

CPP 17: Poster Session I

Topics: Focus: Self-Assembly of Plasmonic Nanostructures (1-4); Molecular Electronics and Excited State Properties (5-10); Organic Electronics and Photovoltaics (11-30); Hybrid and Perovskite Photovoltaics (31-44); Charged Soft Matter, Polyelectrolytes and Ionic Liquids (45-48); Interfaces and Thin Films (49-57), 2D Materials (58-60).

Time: Monday 18:00–20:00

Location: P3

CPP 17.1 Mon 18:00 P3

Plasmonic behaviour of surface modifications of γ -AlOOH nanoparticles and their effect on the particles Hamaker constant — •DOROTHEE SILBERNAGL¹, MATEUSZ DUDZIAK¹, ANNA MARIA MANZONI¹, and HEINZ STURM^{1,2} — ¹Bundesanstalt für Materialforschung und -prüfung, Unter Den Eichen 87, 12205, Berlin, Germany — ²Institute for Machine Tools and Factory Operations (IWF), TU Berlin, Pascalstr. 8-9, 10587 Berlin, Germany

Boehmite (γ -AlOOH) nanoparticles (BNP, particle size appr. 14nm) are known for their extremely low Hamaker constant A, which results in low interparticle van der Waals forces. However, surface modified BNPs (modifications are acidic acid BNPA, lactic acid BNPL and stearic acid BNPS) exhibit a gradually increased Hamaker constant A and therefore increased interparticle van der Waals forces. This was measured by atomic force microscopy force distance curves (AFM FDC). For this experiment an unmodified BNP agglomerate of approximately 50um diameter was attached to an AFM cantilever and measured against pressed BNPs without and with different surface modifications. This set-up provides a sphere/plane geometry, necessary to calculate the Hamaker constant A of each material pairing from the FDCs attractive regime. Electron energy loss spectroscopy (EELS) measurements in the low energy region (up to 80eV) of unmodified and surface modified BNPs were performed to understand the origin of the increased van der Waals forces. As a result, additional plasmon bands were found in the region below 10eV for surface modified BNPs, which contribute to the attractive forces between particles.

CPP 17.2 Mon 18:00 P3

Liquid phase (S)TEM of DNA origami gold nanoparticle hybrids — •A. ONG¹, D. POHL¹, T.K. JEONG^{2,3}, A. HEERWIG^{2,3}, M. MERTIG^{2,3}, and B. RELLINGHAUS¹ — ¹Dresden Center for Nanoanalysis (DCN), cfaed, TU Dresden, Germany. — ²Physical Chemistry, TU Dresden, Germany — ³Kurt-Schwabe-Institut für Mess- und Sensortechnik Meinsberg e.V., Germany

DNA origami pads with site-specific patterns of ssDNA are flexible molecular templates for gold nanoparticles to self-assemble into functional supracolloidal structures [1]. The structure-property relation of supracolloidal structures play a significant role in constructing novel materials with desired properties for application in devices [2]. However, this relation has not been adequately understood. The study focuses on investigating the self-assembly and kinetic processes in supracolloidal structures using (scanning) transmission electron microscopy [(S)TEM] both in vacuum and in the liquid phase. Images of gold nanoparticles attached to DNA origami were acquired under vacuum and in-situ in the liquid phase, highlighting the possibility of real-time visualizations at the nanometer scale in different environments. The measured distances between gold nanoparticles in liquid confirm the intended templating mechanism. Financial support by DFG through RTG 2767 and by the EU Horizon 2020 Research & Innovation Programme grant agreement no. 964248 is gratefully acknowledged.

[1] J. Zessin et al. Nano Lett. (2017)17, 5163.

[2] T. Woehl, ACS Nano (2019) 13, 12272.

CPP 17.3 Mon 18:00 P3

Probing photoluminescent polymers using plasmonic self-assembly — •ONIMA BISHT^{1,3}, SEZER SEÇKIN¹, and TOBIAS KÖNIG^{1,2} — ¹Leibniz-Institut für Polymerforschung e.V., Hohe Straße 6, 01069 Dresden, Germany — ²Center for Advancing Electronics Dresden (cfaed), Technische Universität Dresden, 01062 Dresden, Germany — ³Department of Physics, Indian Institute of Technology Delhi, Hauz Khas, New Delhi, 110016, India

Surface Enhanced Raman Spectroscopy (SERS) is an advantageous and indispensable technique for detection and sensing applications. Although SERS substrates have been fabricated using several top-down approaches, these methods are limited by scalability, uniformity, and high instrumentation costs. Recent developments in template-assisted

self-assembly (TASA) techniques have facilitated us to fabricate low-cost, scalable, and uniform gratings consisting of plasmonic nanoparticle chains. [König et al., Adv. Funct. Mater. 2021, 2105054] With the support of the finite-difference time-domain (FDTD) method, we have rationally designed the colloidal grating to benefit from the coherent interaction between Rayleigh anomalies and various plasmon modes. We will combine these modes with the quantum emitter, which we used previously as an efficient gain component for optoelectronic devices. [König et al., Adv. Optical Mater. 2020, 2001280] Finally, we use this overlap of the plasmonic modes with the photoluminescence of the emitters for nonlinear effects such as lasing, strong coupling, and ultra-high SERS sensitivity.

CPP 17.4 Mon 18:00 P3

Influence of thermal effects on a combinatorial plasmonic nanostructure for bio-detection — •TIANFU GUAN¹, SUZHE LIANG¹, YUSUF BULUT^{1,2}, KRISTIAN RECK³, MATTHIAS SCHWARTZKOPF², JONAS DREWES³, THOMAS STRUNSKUS³, FRANZ FAUPEL FAUPEL³, STEPHAN V. ROTH^{2,4}, and PETER MÜLLER-BUSCHBAUM^{1,5} — ¹TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — ²DESY, 22607 Hamburg, Germany — ³CAU, Chair for Multicomponent Materials, Faculty of Engineering, 24143 Kiel, Germany — ⁴Department of Fiber and Polymer Technology, KTH, SE-100 44 Stockholm, Sweden — ⁵MLZ, TUM, 85748 Garching, Germany

In recent decades, Au nanoparticles (NPs) have been utilized in a wide range of sensor applications, such as photodetection, bio-detection, and thermal-detection, because of their unique optical and chemical properties. Among the optical sensors, surface-enhanced Raman spectroscopy (SERS) has attracted extensive attention being used in the identification of unknown substances in analytical chemistry. In this work, we investigate in situ sputter deposition of Ag on highly ordered Au NPs substrates as probed by grazing incidence small angle X-ray scattering (GISAXS). In addition, we explore the effect of temperature on the silver growth kinetics on different sizes of Au NPs substrates. Furthermore, by correlating the growth steps of the composite Au/Ag nanostructures with their SERS performance, we obtain the plasmonic hot spot performance corresponding to the combined nanostructure.

CPP 17.5 Mon 18:00 P3

Understanding the Double Doping of Organic Semiconductors Via State Energy Renormalization upon Charging — •ROSS WARREN¹, EUNKYUNG CHO², HONG LI², JEAN-LUC BREDAS², and NORBERT KOCH^{1,3} — ¹Institut für Physik & IRIS Adlershof, Humboldt-Universität zu Berlin, 12489 Berlin, Germany — ²Department of Chemistry and Biochemistry, The University of Arizona, Tucson, Arizona 85721-0088, United States — ³Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, 12489 Berlin, Germany

The double ionisation of dopants is a recent experimental observation that allows the doping efficiency to rise above 100%. This is exciting because high conductivities can be achieved with fewer dopant molecules, meaning less disruption to the resulting film's microstructure. However, the current models of doped organic semiconductors based on Fermi-Dirac statistics fail to explain the double ionization of dopants and also the analogous situation of bipolaron formation on a host polymer. Here, we address this shortcoming by considering the renormalization of the state energies upon electron transfer between host and p-dopant. We vary the model parameters - the reorganization energy and evolutions of ionization energies and electron affinities upon charging - and plot the fractions of doubly ionized, singly ionized, and neutral species. We find good agreement with experiment. Finally, we suggest that the state energy renormalization upon charging is the key parameter to be minimized for double ionization of dopants or maximized to avoid formation of bipolarons on the host.

