the past years. Due to the unique properties of lead halide perovskites such as high defect tolerance, high absorption coefficient and tunable band gap, they are considered a highly promising class of materials for optoelectronic devices and photovoltaics. One of the issues that is hindering the perovskites application is possessing small Stokes shifts or self-absorption. Therefore, developing lead halide perovskites with large Stokes shifts is a significant venture.

There are a number of approaches used to control the Stokes shifts in semiconductors including chemical composition, size, temperature, and other reaction conditions. In this work, structural modifications were introduced into inorganic lead halide perovskite as a way of obtaining high Stokes shift, we characterize the obtained particles optically, and structurally. Moreover, scanning electron microscope (SEM) was used to measure the change in particle size as a result of introducing modifications.

The successful incorporation of the synthesized particles into transparent or semitransparent films could be used to enhance the performance of the currently available solar cells in the market.

CPP 28.39 Wed 11:30 Poster C

**Charge transfer and recombination in hole transport/perovskite bilayers probed by photoluminescence** — ●LUKAS SCHÄFER, PATRICK DÖRFLINGER, OLGA TRUKHINA, and VLADIMIR DYAKONOV — Experimental Physics 6, Julius-Maximilians-Universität Würzburg, 97074 Würzburg, Germany

Hole transport materials (HTMs) play a crucial role in enhancing the performance of perovskite solar cells by selectively extracting holes from the active layer. While their charge extraction capabilities positively impact solar cell efficiency, surface recombination at the perovskite interface can hinder overall performance. In this study, we employ steady-state PL (SSPL) as well as time-resolved PL (TRPL) experiments on HTM/perovskite bilayers to assess the charge extraction capability and the surface recombination. We demonstrate the quenching of the photoluminescence quantum yield of these bilayers which is characteristic for the extraction of charges and their non-radiative recombination at the HTM/perovskite interface. Furthermore, the bilayers exhibit a faster decay in TRPL transients compared to pristine perovskite. This can be indicative for charge extraction and surface recombination. SSPL and TRPL have proven to be useful tools to characterize novel HTMs for perovskite solar cell applications and to gain insights into the processes at the interface between the perovskite and the HTMs.

CPP 28.40 Wed 11:30 Poster C

**Influence of additives on the recombination dynamics in lead-halide perovskite absorbers probed by TRMC and SSMC** — ●MECHTHILD SEIDL<sup>1</sup>, PATRICK DÖRFLINGER<sup>1</sup>, MOHAMMAD KHAJA NAZEERUDDIN<sup>2</sup>, and VLADIMIR DYAKONOV<sup>1</sup> — <sup>1</sup>Experimental Physics 6, Julius-Maximilians-Universität Würzburg, 97074 Würzburg, Germany — <sup>2</sup>Group of Molecular Engineering of Functional Materials, Institute of Chemical Sciences and Engineering, EPFL Valais, Sion 1950, Switzerland

Perovskites have attracted attention due to the possibility of using them as a top cell with a wide bandgap in tandem solar cells. However, a significant challenge associated with perovskites is their instability. One promising approach to enhance their performance and stability involves the incorporation of additives. Two contactless measurement techniques, time-resolved microwave conductivity (TRMC) and steady-state microwave conductivity (SSMC) are used to characterize and understand the influence of the additives. Both techniques use the interaction of light-induced charge carriers with an electromagnetic field inside a cavity to measure a change in conductance. SSMC provides insight into the dominant charge carrier recombination pathway, while TRMC is employed to determine the mobility and lifetime of generated charge carriers in the perovskite. An understanding of the influence of the additives on these optical properties is essential to improve the solar cell's performance further.