CPP 17.6 Mon 18:00 P3

Temperature Dependent Photoluminescence of β -Phase Zinc Phthalocyanine Single Crystals — •KILIAN STRAUSS¹, LISA SCHRAUT-MAY¹, SEBASTIAN HAMMER^{1,2}, KILIAN FRANK³, BERT NICKEL³, and JENS PFLAUM¹ — ¹Experimental Physics VI, Julius-Maximilians-Universität of Würzburg — ²Department of Physics, Ludwig Maximilian University, Munich — ³Departments of Physics and Chemistry, McGill University, Montreal, Canada

The photophysical properties of organic crystals are strongly dependent on the interactions between the comprising molecules. We chose zinc phthalocyanine (ZnPc) in its crystallographic β -phase as a model system to investigate the excitonic coupling as a function of crystallographic direction. For this purpose, we performed polarization dependent photoluminescence (PL) measurements from 5 K to 300 K on needle-shaped single crystals grown by horizontal vapour deposition. A gradual optical transition from a J- to H-aggregate like behavior occurs on cooling down to 100 K. Upon further cooling, we find the emergence of superradiant luminescence typical for exciton delocalization in J-aggregates. This optical transition is induced by an anisotropic thermal compression of the crystal lattice.

We thank the Bavarian Research Network SolTech for financial support.

CPP 17.7 Mon 18:00 P3

On the Parametrization of Exciton-Phonon Coupling Matrix Elements by Ab Initio Methods — •MAXIMILIAN FRANZ XAVER DORFNER and FRANK ORTMANN — Department of Chemistry, Technische Universität München, 85748 Garching b. München, Germany

The accurate description of optical or transport properties of organic semiconductors, such as small molecules or polymers requires, besides the electronic degrees of freedom, also the incorporation of the nuclear motion into the theoretical treatment. This is because in these materials the electrons and the core movement are significantly coupled to each other.

This interaction co-determines macroscopic observables, like absorption cross-sections, charge carrier mobilities, or electronic relaxation time-scales. Close to the equilibrium configuration, the interplay of the electronic degrees of freedom and the nuclei can be cast into the form of a Holstein-Peierls model. In this representation, the interaction is characterized by a set of coupling constants, which are typical for a given molecule and dictate behavior in a range around the equilibrium configuration.

Here we present a novel scheme and an implementation for the computation of these effective coupling constants based on the CP2K software package. We benchmark our implementation for a number of molecules and study their non-radiative electronic relaxation behavior by the use of a matrix product state approach.

CPP 17.8 Mon 18:00 P3

Unraveling Structural Dynamics in Excimer Formation Using Ultrafast Electron Diffraction — •SEBASTIAN HAMMER¹, LAURENZ KREMEYER¹, TRISTAN BRITT¹, MAXIMILIAN RÖDEL², SYED ALI HASSAN¹, JENS PFLAUM^{2,3}, and BRADLEY SIWICK¹ — ¹Departments for Physics and Chemistry, McGill University, Montreal, QC H3A 2K6, Canada — ²Experimental Physics VI, University of Würzburg, 97074 Würzburg — ³Bayerisches Zentrum für Angewandte Energieforschung (ZAE Bayern), 97074 Würzburg

Excimer formation, *i.e.* the formation of an excited dimer state which is accompanied by structural deformations in the local inter-molecular geometry, is a common phenomena in molecular solids and crucially determines the opto-electronic properties of the material. While the process is understood well on a theoretical level [1], direct observational evidence of the underlying structural dynamics are experimentally challenging.

In recent years, the technique of ultrafast electron diffraction (UED) has proven to be capable of unraveling the structural dynamics of molecular single crystals after photo-excitation [2]. Using the prototypical excimer system zinc-phthalocyanine in its crystallographic α -phase [3], we show that UED experiments on polycrystalline thin-films can disclose the structural dynamics accompanying excimer formation. We gratefully acknowledge funding from the DFG (Project 490894053).

[1] Bialas et al. *J. Chem. Phys. C* **126** 4067-4081 (2022)

[2] Gao et al. *Nature*. **496** 343-346 (2013)

[3] Hammer et al., *Mater. Horiz.*. (2022)

CPP 17.9 Mon 18:00 P3

Influence of Ligands and Linker on the Optoelectronic Properties of Phenazine-based Iron Spin-Crossover Complexes

— •LYDIA PLOSS¹, FLORIAN DAUMANN², KONSTANTIN SCHÖTZ¹, GERALD HÖRNER², BIRGIT WEBER², and ANNA KÖHLER^{1,3} — ¹Experimental Physics II, University of Bayreuth — ²Anorganische Chemie IV, University of Bayreuth — ³Bayreuth Institute of Macromolecular Research, University of Bayreuth

Spin-crossover (SCO) complexes are a class of materials - typically organo-metallic complexes - whose electronic ground state can be switched between a high spin (HS) and a low spin (LS) state by external stimuli, e.g., by varying the temperature. This possibility renders them promising candidates for applications such as molecular switches or sensors.

An easy way to read out sensors is, e.g., by using photoluminescence (PL) spectroscopy. Recently, an iron-based SCO complex was found that shows PL in both spin states.¹ This is remarkable since most SCO complexes show PL in only one of the two spin states or are not luminescent at all. To understand what defines the optical properties of such compounds, we systematically vary ligands and linker molecules of the complexes and investigate their influence on the optical properties of the resulting complexes, using absorption and temperature-dependent PL spectroscopy.

¹Lochenie et al., *J. Am. Chem. Soc.* 2018, 140, 2, 700-709

CPP 17.10 Mon 18:00 P3

Multichromophore Macrocycles of Perylene Bisimide Dyes as Fluorescent OLED Emitters — •THEODOR KAISER¹, BJÖRN EWALD¹, ULRICH MÜLLER¹, PETER SPEST², MATTHIAS STOLTE², FRANK WÜRTHNER², and JENS PFLAUM¹ — ¹Experimental Physics VI, University of Würzburg — ²Institut für Organische Chemie and Center for Nanosystems Chemistry, University of Würzburg

While fluorescent organic emitters exhibit an efficient and bright singlet decay their efficiency in Organic Light Emitting Diodes (OLEDs) is limited by the lifetime and non-radiative loss pathway of triplet dark states. Therefore OLED applications are mainly based on phosphorescent emitters harvesting triplet excitons for light emission. In order to increase the efficiency of fluorescent OLEDs we present a novel approach for the chemical design of fluorescent emitters based on multichromophore macrocycles of perylene bisimide dyes (PBIs). By linking individual PBI chromophores in macrocyclic architectures, biexcitonic coupling can lead to an efficient transformation of triplet dark states by processes like triplet-triplet annihilation (TTA). This allows for an efficient bright electrical operation in OLED devices as the lifetime of dark states is drastically reduced. As recently reported by our groups trimeric perylene bisimides can even produce non-classical electrically driven single photon emission at room temperature [1], which has so far only been reported for phosphorescent emitters. Therefore these emitters offer new options for the application of strictly fluorescent materials in classical and non-classical OLED devices.

[1] Ulrich Müller et al., *Adv. Optical Mater* 2022, 10, 2200234.

CPP 17.11 Mon 18:00 P3

Investigation of Metal-Insulator Transitions in Organic Field-Effect Transistors of an n-Type Organic Semiconductor — •PAUL SCHLACHTER¹, MAXIMILIAN FRANK¹, MATTHIAS STOLTE², FRANK WÜRTHNER², and JENS PFLAUM^{1,3} — ¹Experimental Physics VI, University of Würzburg, 97074 Würzburg — ²Institut für Organische Chemie and Center for Nanosystems Chemistry, University of Würzburg, 97074 Würzburg — ³ZAE Bayern, 97074 Würzburg

Metal-insulator transitions in organic materials offer many exciting applications and are therefore gaining increasing scientific as well as technological interest. In this work, we aim to investigate electronic field-effect-induced phase transitions (semiconductor \rightarrow conductor \rightarrow insulator) in organic single crystals (especially Cl₂NDI [1]) of high electron mobility. The long-range order of their molecular entities in combination with a preferred (001) gliding plane geometry provides the pre-condition of a nearly defect-free interface for studying quasi-two-dimensional electron gas formations. For this purpose, we use an electrolyte as a top gate in addition to a dielectric conventional back gate. By simultaneously varying the bottom and top gate voltages, respectively, we aim to control the charge carrier density and thereby to gain deeper insights into Mott physics. First results on these efforts will be presented and evaluated with respect to the possible implementation in Mott field-effect transistors.

[1] Tao He et al., *Nat. Commun.* 2015, 6, 5954

CPP 17.12 Mon 18:00 P3

On the orientation mechanism of non-polar dyes in light-emitting guest-host systems — •BINH-MINH NGUYEN, MARKUS

SCHMID, JOHANN KIRSCH, and WOLFGANG BRÜTTING — Experimental Physics IV, Institute of Physics, University of Augsburg, 86159 Augsburg, Germany

After many years of development, OLEDs have continuously been optimized to reach higher efficiency, for which the horizontal orientation of the emitter molecules is one of the dominant factors [1]. For the purpose of studying intrinsic orientation without electrostatic interaction, our work considers non-polar dyes, namely TTPA, BSBCz, DIP and DBP. While the emitter orientation has been studied in neat film as a basic approach, their behavior in guest-host systems has not been studied widely. In this work we focus on the correlation between emitter concentration and its orientation. With the results from experimental and simulation study, we also discuss the possible orientation mechanism of emitter molecules on the substrate surface in terms of molecular structure, possibility to form crystallites and the effective glass transition temperature of the guest-host system. We observe that isotropic structure of the emitter as well as the crystallized and aggregated molecules are not favorable for horizontal orientation. However, molecules having a rod-like structure have the tendency to arrange horizontally to the substrate. These results contribute to a further understanding of orientation of non-polar emitter molecules.

[1] Brütting et. al, Physical Review Applied, 2017, 8(3), 037001.

CPP 17.13 Mon 18:00 P3

Self-heating in OLED Lighting — ●ANTON KIRCH^{1,2}, AXEL FISCHER¹, MATTHIAS LIERO³, JÜRGEN FUHRMANN³, ANNEGRET GLITZKY³, LUDVIG EDMAN², and SEBASTIAN REINEKE¹ — ¹Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP), TU Dresden, Germany — ²Department of Physics, Umeå University, Sweden — ³Weierstrass Institute Berlin, Germany

For bright area light sources, such as OLED lighting tiles, the electric resistivity of transparent electrodes induces a non-uniform current distribution within the device. At high driving currents, the interaction between conductivity, heat, and power dissipation results in a positive electrothermal feedback loop, which drastically exacerbates inhomogeneities in local device temperature and luminance.

Such nonlinear behavior induces unprecedented electrothermal effects that compromise the performance of bright area light sources. In this contribution, we present how Joule self-heating squeezes temperature and current into a tiny device region, while the remainder of the active area decreases in luminance (Switch-back effect) [1]. We further introduce how the dimension of the active area governs the current-voltage characteristics of the OLED and how two and even three stable operating branches develop (tristability) that can promote destructive incidences [2].

References

[1] Kirch et al., Light: Science & Applications 9, 5 (2020)

[2] Kirch et al., Adv. Func. Mat. 31, 47 (2021)

CPP 17.14 Mon 18:00 P3

Organic Photoconductors based on Rubrene Thin-Films — ●JONAS SCHROEDER, RISHABH RISHABH, JOHANNES BENDUHN, and KARL LEO — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute for Applied Physics, Technische Universität Dresden, Nöthnitzer Str. 61, 01187 Dresden, Germany

Thin films of organic semiconductors possess huge potential for large-scale industrial applications. However, the limited possibilities of crystal growth directly on the substrates often restrict device concepts but also achievable device performance. Here, we use vacuum-deposited rubrene in combination with a thermal post-treatment to fabricate different morphologies of polycrystalline thin films. To take advantage of the high in-plane mobility ($3\text{ cm}^2\text{ V}^{-1}\text{ s}^{-1}$) of the well-known orthorhombic rubrene phase in light detection applications, we employ photoconductive detectors in which the contacts are placed laterally on the sides of the active material. This allows for decoupling of the filtering of the incident light from the channel geometry and a photocurrent gain due to the natural imbalance of electron and hole mobilities in organic semiconductors. We show performance benchmarks of prototypical photoconductive organic photodetectors and relate these to the optical and electrical properties of the used rubrene thin films.

CPP 17.15 Mon 18:00 P3

Optimizing narrowband OPDs for wavelength range from 700 nm to 1100 nm — ●FRED KRETSCHMER, LOUIS CONRAD WINKLER, JAKOB WOLANSKY, JOHANNES BENDUHN, and KARL LEO — Technische Universität Dresden, Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute of Applied

Physics (IAP), Dresden, Germany

In recent years, organic photodetectors have attracted particular interest, due to their advantageous properties, such as cheap manufacturing costs and high performance, compared to inorganic devices. Particularly important is the narrowband photo-response, which enables the detection of small wavelength ranges, making optical filters obsolete and allowing miniature detector compositions. Narrowband spectroscopic sensors are an integral part of modern society, for example, in food quality monitoring, signal communication, or medical imaging.

In this contribution, microcavity-enhanced organic photodetectors in the visible and near-infrared wavelength range are investigated. For these devices, the active and transport layer thickness are varied and analysed for the donor material Rubrene and Spiro-MeO-TPD. Therefore, performance parameters such as the external quantum efficiency, the specific detectivity, the dark current, the response speed, and parasitic side effects are investigated and examined, leading to concrete device guidelines which can increase the performance of narrowband organic photodetectors. In a next step, we are planning to complement these detectors with infrared light-emitting diodes for a fully organic, spectroscopic sensing system.

CPP 17.16 Mon 18:00 P3

Humidity Stable Thermoelectric Hybrid Materials for A Self-Powered Sensing System — ●SUO TU¹, TING TIAN¹, TIANXIAO XIAO¹, SHANSHAN YIN¹, JULIAN HEGER¹, GUANGJIU PAN¹, SHUJIN HOU², ALIAKSANDR BANDARENKA², MATTHIAS SCHWARTZKOPF³, STEPHAN ROTH³, and PETER MÜLLER-BUSCHBAUM^{1,4} — ¹Technical University of Munich, TUM School of Natural Sciences, Department of Physics, Chair for Functional Materials, 85748 Garching — ²Technical University of Munich, TUM School of Natural Sciences, Department of Physics, Physik der Energiewandlung und -speicherung, 85748 Garching — ³DESY, 22607 Hamburg — ⁴MLZ, TUM, 85748 Garching

Highly sensitive and humidity-resistive detection of the most common physical stimuli is of primary importance for practical application in a real-time monitoring. Here, we report a simple yet effective strategy to achieve a highly humidity-stable hybrid composite that enables simultaneous and accurate pressure and temperature sensing in a single sensor. The improved electronic performance was due to the enhanced planarity of PEDOT and charge transfer between PEDOT:PSS and multi-walled carbon nanotubes (MWCNT) by strong π - π interaction. The preferred electronic pathway induced by robust morphology in the hybrid composite is responsible for the high humidity stability. These observations have been recognized by Grazing-incidence wide/small-angle X-ray scattering (GIWAXS/GISAXS), Raman, FTIR, and electrochemical impedance spectroscopy (EIS).

CPP 17.17 Mon 18:00 P3

New insights into the P3HT:PCBM bulk-heterojunction — ●SHAHIDUL ALAM¹, CHRISTOPHER E. PETOUKHOFF¹, HAYA ALDOSARY¹, XINYU JIANG², TOMÁŠ VÁRY³, WEJDAN ALTHOBAITI¹, SANDRA P. GONZALEZ LOPEZ¹, WEJDAN ALSUFYANI¹, PETER MÜLLER-BUSCHBAUM², VOJTECH NÁDAŽDY⁴, HARALD HOPPE⁵, and FRÉDÉRIC LAQUAT¹ — ¹KAUST Solar Center (KSC), Kingdom of Saudi Arabia — ²TU Munich, Germany — ³STU Bratislava, Slovak Republic — ⁴Slovak Academy of Sciences, Bratislava, Slovak Republic — ⁵FSU Jena, Germany

Here, we studied the influence of thermal annealing on blends of well-known regio-random and regio-regular P3HT conjugated polymers and fullerene derivative [6,6]-phenyl-C60-butyric acid methyl ester (PC60BM). Several advanced microscopic and spectroscopic techniques were applied to investigate the thermal annealing effects on the structural, morphological, and energetic states, e.g., grazing-incidence wide-angle x-ray scattering, polarized light microscopy, hyperspectral photoluminescence spectroscopy, and photo-deflection spectroscopy. Furthermore, the blends' density of states (DOS) distribution was studied using energy resolved-electrochemical impedance spectroscopy. Coupled transfer matrix methods and drift-diffusion simulations were employed to see the impact of DOS on the solar cells' device parameters.

CPP 17.18 Mon 18:00 P3

Crystal Orientation and Surface Morphology in Thin Films of Poly-[3-(6-trifluorohexyl)thiophene] on Silicon and Graphene — ●ALEXANDER MUCH¹, ROBERT KAHL¹, FLORIAN MEICHSNER², MUKUNDAN THELAKKAT², THOMAS THURN-ALBRECHT¹, and OLEKSANDR DOLYNCHUK¹ — ¹Experimental Polymer Physics, Martin Luther University Halle-Wittenberg — ²Applied Functional Polymers,

University of Bayreuth

Semiconducting polymers gained much interest for use in electronic devices due to their easy processing from solution and mechanical flexibility. To improve the efficiency of organic electronic devices, it is crucial to understand and control the crystal orientation in thin films.