CPP 28.41 Wed 11:30 Poster C

**Monolithic series interconnection of perovskite CIGSe tandem modules by laser patterning: Process development and material characterization** — ●NICOLAS OTTO<sup>1</sup>, CHRISTOPH SCHULTZ<sup>1</sup>, GUILLERMO FARIAS-BASULTO<sup>2</sup>, OLIVER FISCHER<sup>3</sup>, RUT-

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Perovskite and chalcopyrite based solar cells for 2-T tandem devices enables efficiencies beyond the SQ limit for single junction cells. Both materials can be electrically interconnected by monolithic series interconnection, which comprises alternating layer deposition and layer patterning steps (P1, Isocut, P2, and P3). The goal is to develop suitable patterning parameters for each of the four scribe lines by systematic variation of the laser fluence. Suitable process windows were determined by analyzing the electrical functionality of the scribe lines, their geometry (using laser-scanning microscopy), and photo-activity (using intensity dependent photoluminescence imaging of the individual sub-cells) as well as alterations in the material composition in the scribe line vicinities (using energy-dispersive x-ray spectroscopy, EDX).

CPP 28.42 Wed 11:30 Poster C

**Temperature Dependent Photoluminescence Studies of Metal-Free Phthalocyanine Single Crystals** — ●LUISE PÄTZOLD<sup>1</sup>, LISA SCHRAUT-MAY<sup>3</sup>, and JENS PFLAUM<sup>1,2</sup> — <sup>1</sup>Experimental Physics VI, University of Würzburg, 97074 Würzburg — <sup>2</sup>CAE Bayern, 97074 Würzburg

The opto-electronic properties of organic materials depend not only on the individual molecules, but also on their interaction in the crystalline lattice [1]. As a representative, the material class of phthalocyanines (Pc) is studied in various research fields because of the possibility to steer its opto-electronic and structural properties by choice of the central metal atom, chemical substitution of its periphery and, thus, aggregate packing [2]. This distinguishes Pc compounds to investigate the excitonic coupling between neighboring molecules under various conditions. We have grown  $\beta$ -phase single crystals of metal-free H<sub>2</sub>-phthalocyanine (H<sub>2</sub>-Pc) by horizontal vapor phase deposition. Polarization dependent photoluminescence (PL) measurements provide insights into the anisotropic coupling of the photoexcited molecules within the crystallographic (101) plane. Furthermore, changes in the excitonic coupling are investigated as function of temperature down to 5 K. The results will be discussed in comparison to metal-centered zinc-phthalocyanine (Zn-Pc), where a super-radiant PL enhancement is observed below 80 K which is related to a discontinuous change in inter-molecular coupling at cryogenic temperatures.

[1] Hestand et al., Chem. Rev. (2018)

[2] Rödel et al., J. Phys. Chem. C (2022)

CPP 28.43 Wed 11:30 Poster C

**Influence of the Atmosphere on the Phosphorescence of a Brominated Diphenylphosphine Oxide-Ethyl Naphthalene-imide Dyad** — MARVIN MALCHAU<sup>1</sup>, PAUL M. REICHSTEIN<sup>2</sup>, WERNER REICHSTEIN<sup>3</sup>, and ●LOTHAR KADOR<sup>1</sup> — <sup>1</sup>University of Bayreuth, Institute of Physics and BIMF, 95440 Bayreuth, Germany — <sup>2</sup>University of Bayreuth, Macromolecular Chemistry I and BIMF, 95440 Bayreuth, Germany — <sup>3</sup>University of Bayreuth, Bayreuth Materials Center (BAYMAT), 95440 Bayreuth, Germany

The non-brominated diphenylphosphine-ethyl naphthaleneimide dyad (DPPENI) acts as a sensitive sensor for cumulative exposure to oxygen, since, under simultaneous irradiation of UV or blue light, the diphenylphosphine unit is oxidized to diphenylphosphine oxide; as a consequence, blue fluorescence emission is turned on in the originally non-fluorescing compound. [1] Upon bromination of the naphthaleneimide unit, strong phosphorescence is emitted in addition to the fluorescence. We studied the intensity and lifetime of the phosphorescence of the fully oxidized Br-DPPENI dyad in atmospheres of air, argon, helium, nitrogen, and oxygen as a function of pressure between vacuum and 1 bar. The experiment was performed in the frequency domain with a two-channel lock-in amplifier and the data were analyzed with the polar-plot or phasor technique. Reversible phosphorescence quenching due to triplet-triplet annihilation was found in the presence of atmospheric or pure oxygen, whereas the other gases had no effect.