As recently found in films of poly-(3-hexylthiophene) (P3HT) on graphene, the interfaces to vacuum and graphene induce edge-on and face-on orientation, respectively [1]. We propose to influence the crystal orientation in polythiophenes by increasing the polarity of the end group of the side chains. Thereby, melt-crystallized thin films of poly-[3-(6-trifluorohexyl)thiophene] (P3CF3HT) studied by GIWAXS showed an increased and thickness-dependent tendency to face-on orientation not only on graphene, but also on silicon, which is inactive for P3HT. Furthermore, the film surface morphology probed by AFM strongly depends on the crystal orientation and the substrate. Our results validate the approach and open a pathway to control molecular orientation in polythiophenes.

[1] Dolynchuk et al., *Macromolecules* **54**, 5429-5439, 2021

CPP 17.19 Mon 18:00 P3

Influence of amphiphilic additives on P3HT:PC60BM organic solar cells — ●JOSE PRINCE MADALAIMUTHU^{1,2}, ZHUO XU^{1,2}, ULRICH S. SCHUBERT^{1,2}, and HARALD HOPPE^{1,2} — ¹Laboratory of Organic and Macromolecular Chemistry (IOMC), Friedrich Schiller University Jena, Humboldtstr. 10, D-07743 Jena, Germany — ²Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich Schiller University Jena, Philosophenweg 7a, D-07743 Jena, Germany

The mechanical stability of the layer stack is a significant barrier to the continued functioning of flexible OPVs. Delamination processes have the potential to significantly reduce photovoltaic performance. High-crystallinity polymers retain blend morphologies for a long time but yield brittle thin films. Amorphous polymers produce more flexible films but have less morphological stability. Device performance is associated with high crystallinity and superior charge carrier mobility. Furthermore, the elasticity required for mechanical stability is often improved with more amorphous polymers. This seems to split the necessary material characteristics in two. The objectives of the investigations are to improve mechanical resilience by lowering the tensile modulus and reducing crystallization by introducing tiny amounts of amphiphilic plasticizers. The effect of amphiphilic small molecule additions in donor-acceptor blends was investigated for toluene sulfonic acid (TSA) and then with a series of perylenes with systematically varying amphiphilicity. Enhancing the device's performance and long-term stability illustrates that the active layer's morphology can be regulated by the presence of amphiphilic additives.

CPP 17.20 Mon 18:00 P3

Enhanced air stability of green-solvent polymer solar cells with green-fluorescent polymer EH-P — ●ZERUI LI¹, SERGEI VAGIN², KUN SUN¹, MORGAN LE DÜ¹, MANUEL A. REUS¹, and PETER MÜLLER-BUSCHBAUM^{1,3} — ¹Technical University of Munich, TUM School of Natural Sciences, Department of Physics, Chair for Functional Materials, James-Franck-Str. 1, 85748 Garching, Germany — ²Technical University of Munich, TUM School of Natural Sciences, Department of Chemistry, Chair of Macromolecular Chemistry, James-Franck-Str. 1, 85748 Garching, Germany — ³Technical University of Munich, MLZ, Lichtenbergstr. 1, 85748 Garching, Germany

The rapid development of materials has promoted that the efficiency of polymer solar cells (PSCs) reached over 20%, which is highly close to the application requirement. While the relative poor stability of PSCs slows down their commercial progress. Nowadays the research of stability in nitrogen or vacuum received much attention, while the inevitable contact of air would also cause undesirable effect on the device performance. Here, we select a green-solvent based material system PBDB-TF-T1:BTP-4F-12 as research model. Firstly the degradation of solar cells in air was observed and the mechanism was investigated. Then a green fluorescent polymer additive could EH-P was explored and it's found that it could improve the air-illumination stability of these solar cells. The doped solar cells shown obvious advantaged performance compared than reference ones after 24-hours-illumination in air. Such a material shows great potential in real application and provides guidance in exploring new additive.

CPP 17.21 Mon 18:00 P3

Calculation of intra-molecular transition rates depending on structural parameters with DFTB — ●FABIAN TEICHERT, ROBIN SILLIGMANN, FLORIAN GÜNTHER, and ANGELA THRÄNHARDT — In-

stitute of Physics, Chemnitz University of Technology, Chemnitz, Germany

Organic semiconductors become increasingly important for electronic applications. The large number of organic materials and their combinations make it useful to investigate properties like current-voltage characteristics using simulations in order to find suitable material combinations for applications. We investigate the transition rates of electrons between two organic molecules, especially between thiophene, zinc porphyrin and PCBM. For this, we calculate HOMO and LUMO states and energies, reorganisation 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) zinc porphyrin and PCBM. We show reorganisation 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 17.22 Mon 18:00 P3

Charge transfer characteristics of an optically-driven conjugated molecular system — VLADYSLAV SAVCHENKO and ●OLGA GUSKOVA — IPF Dresden, Dresden, Germany

Recently [1], we have simulated E/Z isomers of two azobenzene-bithiophene (azo-bt) molecular switches in-between an anchoring surface and a gold STM tip. One of these switches has been previously synthesized [2], another one represents a structural isomer of [2], where azo and bt blocks have been swapped along the molecule. Here, we focus on the intermolecular charge transfer within chemisorbed monolayer because this aspect is still unexplored. First, DFT method is applied to define the reorganization energies for electron and hole transfer and the transfer integrals for stacked molecules using energy splitting in dimer approach. Further, the charge carrier mobility is evaluated. The results show, that the position of azo and bt favors either hopping of electrons or holes. For example, both isomers of the molecule with swapped blocks [1] are prone to the electron transfer, whereas for switch [2] the UV light stimulus toggles the main charge carrier from electron to hole. Interestingly, that molecule [2] possesses a non-zero mobility for the hopping distances $h < 0.5$ nm, which requires densely packed layers. On contrary, relatively high electron transfer is predicted for molecule [1] even for sparsely anchored switches (h ca. 1 nm); the UV light turns off the hole hopping at distances $h > 0.5$ nm as well. This work is supported by DFG, grant GU1510/5-1. [1] Savchenko V., Guskova O. *Herald of TvSU. Series: Chem.* 3(45) 2021, 7. [2] Karpe S., et al. *Chem. Commun.* 46, 2010, 3657.

CPP 17.23 Mon 18:00 P3

Critical Conditions in Transfer Matrix Methods — ●REINHARD SIGEL — Independent Scientist, Markdorf, Germany

The propagation of light in a layered refractive index profile is well described by transfer matrix methods (TMMs) [1]. Critical conditions (CC) occur when the wave vector perpendicular to the layering becomes zero. This case can be encountered in a total reflection geometry. Conventional TMMs become singular for CC. We discuss the divergence of layer amplitudes when one approaches CC. It is furthermore elucidated, how this divergence shows up in different experiments. New types of basis functions for a TMM based on virtually linear functions to circumvent the singularity have been introduced recently [2].

[1] J. Lekner, *Theory of reflection of electromagnetic and particle waves*, Martinus Nijhoff Publisher, Dordrecht, 1987.

[2] R. Sigel, *Light Propagation in Layered Media in a Total Reflection Geometry: A Transfer Matrix Method Using Virtually Linear Basis Functions to Handle Critical Conditions*, *J. Opt. Soc. Am. A*, accepted.

CPP 17.24 Mon 18:00 P3

Surface doping of rubrene single crystals by molecular electron donors and acceptors — ●CHRISTOS GATSIOS¹, ANDREAS OPITZ¹, SEBASTIAN HAMMER³, JENS PFLAUM³, YADONG ZHANG⁴, STEPHEN BARLOW⁴, SETH R. MARDER⁵, and NORBERT KOCH^{1,2} — ¹Institut für Physik & IRIS Adlershof, Humboldt-Universität zu Berlin, 12489 Berlin, Germany — ²Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, 12489 Berlin, Germany —

³Experimentelle Physik VI, Julius-Maximilians-Universität Würzburg, 97074 Würzburg, Germany — ⁴Renewable and Sustainable Energy Institute (RASEI), University of Colorado, Boulder, CO 80309, USA — ⁵Renewable and Sustainable Energy Institute (RASEI), Department of Chemical and Biological Engineering, Department of Chemistry, and Materials Science and Engineering Program, University of Colorado, Boulder, CO 80309, USA

Molecular doping can be used as a method to control the electronic energy levels and charge carrier densities of the organic semiconductor via charge transfer interactions with electron-donating or electron-accepting molecules. This work seeks to understand the mechanisms of interface engineering by focusing on the surface doping of rubrene single-crystals by molecular electron donors (CoCp2) and acceptors (Mo(tfd-CO2Me)3). Our angle-resolved photoemission results show that deposition of molecular dopants on rubrene shifts the valence band with respect to the Fermi level, thus changing the p- (n-) character of the surface, while the electronic band parameters remain essentially unaffected.

CPP 17.25 Mon 18:00 P3

Electronic structure of singlet fission donor-acceptor complexes — ●KARIN S. THALMANN¹, PEDRO B. COTO², and MICHAEL THOSS¹ — ¹Institute of Physics, University of Freiburg, Germany — ²Spanish National Research Council (CSIC), Madrid, Spain

Singlet fission (SF) is a photophysical process in molecular materials describing the spin-allowed conversion of a singlet exciton to two triplet excitons [1]. Due to its ability to multiply charge carriers and its potential usage in solar cells to circumvent the Shockley-Queisser limit [2,3], SF has received significant attention recently. For future applications in energy conversion, the molecule exhibiting SF has to be combined with an electron acceptor to extract the energy of the two triplet excitons. As an example, we consider the complex of two covalently linked diazadiborane chromophore units as the SF exhibiting donor and tetracyanoquinodimethane as the acceptor molecule. Using multireference perturbation theory techniques, we analyze the electronic structure of the complex, in particular the electronically excited states, which include locally excited, charge transfer, and multiexcitonic states. Furthermore, we study the influence of the acceptor on the electronic structure of the donor molecule.

[1] M. B. Smith, J. Michl, *Chem. Rev.* **110**, 6891 (2010).

[2] W. Shockley, H. J. Queisser, *J. Appl. Phys.* **32**, 510 (1961).

[3] A. J. Baldacchino et al., *Chem. Phys. Rev.* **3**, 021304 (2022).

CPP 17.26 Mon 18:00 P3

Recyclable-refabricated efficient solar cells with cellulose-based materials — ●SHUXIAN XIONG^{1,2}, MARIE BETKER^{1,3}, BENEDIKT SOCHOR¹, CONSTANTIN HARDER^{1,2}, YUSUF BULUT^{1,2}, L. DANIEL SÖDERBERG³, PETER MÜLLER-BUSCHBAUM^{2,4}, and STEPHAN V. ROTH^{1,3} — ¹DESY, 22607 Hamburg, Germany — ²TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — ³KTH Royal Institute of Technology, 10044 Stockholm, Sweden — ⁴MLZ, TUM, Garching, Germany

Cellulose-based nanomaterials are used in a variety of potential applications, particularly in green electronics and optoelectronic devices, due to their sustainability, low cost and the ease of chemical functionalization. For recycling and prefabrications of cellulose-based solar cells, we propose the fabrication of green, fully sprayed solar cells based. The electrode material using conductive inks laminated with cellulose is easy to fabricate in large-area solutions. Preferably chlorine-free solvents are used in the active layer, and solvent engineering and post-treatment are used to control the morphology and aggregation to achieve high performance and environmental recyclability. The solar cells are planned to be recycled using the most environmentally friendly physical and chemical methods. The solar cell materials should be recycled to the maximum extent possible, and the recycled materials are then used to refabricate the solar cells and evaluate them in terms of morphology and efficiency.

CPP 17.27 Mon 18:00 P3

Towards needleless Electrospinning of a non-toxic, textile Dye-sensitized solar cell — ●MARIUS DOTTER — FH Bielefeld, University of Applied Sciences, Bielefeld, Deutschland

Photovoltaics can be used not only to feed energy into the power grid, but also to provide opportunities for applications on a smaller scale and for the autonomous supply of small electrical devices. In some cases, optimized efficiency can be dispensed with in favor of more cost-

effective variants. Dye-sensitized solar cells (DSSC) offer a good option in this regard. They are also more effective indoors, because of a better conversion of stray light than semiconductor cells. Another idea is to make previously unused areas usable, with textiles such as tarpaulins, umbrellas and awnings being of particular interest. This niche, which has hardly been used so far, is to be filled by a textile DSSC, relying on needleless electrospinning for the textile haptics. This process, in which a polymer solution is formed into fine nanofibers using high voltage, which are then arranged in a disordered manner to form a nanofiber mat, enables simple and industrially scalable production of the DSSC components with a textile feel. In addition, simple production with non-toxic materials can also enable later reuse or simple recycling. In this context, this poster shows the general concept and progress of the work on the front electrode, which is based on a currently submitted paper.

CPP 17.28 Mon 18:00 P3

Exploring the kinetics of pseudo-bilayer architecture formation during sequential deposition via slot die coating — ●JINSHENG ZHANG¹ and PETER MÜLLER-BUSCHBAUM^{1,2} — ¹TUM School of Natural Sciences, Chair for Functional Materials, Garching — ²MLZ, TUM, Garching

Recently, organic solar cells have received increasing attention due to obvious advantages such as flexibility and being lightweight. Among the different types of structures of the active layer, typically planar and bulk heterojunction geometries are used, which introduces intrinsic shortcomings. The newly developed pseudo-bilayer structure can perfectly combine their strengths and circumvent the drawbacks. Unfortunately, most of the pseudo-bilayer are still prepared by spin coating and rarely by printing methods such as slot die coating. Besides these studies mainly focus on selecting solvents, adding third components and studying the vertical morphology. The kinetics of forming the pseudo-bilayer architecture with slot-die coating are still unknown. Here we select the donor acceptor system PM6 and Y6 and the solvents CB and CF. First, PM6 is printed on the substrate and then Y6 is printed on top of PM6. During the deposition, in situ GIWAXS, in situ GISAXS, and in situ UV-vis absorption is carried out to study the formation of the pseudo-bilayer.

CPP 17.29 Mon 18:00 P3

Flash-lamp processing of charge extraction layers for polymer solar cells — ●AURELIEN SOKENG DJOUMESSI^{1,2}, JOSE PRINCE MADALAIMUTHU^{1,2}, SHAHIDUL ALAM^{1,2,3}, AMAN ANAND^{1,2}, ANASTASIA SICHWARDT^{1,2}, PETER FISCHER⁴, ROLAND RÖSCH^{1,2}, ULRICH S. SCHUBERT^{1,2}, and HARALD HOPPE^{1,2} — ¹Laboratory of Organic and Macromolecular Chemistry (IOMC), Friedrich Schiller University Jena, Humboldtstrasse 10, 07743 Jena, Germany — ²Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich Schiller University Jena, Philosophenweg 7a, 07743 Jena, Germany — ³King Abdullah University of Science and Technology (KAUST), KAUST Solar Center (KSC), Physical Sciences and Engineering Division (PSE), Material Science and Engineering Program (MSE), Thuwal 23955-6900, Kingdom of Saudi Arabia — ⁴Institute of Materials Engineering, Technical University of Ilmenau, Gustav-Kirchhoff-Str. 6, 98693 Ilmenau, Germany

Despite the benefits of thermal annealing (TA) in the fabrication of polymer solar cells, the high processing temperatures are not compatible with high throughput manufacturing techniques such as roll-to-roll, which commonly used flexible substrates. Therefore, techniques such as flash lamp annealing (FLA), which do not negatively affect the plastic substrate are needed. Herein, the FLA was successfully applied to PEDOT:PSS and SnO₂ films used as interfacial layers in PM6:Y6-based solar cells, yielding device performances comparable to or even better than the devices treated with TA on a hotplate. Even at prototype size, the FLA is clearly more energy-efficient than the TA.

CPP 17.30 Mon 18:00 P3

Validating novel solar cells in space — ●LUKAS V. SPANIER¹, LENNART K. REB¹, MICHAEL BÖHMER², CHRISTOPH DREISSIGACKER³, ZERUI LI¹, EMANUEL ANWANDER¹, AHMED KRIFA², and PETER MÜLLER-BUSCHBAUM^{1,4} — ¹Technical University of Munich, TUM School of Natural Sciences, Department of Physics, Chair for Functional Materials, Garching, Germany — ²Technical University of Munich, TUM School of Natural Sciences, Department of Physics, Central Technology Laboratory, Garching, Germany — ³Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), Köln, Germany — ⁴Technical University of Munich,

Heinz Maier-Leibnitz Zentrum (MLZ), Garching, Germany

The exploration of the outer solar system so far relied heavily on the use of scarce, highly radioactive plutonium stockpiles for power generation, as traditional solar cells have a too low power-to-mass ratio in low light environments to be suitable for those missions. Latest advances in organic and perovskite solar cells now open up the possibility of utilizing them on lightweight foils as photovoltaic solar sails for efficient power generation in low solar irradiation conditions.

We report the deployment of various organic and hybrid solar cell systems on a sounding rocket and their operation in outer space. We investigate the environmental influences during ascent, exposure to space, and reentry on the photovoltaic performance. We further study and compare the changes in morphology and optoelectronic behavior at various stages during the space mission, isolating different external impact factors.