[1] R. Shritz et al., Chem. Eur. J. **21**, 11531 (2015).

CPP 28.44 Wed 11:30 Poster C

**Intramolecular Barrier for Stilbene Photoisomerization from**



**Temperature- and Viscosity-Dependent Transient Absorption** — ●DARIA SCHRIEVER<sup>1</sup>, ALEXANDER L. DOBRYAKOV<sup>2</sup>, J. LUIS PEREZ LUSTRES<sup>1</sup>, MARTIN QUICK<sup>3</sup>, ILYA N. IOFFE<sup>4</sup>, and SERGEY A. KOVALENKO<sup>3</sup> — <sup>1</sup>Fachbereich Physik, Freie Universität Berlin — <sup>2</sup>Moscow — <sup>3</sup>Institut für Chemie, Humboldt Universität zu Berlin — <sup>4</sup>Moscow

The photoisomerization of stilbene is investigated by means of fs broadband transient absorption in solution and compared to the RRKM and Kramers reaction rate theories [1]. To this end, it is necessary to extract the intramolecular barrier from the experimental one, which contains the viscosity contribution. Reaction dynamics is measured in a range of temperatures and non-polar solvents of various viscosities. In this way, the barrier height remains virtually unaffected by polar interactions between the surrounding solvent and the polar transition state of the isomerization reaction. In parallel, viscosity activation energies are obtained from the rotational diffusion times of the stilbene molecule. It is found that the isomerization time constant is proportional to  $\eta^\alpha$ , with  $\alpha = 0.3$ . An average barrier of 1236 cm<sup>-1</sup> is obtained, in good agreement with the gas phase results: 1398 cm<sup>-1</sup> [2].

[1] S. A. Kovalenko, A. L. Dobryakov, *Chem. Phys. Lett.* **2013**, 570, 56-60. [2] J. S. Baskin *et al*, *J. Phys. Chem.* **1996**, 100, 11920-11933.

CPP 28.45 Wed 11:30 Poster C

**Extension of parametrization for long-range corrected DFTB and its application on organic photovoltaics** — ●WENBO SUN<sup>1</sup>, TAMMO VAN DER HEIDE<sup>1</sup>, CARLOS R. LIEN-MEDRANO<sup>1</sup>, THOMAS FRAUENHEIM<sup>2</sup>, and BÁLINT ARADI<sup>1</sup> — <sup>1</sup>University of Bremen, Bremen 28359, Germany — <sup>2</sup>Constructor University, Bremen 28759, Germany

In recent years, the field of organic photovoltaics (OPV) has witnessed significant progress, marked by the synthesis of novel donor and acceptor molecules. To gain deeper insights into the mechanisms of OPV and predict the electronic properties of molecules, theoretical computational methods are frequently employed. However, the application of Density Functional Theory (DFT) calculations faces limitations when dealing with large systems, such as dimers of donor-acceptor molecules or aggregates, due to their computational requirements. As an alternative, the Density Functional Tight Binding (DFTB) method is an approximation to Kohn-Sham DFT, usually being orders of magnitudes faster. For the description of charge transfer excited states by DFTB, the incorporation of long-range corrected hybrid functionals into DFTB (LC-DFTB) becomes essential.

Based on the existing ob2-1-1 parameter set [1] containing the chemical elements C, H, N, and O, the present work extends these parameters to include S, F, and Cl. The extension of parametrization broadens the scope for investigating novel OPV molecules via LC-DFTB, such as non-fullerene acceptor Y6, as well as small-molecule donors BTR and BTR-Cl, along with their respective dimers and aggregates.

[1] *J. Chem. Theory Comput.*, 2018, 14, 115-145.