CPP 17.31 Mon 18:00 P3

In situ study of superlattice self-assembly during slot-die coating of perovskite quantum dot films. — ●DAVID P. KOSBAHN¹, MANUEL A. REUS¹, CHRISTOPHER R. EVERETT¹, GUANGJIU PAN¹, MATTHIAS SCHWARTZKOPF², STEPHAN V. ROTH^{2,3}, and PETER MÜLLER-BUSCHBAUM^{1,4} — ¹TUM School of Natural Sciences, Chair for Functional Materials, Garching — ²DESY, 22607 Hamburg — ³Department of Fibre and Polymer Technology, KTH, Stockholm, Sweden — ⁴MLZ, TUM, Garching

Research into quantum dots (QDs) of metal halide perovskites has become increasingly popular due to their stability and tunable optoelectronic properties. Their controllable surface chemistry and simple preparation make them a promising alternative to bulk perovskite solar cells. The power conversion efficiency of $\text{Cs}_x\text{FA}_{1-x}\text{PbI}_3$ QD solar cells has been steadily rising, up to a recent record efficiency of more than 16%. However, the alignment and self-assembly of the colloidal precursor into a superstructure during film fabrication via slot-die coating is not yet well-understood. In this work, we study the formation of perovskite QD films using in situ grazing-incidence X-ray scattering on different substrates and at different temperatures, to achieve a better understanding of the kinetic processes during solvent evaporation.

CPP 17.32 Mon 18:00 P3

Steady-State Microwave Conductivity (SSMC) on ionic liquid doped lead halide perovskites — ●PATRICK DÖRFLINGER¹, YONG DING², MOHAMMAD KHAJA NAZEERUDDIN², and VLADIMIR DYAKONOV¹ — ¹Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — ²Group for Molecular Engineering of Functional Materials, Institute of Chemical Sciences and Engineering, EPFL Valais, Sion 1950, Switzerland

Knowledge of the charge carrier lifetime and recombination behavior in perovskite solar cells is crucial, as non-radiative recombination processes still limit solar cell efficiencies. Here we present a technique to probe the charge carrier recombination. Of particular interest is the dominant charge carrier recombination pathway, which enables to quantify non-radiative recombination in the perovskite bulk. Furthermore, simultaneous photoluminescence measurements allow for estimating the doping density and determining the radiative efficiency at different charge carrier densities. As an example, the SSMC technique is applied to investigate the influence of ionic liquid additives, which are known to improve the stability of perovskite solar cells and the optoelectronic properties of perovskite absorbers.

CPP 17.33 Mon 18:00 P3

Giant Electrostriction in Lead Halide Perovskite MAPbI_3 Films as Measured with Double-Modulated Interferometry — ●PHILIPP RAMMING¹, MARVIN MALCHAU², EMMA RAULAND¹, ANNA KÖHLER¹, and LOTHAR KADOR² — ¹Experimental Physics II, University of Bayreuth, Germany — ²Institute of Physics and BIMF, University of Bayreuth, Germany

Hybrid lead halide perovskite semiconductor MAPbI_3 and similar materials have attracted much recent interest for photovoltaic devices. Upon application of moderate electrical fields, MAPbI_3 exhibits very large electrostriction effects. The thickness variation was measured with high precision using a double-modulation interferometer set-up. Phase modulation of the laser light and mechanical modulation of the interferometric path difference were employed. With field strengths on the order of 100 kV/cm, the relative thickness change of a polycrystalline film of 1 micron thickness can be as large as several per cent. The electrostriction varies with the square of the field strength;

it is strongest at very low frequencies below one Hertz and decreases quickly at higher frequencies. The effect is compared to recently published data obtained on perovskite single crystals.

CPP 17.34 Mon 18:00 P3

First-principles study of the electronic and optical properties of perovskite solution precursors — ●FRIEDRICH SCHÜTT¹, ANA M. VALENCIA^{1,2}, and CATERINA COCCHI^{1,2} — ¹Carl von Ossietzky Universität, Institut für Physik, Oldenburg, Germany — ²Humboldt-Universität zu Berlin und Iris Adlershof, Berlin, Germany

Metal halide perovskites have shown great promise for next-generation opto-electronic applications but the predominant employment of Pb poses a problem in terms of environmental sustainability of these compounds. Replacing Pb with Sn represents a viable solution, however, despite recent efforts in this direction [1], knowledge of Sn-based perovskites and precursors is to date still insufficient. In a first-principles work based on time-dependent density-functional theory coupled to the polarizable continuum model, we systematically investigate electronic and optical properties of SnI_2M_4 complexes, with M being common solvent molecules. We find that the structural, electronic, and optical properties are strongly affected by the choice of the solvent. By rationalising the behavior of 14 of such compounds even in comparison with lead-halide counterparts [2,3], we provide useful indications to complement experiments in the choice of the solvent molecules for SnI_2 -based solution complexes and in their characterization towards the production of thin films [4].

[1] Di Girolamo et al., ACS Energy Lett. 6, 959 (2021). [2] Schier et al., Phys. Status Sol. B 258, 2100359 (2021). [3] Procida et al., PCCP 23, 21087 (2021). [4] Schütt et al., in preparation.

CPP 17.35 Mon 18:00 P3

In situ Grazing-Incidence Small-Angle X-ray Scattering Observation of TiOx Sputter Deposition on SnO2 Layer for Perovskite Solar Cells Application — ●XIONGZHUO JIANG¹, ZHUIJUN XU¹, YUSUF BULUT^{1,2}, STEPHAN V. ROTH^{2,3}, and PETER MÜLLER-BUSCHBAUM^{1,4} — ¹TUM School of Natural Science, Chair for Functional Materials, 85748 Garching, Germany — ²Deutsches Elektronen-Synchrotron (DESY), 22607 Hamburg, Germany — ³Department of Fibre and Polymer Technology, KTH, Stockholm, Sweden — ⁴MLZ, TUM, 85748 Garching, Germany

It is crucial for the efficiency perovskite solar cells to promote the charge transport and suppress the non-radiation recombination in the hole blocking layer (HBL) and at the interface between the HBL and the active layer. Here, TiOx layers are deposited onto a SnO2 layer via sputter deposition at room temperature, forming a bilayer HBL. The structure evolution of TiOx during sputter deposition is investigated via in situ grazing-incidence small-angle X-ray scattering. After sputter deposition of TiOx with suitable thickness on the SnO2 layer, the bilayer HBL shows a suitable transmittance, smoother surface roughness, fewer surface defects and more suitable energy arrangement with active layer, and thus resulting in a lower trap-assisted recombination at the interface between the HBL and the active layer. With this SnO2/TiOx functional bilayer, the perovskite solar cells exhibit higher power conversion efficiencies than the unmodified SnO2 monolayer devices.

CPP 17.36 Mon 18:00 P3

Interfacial engineering via modifications of the electron blocking layer in PbS quantum dot solar cells — ●TIMO PIECUCH¹, HUAYING ZHONG¹, and PETER MÜLLER-BUSCHBAUM^{1,2} — ¹TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — ²MLZ, TUM, Garching, Germany

Colloidal quantum dot solar cells (CQDSCs) have received tremendous attention as next generation solar cells. Best performances up to 15% power conversion efficiency (PCE) have been achieved using lead sulfide quantum dots in a heterojunction cell architecture. PbS is especially efficient in the infrared region, and thus particularly interesting for future applications like space satellites. Research in the last years mainly has focused on improving the absorber layer and the hole blocking layer, but the potential by improving the electron blocking layer (EBL) has recently aroused increasing interest. In order to reduce interfacial charge carrier recombination and capture the large fraction of long wavelength photons at the EBL/active layer interface, the different interfacial energy-level offsets between EBL and absorber layer, tuned by the EBL-QDs size, are investigated using ultraviolet photoelectron spectroscopy (UPS) and absorption spectroscopy. Furthermore, the corresponding photovoltaic performances are characterized

to demonstrate improved interfacial band alignment.

CPP 17.37 Mon 18:00 P3

PbS Quantum Dot Solar Cells for Space Applications — ●JASPER EBEL¹, HUAYING ZHONG¹, and PETER MÜLLER-BUSCHBAUM^{1,2} — ¹TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — ²MLZ, TUM, Garching, Germany

A key performance parameter for photovoltaics (PVs) on space missions is the power-to-weight ratio since launch costs increase drastically with the mass-to-orbit. During the last decades, several promising, light-weight and flexible alternatives to current silicon- and GaAs-based technology have emerged, such as perovskite, organic or colloidal quantum dot (CQD) based solar cells. Lead sulfide (PbS) CQD solar cells are especially interesting due to their easily size-tunable bandgap range in the infrared regime, allowing for the exploitation of previously unused parts of the solar spectrum. This in conjunction with ligand, solvent and interface-customizable opto-electronic properties makes QD solar cells a promising candidate for tandem solar cells reaching high efficiencies. Here, by mimicking heat and illumination cycles experienced in orbit, we analyse the performance and structural integrity of PbS CQD solar cells under lab conditions to explore the viability of their use for space applications. Repeating this experiment for various solvents, we test a range of devices to investigate their effects on the stability.

CPP 17.38 Mon 18:00 P3

Hybrid Energy Harvester Based on the Combination of Triboelectric Nanogenerator and PbS Quantum Dot Solar Cell — ●TIANXIAO XIAO¹, WEI CHEN¹, WEI CAO¹, and PETER MÜLLER-BUSCHBAUM^{1,2} — ¹TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — ²MLZ, TU München, 85748 Garching, Germany

Developing clean energy lies in the heart of sustainable development of human society. Triboelectric nanogenerator (TENG) originating from Maxwell's displacement current is a new type of energy harvester for harnessing ambient mechanical energy based on the coupling of triboelectrification and electrostatic induction effect. Compared with other counterparts, owing to the light-weight, low-cost, and easy fabrication, TENG has become one of the most promising candidates in replacement of conventional fossil fuels and attracted worldwide attention in the past years. However, to further increase the energy harvesting efficiency and broaden application fields, integrating the TENG with other kinds of energy harvesters in one device is a possible way to meet these needs. In the present work, a TENG based hybrid energy harvester is designed and fabricated on the flexible polyethylene terephthalate (PET) substrate. This hybrid device consists of a single-electrode mode TENG component and a PbS quantum dot (QD) based solar cell component, which can harness both mechanical and solar energy from ambient environment to directly generate electricity.

CPP 17.39 Mon 18:00 P3

Improved surface passivation of AgBiS₂ quantum dots for photovoltaic applications — ●PETAR LOVRIC¹, HUAYING ZHONG¹, and PETER MÜLLER-BUSCHBAUM^{1,2} — ¹TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — ²Heinz Maier-Leibnitz-Zentrum (MLZ), TUM, Garching, Germany

AgBiS₂ colloidal quantum dots (QDs) are a non-toxic alternative for the commonly used PbS QDs for photovoltaic applications. Similar to its PbS QDs, they show great promise due to a tunable bandgap and solution processing, but what makes them stand out is the abundance of materials as well as a high absorption coefficient, which enables to greatly reduce the thickness of the active layer to around 35 nm. Additionally, studies have shown that they are more stable in water and can effectively harvest photons in the near-infrared part of the solar spectrum. One of major issue that impedes the development of AgBiS₂ based photovoltaics is QD surface defects induced recombination losses. Here, we aim to improve the surface passivation of individual QDs and improve the charge transport in the QD films using surface ligand treatment with ZnI, mercaptocarboxylic acid (MPA) and TBAI as surface ligands. The optical and electrical properties of corresponding QDs films are characterized utilizing FTIR, XPS and UPS techniques, and further the corresponding device performances are investigated.

CPP 17.40 Mon 18:00 P3

Effect of ground state charge transfer and photoinduced

charge separation on the energy level alignment at metal halide perovskite / organic charge transport layer interfaces — ●LENNART FROHLOFF¹, FENGSHUO ZU¹, DONGGUEN SHIN¹, and NORBERT KOCH^{1,2} — ¹Institut für Physik & IRIS Adlershof, HU Berlin — ²Helmholtz-Zentrum Berlin

A proper energy level alignment at semiconductor interfaces is of paramount importance for realising high performance in perovskite solar cells. Therefore, we investigated the interface between a modern triple cation perovskite and a prototypical electron acceptor molecule in great detail. Strong band bending on both sides of the junction as well as negatively charged species of the organic molecule were evidenced by the means of photoemission spectroscopy, indicating a ground-state charge rearrangement across the interface. The band bending leads to significantly altered charge extraction offsets as compared to a hypothetical vacuum level alignment and flat band conditions. Additionally, we present direct evidence of a reversible reduction of the electron extraction offset under white light illumination as compared to the dark condition. The energy levels of the organic semiconductor were observed to rigidly shift to lower binding energy by up to 0.26 eV whilst the perovskite energy levels remain essentially unchanged. Consequently, we emphasise the necessity to determine the energy level alignment at interfaces involving perovskites not only in the electronic ground state but also under device operating conditions to allow for a reliable correlation to the performance of the device.

CPP 17.41 Mon 18:00 P3

Active layer aging for the fabricating durable perovskite solar cells with improved reproducibility — ●YUQIN ZOU¹ and PETER MÜLLER-BUSCHBAUM^{1,2} — ¹TUM School of Natural Sciences, Chair for Functional Materials, Garching — ²MLZ, TUM, Garching

Solution processing of semiconductors is a highly promising approach for the fabrication of cost-effective electronic and optoelectronic devices. Although hybrid perovskites have potential in various device applications, challenges remain in the development of high-quality materials with simultaneously improved processing reproducibility and scalability. Here, we report a facile and practical aging treatment method to modulate crystal growth over the entire film to produces homogeneous films with high crystallinity, low defects and full-coverage. The resulting aged perovskite solar cells (PSCs) exhibits superior electronic properties: fast charge carrier transport, efficient charge extraction and low carrier recombination. The average power conversion efficiency (PCE) of MAPI-based PSCs greatly increase from 16.38% to 17.26% with high reproducibility. In addition, the aged PSCs maintain 80% of their initial PCE after 18 hours of operation under ambient and vacuum conditions, respectively, which illustrates their feasibility in scalable fabrication. Aging treatment effectively prevents the uneven performance and low reproducibility of PSCs arising from variations in the preparation environment (temperature, humidity). Thus, this method opens a new and effective avenue to improving the quality of perovskite films and photovoltaic devices in a scalable and reproducible manner.

CPP 17.42 Mon 18:00 P3

Investigating the Impact of Surfactants on Perovskite Film Formation Using In Situ Optical Spectroscopy — ●TOBIAS SIEGERT, SIMON BIBERGER, KONSTANTIN SCHÖTZ, ANNA KÖHLER, and FABIAN PANZER — Soft Matter Optoelectronics (Experimental Physics II), University Bayreuth, Germany

Recent reports have shown that adding surfactants in the solution processing of halide perovskites, e.g. by blade-coating, can improve the morphology and optoelectronic properties of the resulting perovskite sample. In general, the crystallization processes of halide perovskites occurring during thin film formation largely determine the final film morphology. Thus, here we investigate the change in crystallization dynamics upon addition of surfactants to the precursor solution of halide perovskites. We monitor the film formation processes by multimodal optical in situ spectroscopy[1] to gain detailed insights about the film formation process of halide perovskites.[2-4] This finally allows us to elucidate the exact role and the impact of the presence of surfactants during solution processing on the crystallization behavior of the perovskite.

- [1] Buchhorn, Wedler, Panzer. J. Phys. Chem. A 2018
- [2] Chauhan, Zhong, Köhler, Panzer et al. J. Mater. Chem. A. 2020
- [3] Schötz, Greve, Panzer et al. Adv. Optical Mater. 2021
- [4] Biberger, Panzer et al. J. Mater. Chem. A. 2022

CPP 17.43 Mon 18:00 P3

Exploring the impact of nucleation seeds on the defect formation of printed hybrid perovskite films — ●ALTANTULGA BUYAN-ARIVJIKH¹ and PETER MÜLLER-BUSCHBAUM^{1,2} — ¹TUM School of Natural Sciences, Chair for Functional Materials, Garching — ²MLZ, TUM, Garching

In the research of next-generation solar technologies, perovskite-based devices are prominent candidates due to their lucrative power conversion efficiencies and ease of fabrication. Such devices typically contain a polycrystalline perovskite layer grown via various coating methods. Due to the short timeframe of the growth process, the formation of defects is inevitable, leading to increased non-radiative recombination and decreased extraction of photogenerated charge-carriers. One route to counteract the extensive formation of defects would be the addition of external seeds in the precursor solutions, leading to more controlled nucleation and improved crystallinity of the thin film. In this study, different nucleation seeds in the precursor solutions were used for the fabrication of polycrystalline perovskite thin films via slot-die coating. The effect of the seeds on the formation of defects in the film was explored via optical spectroscopical methods such as UV-vis & PL spectroscopy.