CPP 28.46 Wed 11:30 Poster C

**Behaviour of metal-containing films of chitosan-based films in aqueous solutions** — ●SNEGIREVA ANASTASIA — Moscow, Russia

The behaviour of biologically active coating materials in aqueous solutions is an important feature for determining the area of application and the possibility of use as a drug. The dynamics of the change in these parameters over time under standard conditions for storing the materials determines one of the parameters for the shelf life of the foils obtained. Films containing iridium and rhodium were produced by the solution casting method. There are three types of films: chitosan-based, chitosan-gelatin-based and chitosan-agar-based. The degree and the swelling constant were determined both in aqueous solution and in salt buffer solution with a pH value of 7.2, which corresponds to the ion set and the acidity of the organism's biological media. The addition of metal cations to the films changes the character of the solution. Matrices that do not contain salt swell without restriction in both aqueous and buffer solutions. As the metal concentration in the foils increases, the degree of swelling decreases. The swelling rate constant increases. The ability to absorb moisture during storage under standard conditions decreases over a period of two months, which indicates an increase in the strength of the materials.

CPP 28.47 Wed 11:30 Poster C

**Light-Driven Charge Regulation at Oil/Water Interfaces in Nanoemulsions** — ●DANA GLIKMAN and BJÖRN BRAUNSCHWEIG — Institute of Physical Chemistry and Center for Soft Nanoscience, University of Münster, Busso-Peuss-Str. 10, 48149 Münster

Understanding oil/water (o/w) interfaces in nanoemulsions and on a molecular level is of great interest, but often impaired by experimental limitations to probe the internal interfaces in situ. In order to study and to tune nanoemulsions we make use of photoswitchable surfactants. For that we apply arylazopyrazole sulfonate (butyl-AAP) surfactants which can be photoisomerized between *E* and *Z* isomers by visible and UV light. This causes massive changes in the interface tension at the extended o/w interface and a drastic shift in the surfactants' CMC, which we apply to control the stability of the macroemulsions through UV irradiation. Nanoemulsions with a droplet radius of 90 nm were, however, not susceptible to *E/Z* photoisomerization in terms of changes in particle size or in the  $\zeta$ -potential. However, second-harmonic generation in the scattering mode (SHS) shows that the surfactants' surface excess at the nanoscopic o/w interface is changed drastically and reversibly by *E/Z* photoisomerization. The apparent differences in the  $\zeta$ -potential and the changes in surface excess provide evidence for a fixed charge to particle size ratio and the need for counter ion condensation in order to renormalize the particle charge to a critical charge per particle, which is largely different to extended interfaces.

CPP 28.48 Wed 11:30 Poster C

**Time-dependent morphology evolution of templated mesoporous titanium films** — ●GUANGJIU PAN<sup>1</sup>, TIANLE ZHENG<sup>1</sup>, SUZHE LIANG<sup>1</sup>, ALTANTULGA BUYAN-ARIVJIKH<sup>1</sup>, CAROLINE EHGARTNER<sup>2</sup>, NICOLA HÜSING<sup>2</sup>, MATTHIAS SCHWARTZKOPF<sup>3</sup>, STEPHAN V. ROTH<sup>3,4</sup>, and PETER MÜLLER-BUSCHBAUM<sup>1,5</sup> — <sup>1</sup>TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — <sup>2</sup>Universität Salzburg, 5020 Salzburg, Austria — <sup>3</sup>DESY, 22607 Hamburg, Germany — <sup>4</sup>KTH Royal Institute of Technology, SE 100 44 Stockholm, Sweden — <sup>5</sup>TUM, MLZ, 85748 Garching, Germany

Mesoporous transition metal oxides have attracted significant interest due to their excellent properties. The soft templating approach with the sol-gel method is one of the most common approaches for designing mesoporous transition metal oxides. However, the influence of hydrolysis and condensation of precursors on the morphology is still unclear. Commercial metal alkoxide precursors were chosen in this work to demonstrate the influence of the reaction time. A similar morphology transition, from worm-shaped mesopores to ordered spherical mesopores, was observed with increasing sol-gel reaction time for different precursors. The surface morphologies of spin-coated films are probed via scanning electron microscopy and grazing-incidence small-angle X-ray scattering (GISAXS).

CPP 28.49 Wed 11:30 Poster C

**Photo-thermal Expansion of Nanostructured Surfaces in Photoinduced Force Microscopy (PiFM)** — ●SHOHELY ANINDO<sup>1,2</sup>, JESVIN JOSEPH<sup>2,3</sup>, RAINER HEINTZMANN<sup>2,3,4</sup>, DANIELA TÄUBER<sup>3,4</sup>, and CHRISTIN DAVID<sup>1,2</sup> — <sup>1</sup>IFTO, Friedrich Schiller University Jena — <sup>2</sup>Abbe Center of Photonics, Jena — <sup>3</sup>Leibniz Institute of Photonic Technology, Jena — <sup>4</sup>Institute of Chemical Physics, Friedrich Schiller University Jena, Germany

The recently developed Photo-induced Force Microscopy (PiFM) offers high spatial resolution in chemical imaging of polymer films and biomaterials, when combined with mid-infrared illumination. Upon absorption, photo-thermal expansion of the material causes a modulation of the Van der Waals (vdW) force acting between the tip and the sample. This work theoretically investigates the non-linear impact of material properties and surface shape on the tip-sample interaction, heat generation from the presence of a photo-induced electric field, the resulting thermal expansion under different illumination conditions and the change in cantilever oscillation at different detection modes. We compare our results to mid-infrared PiFM images obtained from a poly(methyl methacrylate) (PMMA) nanosphere with a diameter of 100 nm.

CPP 28.50 Wed 11:30 Poster C

**Influence of Polymers on Ice-Polymer Premelting Dynamics** — ●TAKUMI SATO<sup>1</sup>, IKKI YASUDA<sup>1</sup>, YUSEI KOBAYASHI<sup>2</sup>, NORIYOSHI ARAI<sup>1</sup>, and KENJI YASUOKA<sup>1</sup> — <sup>1</sup>Keio University, Kanagawa-ken, Japan — <sup>2</sup>Kyoto Institute of Technology, Kyoto, Japan

As exemplified by ice rinks, even at temperatures below the freezing point, the ice surface undergoes melting, forming a pseudo-liquid layer known as the premelting layer. Such a premelting layer is generated not only at the ice-vapor interface but also at the ice-polymer (rubber) interface, significantly influencing the properties of the ice surface. Ex-



tensive research has been conducted on the premelting layer, which has been observed at the ice-vapor interfaces. However, the behavior of the premelting layer at the ice-polymer interface has not been clarified.

Understanding the behavior of the premelting layer at the ice-polymer interface, is considered to make a substantial contribution to the development of applications such as winter tires for automobiles. However, clarifying the behavior of the premelting layer at the ice-polymer interface due to friction is challenging, given the variability under numerous conditions such as temperature, pressure, velocity, and the surface roughness of the rubber.

In this study, we initiate all-atom molecular simulations at the ice-polymer interface using polymers such as polyethylene. This allows us to analyze the molecular dynamics of the premelting layer, revealing the influence of polymers on the premelting layer and elucidating the physical properties of the premelting layer.

CPP 28.51 Wed 11:30 Poster C

**Advancing Microscopy Techniques for Plastic Analysis in Transmission Electron Microscope and Focused Ion Beam** — ●JUDITH BÜNTE, INGA ENNEN, LAILA BONDZIO, and ANDREAS HÜTTEN — Universität Bielefeld, Dünne Schichten und Physik der Nanostrukturen, Universitätsstr. 25, 33615 Bielefeld, Germany

Plastics play an essential role in various industries. Wanting to reduce plastic waste their analysis is necessary for advancing high-quality recycle usage. While it is easy to downcycle pre-used plastics, we do not want to lose product quality in the recycling process. Here, we present our workflows for plastic analysis using Transmission Electron Microscope (TEM) and Focused Ion Beam (FIB) techniques. The goal is to explore diverse contrast enhancement techniques to unravel complex details of plastic structures. Understanding these structures is important for optimizing recycle usage.

Our toolbox of experimental setups employs state-of-the-art TEM and FIB technologies, providing high-resolution insights into the morphology and composition of plastics. By investigating and comparing contrast enhancement methods, we aim to refine the imaging process and contribute to a more comprehensive understanding of plastic materials.

CPP 28.52 Wed 11:30 Poster C

**Investigation of the impact of dissolved H<sub>2</sub> on the surface properties of ionic liquids** — ●ARSHA CHERIAN<sup>1</sup>, GYÖRGY HANTAL<sup>1</sup>, CHRISTIAN WICK<sup>1</sup>, and ANA-SUNCANA SMITH<sup>1,2</sup> — <sup>1</sup>PULS Group, Institute for Theoretical Physics, IZNF, FAU Erlangen-Nürnberg, 91058 Erlangen, Germany — <sup>2</sup>Group for Computational Life Sciences, Ruder Bošković Institute, Bijenička 54, HR-10000 Zagreb

SILP (Supported Ionic Liquid Phase) catalysis technology focuses on obtaining a heterogenised type of homogeneous catalytic systems where a thin film of ionic liquid (IL) containing a homogeneous catalyst is immobilised on the surface of a porous support material, which is commonly employed in hydrogen-involved catalysis systems. The dissolution of small, non-polar molecules of hydrogen in the ionic liquid film resulting in highly asymmetrical system in terms of molecular structures, is expected to have an influence in the thermophysical properties of IL which can subsequently affect the reaction kinetics and ultimately impact the overall reaction rate. In order to understand this influence of dissolved hydrogen on the surface properties of ILs, molecular dynamics (MD) simulations were conducted using GROMACS software in binary mixtures consisting of an ionic liquid (IL) with pressurized molecular hydrogen, between 298 and 393K over a broad pressure ranging from 1 to 30 MPa. We find that the addition of H<sub>2</sub> results in a decrease in the surface tension of both binary mixtures up to about 6 percent at higher pressures, which is more pronounced at lower temperatures. Furthermore, an enrichment of hydrogen is observed at the liquid-gas interface of these binary mixtures.

CPP 28.53 Wed 11:30 Poster C

**Charge characterization of latex colloids under thoroughly deionized and decarbonized as well as under ambient CO<sub>2</sub> conditions** — ●PETER VOGEL and THOMAS PALBERG — Johannes Gutenberg Universität, Mainz, Germany

We report on the charging behavior of dielectric colloidal particles bearing dissociable surface groups in salt-free aqueous environments in absence and presence of ambient CO<sub>2</sub>. We performed systematic measurements of the low-frequency bulk conductivity in dependence on the particle number density and upon adding neutral electrolytes to determine both the effective and bare particle charges based on our conductivity model assuming independent migration of all ionic

species present in solution. We find that upon equilibration with ambient CO<sub>2</sub> the effective number of freely mobile counterions decreases by about 50%. As function of the electrolyte concentration, the measured conductivity reveals a pronounced difference in the curve shape depending on the presence of CO<sub>2</sub>. Caused by the surface adsorption of molecular CO<sub>2</sub>, we demonstrate the absence of micro-ionic exchange processes in-between the proposed inner and outer part of the electrical double layer as deviated from the strict linear increase in conductivity. Conversely, starting from the deionized and decarbonized state, we observe a pronounced non-linear behavior fully accounted for by our model assumptions.

CPP 28.54 Wed 11:30 Poster C

**Fast on-chip AC Seebeck measurement** — ●ANDREAS WAXWEILER, EJONA SYLA, CLARA WIESNER, MORTEZA SHOKRANI, and MARTIJN KEMERINK — Institute for Molecular Systems Engineering and Advanced Materials, Heidelberg University, 69120 Heidelberg, Germany

Organic thermoelectric generators (OTEGs) show promise as a renewable energy source for small-scale devices. Despite the growing emphasis on improving the Seebeck coefficient (S) of organic materials, a precise and fast measurement of S of organic thin films appears to be lacking: the common DC method for measuring S involves substantial waiting times and must be repeated for multiple temperature gradients, which makes the measurement slow and prone to errors. To overcome this, we propose a fast, robust and easy-to-calibrate Seebeck coefficient measurement utilizing an alternate current (AC) technique. In this method, an oscillating current (frequency  $\omega$ ) is applied to an on-chip thin film heater. The resulting thermal wave (frequency  $2\omega$ ) leads to an AC thermovoltage at the same frequency that is measured by lateral electrodes across the chip. The solution of the 1-dimensional heat equation aligns well with the experimentally measured temperatures at the electrodes, allowing us to be independent of temperature measurements by calibrating the system with the heat equation. As a result, our system requires neither an external heater or cooler, nor a temperature sensor. The measurement times can be drastically decreased to less than a minute, using a chip design that can be fabricated by simple thermal evaporation through a shadow mask.

CPP 28.55 Wed 11:30 Poster C

**The Mueller Matrix for Scattering by Polydisperse Non-Chiral Samples** — ●REINHARD SIGEL — 88677 Markdorf, Germany

Light scattering measurements at a thin film or by an ensemble of particles in a dispersion are versatile tools for sample characterization. To fully exploit the technique for maximum information, the control of polarization of the incident and the detected light is required. Often samples are not ideal but include distributions of the orientation of anisotropic scattering centers and their sizes. Thus, a theoretical description ends up in the Stokes-Mueller formalism [1]. All 16 elements of the Mueller matrix can be measured [2]. It remains a task, however, to make use of such a set of partially interdependent data for a characterization of the sample which produces such scattering. The simplest case are samples without depolarization, where there is no intermixing between two orthogonal linear polarization directions. A size distribution of isotropic scattering centers is sufficient to fit an experimental Mueller Matrix for such a case [3]. To extend the model to depolarization in the simplest case, we assume equal scattering behavior for left and right circularly polarized light. Such equality is to be found for non-chiral samples. It reduces the number of independent parameters, and it is sufficient to consider a common polydispersity distribution of two real parameters for the resulting Mueller matrix.

[1] C.F. Bohren, D.R. Huffman, *Absorption and Scattering of Light by Small Particles* (Wiley, Weinheim 1983).

[2] R.M.A. Azzam, Opt. Lett. 2, 148-150 (1978).

[3] R. Sigel, A. Erbe, Appl. Opt. 47, 2161-2170 (2008).

CPP 28.56 Wed 11:30 Poster C

**Significant reduction in electrical conductivity of PE-DOT:PSS with new Schiff base salts additives** — ●AMNEH MIKAEELI<sup>1,2</sup>, NATHAN JUKAM<sup>2</sup>, ANNA KMIECIAK<sup>3</sup>, ROBERT SZCZESNY<sup>3</sup>, ARNE LUDWIG<sup>2</sup>, BAYRAM GUNDUZ<sup>4</sup>, ANDREAS D. WIECK<sup>2</sup>, and MICHAL PAWLAK<sup>1</sup> — <sup>1</sup>Faculty of Physics, Astronomy, and Informatics, Nicolaus Copernicus University in Torun, Grudziadzka 5, 87-100 Torun, Poland — <sup>2</sup>Chair of Applied Solid-State Physics, Faculty of Astronomy and Physics, Ruhr-University Bochum, D-44780, Bochum, Germany — <sup>3</sup>Faculty of Chemistry, Nicolaus Copernicus University in Torun, Gagarina 7, 87-100 Torun, Poland —

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PEDOT:PSS layers were prepared with three different additives. In particular, the conductivity effects of additives on PEDOT:PSS layers were examined depending on temperature. The conductivity values

of PEDOT:PSS layers increase significantly with increasing temperature. These results confirm that PEDOT:PSS exhibits semiconductor properties. Additionally, there appears to be a significant difference, although not a vast difference between the conductivities of PEDOT:PSS for the three different additives. All these results show that both additives and especially temperature change the conductivities of PEDOT:PSS.