CPP 17.44 Mon 18:00 P3

In-situ observation of growth mechanisms during printing of 2D perovskite films — ●KUN SUN¹, RENJUN GUO¹, LINUS F. HUBER¹, MANUEL A. REUS¹, JUNGUI ZHOU¹, MATTHIAS SCHWARTZKOPF², STEPHAN V. ROTH^{2,3}, and PETER MÜLLER-BUSCHBAUM^{1,4} — ¹TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — ²DESY, 22607 Hamburg, Germany — ³Department of Fiber and Polymer Technology, KTH, SE-100 44 Stockholm, Sweden — ⁴MLZ, TUM, 85748 Garching, Germany

Two-dimensional (2D) metal halide perovskites have emerged as a promising candidate for perovskite solar cells (PSCs) due to their remarkable stability compared with their 3D counterparts. However, solution-based spin-coating as fabrication method is not adequate in terms of upscaling. In this regard, the slot-die coating technique, having minimal expenditure and low costs, is a well suitable upscaling method to speed up the commercialization of PSCs. Nevertheless, a fundamental understanding of the film formation during printing is yet not well understood, which causes printed solar cells to stay behind in device efficiencies. Here, we investigate the nucleation and growth of 2D perovskite films during slot-die coating with in-situ grazing incidence wide angle X-ray scattering (GIWAXS) in combination with photoluminescence (PL) during printing. In addition, the crystallite orientation and phase distribution of 2D perovskite containing different dimensionality are well elucidated.

CPP 17.45 Mon 18:00 P3

Design, fabrication and application of PEO-based solid polymer electrolytes for all-solid-state lithium batteries — ●YINGYING YAN¹ and PETER MÜLLER-BUSCHBAUM^{1,2} — ¹TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — ²Heinz Maier-Leibnitz-Zentrum (MLZ), TUM, Garching, Germany

All-solid-state lithium batteries (ASSLBs) have received extensive attention as one of the most promising power sources for flexible and wearable electronics, mainly because of their high flexibility, high energy density and reliable safety. However, the practical application of ASSLBs has been hindered by the poor interfacial stability and inferior ionic conductivity. Therefore, the exploration of advanced solid electrolytes with superior interfacial compatibility/ionic conductivity is an important research topic for all-solid-state batteries. Solid polymer electrolytes (SPEs) exhibit great potential in developing solid-state batteries, specifically for PEO and PEO-based derivatives, because of their superior interfacial compatibility, outstanding solubility against lithium salts, wide electrochemical windows and high ionic conductivity. At the same time, solid fillers, as an important component in SPEs, play a crucial role in determining the overall electrochemical properties. As a consequence, we start from PEO-based materials and prepare SPEs by adding plastic additives and solid fillers with good structure. The electrochemical performance and structural stability of SPEs are elucidated by a combination of electrochemical characterization and morphological structural characterization.

CPP 17.46 Mon 18:00 P3

Study of PEO Composite Electrolyte in All-solid-state Lithium Batteries — ●YUXIN LIANG¹, ZHUIJUN XU¹, KUN SUN¹,

TIANFU GUAN¹, FABIAN A.C. APFELBECK¹, PAN DING², IAN SHARP², MATTHIAS SCHWARTZKOPF³, STEPHAN V. ROTH^{3,4}, and PETER MÜLLER-BUSCHBAUM^{1,5} — ¹TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — ²TUM Walter Schottky Institute, Experimental Semiconductor Physics, Garching, Germany — ³DESY, 22607 Hamburg, Germany — ⁴KTH Royal Institute of Technology, Stockholm Sweden — ⁵MLZ, TUM, 85748 Garching

Lithium batteries (LBs) with composite electrolyte present good ionic conductivity, flexibility and intimate contact with electrodes. However, lithium dendrites will grow and the Coulombic efficiency (CE) will decrease with Li plating and stripping. Moreover, the poly(ethylene oxide) (PEO)-based electrolyte undergoes serious oxidation on the cathode side at high voltage and cause the battery collapse. Strategies have been applied to alleviate the abovementioned challenges, nevertheless, fundamental research on the degradation mechanism of the PEO electrolyte is still lacking. It is of great value to get a deeper understanding and therefore optimize the electrolyte for high voltage LBs. Herein, we select PEO/Al₂O₃ as composite electrode to understand the degradation process. The Li/cathode cells are assembled to observe the battery performance and grazing incidence wide-angle X-ray scattering (GIWAXS) is used to detect morphology changes of the electrolyte before and after cycling.

CPP 17.47 Mon 18:00 P3

Influence of Al₂O₃ concentration in poly(propylene carbonate) based solid polymer electrolyte — ●THIEN AN PHAM^{1,2}, RALPH GILLES¹, and PETER MÜLLER-BUSCHBAUM^{1,2} — ¹MLZ, TUM, Garching, Germany — ²TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany

Solid polymer electrolytes (SPE) have emerged as promising electrolyte material group for all-solid-state batteries that allow the operation with Li metal anodes. Representing one of the main obstacles for Li metal anodes, Li dendrite growth can lead to short circuits which ultimately prevent the usage with liquid electrolytes. SPE offer higher mechanical stability compared to their liquid counterparts and thus, increase the general safety of Li metal batteries.

In this work, poly(propylene carbonate) based solid polymer electrolytes were synthesized with Lithium bis(trifluoromethanesulfonyl)imide (LiTFSI) as Li salt and varying Al₂O₃ concentrations via solution casting. The addition of Al₂O₃ has shown to increase the ionic conductivity of SPEs while simultaneously improve the mechanical stability. Furthermore, small angle X-ray scattering and FTIR were used to study the influence of Al₂O₃ on the structure of the SPE.

CPP 17.48 Mon 18:00 P3

Investigating Thermoelectric Properties of a Sodium-based, Solid Polymer-Electrolyte — ●JULIAN-STEVEN SCHILLING, MAXIMILIAN FRANK, and JENS PFLAUM — Experimental Physics VI, University of Würzburg, 97074 Würzburg

Motivated by the large amount of available waste heat and the need to use energy more efficiently, the development of thermoelectric generators is becoming increasingly important. Their efficiency is characterized by the thermoelectric figure-of-merit z which includes the electrical conductivity σ , the thermal conductivity κ and the Seebeck coefficient S , respectively, and, at a given temperature T , is given by $zT = \frac{S^2\sigma}{\kappa}T$. In contrast to electronic thermoelectric materials, ionic systems promise larger Seebeck coefficients due to lower mobility of the participating charge carriers. Therefore, ionic electrolytes based on organic polymers are of interest due to their expected good thermoelectric performance. In this work, first results on the thermoelectric properties of a methacrylate-based solid polymer electrolyte utilizing sodium as conducting salt are presented. By means of impedance spectroscopy in a frequency range from 100 mHz to 500 kHz we analyzed the mechanisms governing the electrical conductivity in the technologically relevant temperature range from 273K to 353K. Complementary, thermovoltage measurements as function of temperature enable the determination of the Seebeck coefficient and, together with impedance spectroscopy data, reveal strategies how the electronic and ionic transport properties can be modified by the respective salt concentration as well as by the ratio of different carbon-based additives.

CPP 17.49 Mon 18:00 P3

In-situ force measurements on a gold working electrode in lithium-ion electrolytes — ●SABRINA KERZ, THOMAS TILGER, and REGINE VON KLITZING — Department of Physics, Technische Univer-

sität Darmstadt, Darmstadt, 64289, Germany

Batteries have gained a great importance in recent years. They play a vital role in our every-day lives e.g. in mobile-devices and are an important pillar in the transition to renewable energies.

For these applications the solid electrolyte interface (SEI) at electrodes is of great interest. The Gouy-Chapman-Stern (CGS) model describes the interactions of the electrolyte with the charged electrode surface as an interplay between direct adsorption (Stern Layer) and a diffuse double layer. DLVO theory describes the diffuse double layer at the electrode's surface.

In-situ colloidal probe atomic force microscopy (CP-AFM) measures the force between a silica particle and the SEI. The obtained force curves are analyzed using DLVO theory. In a three-electrode setup different potentials are applied between a gold surface (working electrode) and a reference electrode. Thus, changes in the structure of the SEI with varying potentials and salt concentrations are examined.

CPP 17.50 Mon 18:00 P3

High-concentration Lithium-ion Electrolyte Overcomes the Challenges of High-temperature Lithium Batteries — •TIANLE ZHENG^{1,2}, YA-JUN CHENG², and PETER MÜLLER-BUSCHBAUM^{1,3} — ¹TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — ²Ningbo Institute of Materials Technology & Engineering, CAS, Ningbo, 315201, P. R. China — ³TUM, MLZ, 85748 Garching, Germany

Conventional Li-ion batteries are severely constrained in high-temperature applications due to the low thermal stability of the electrolyte/electrode interface and electrolyte decomposition in the cell. Herein, we demonstrate a new electrolyte that achieves an excellent stable long-term cycling at 100 °C, well beyond the typical 60 °C limits of normal conventional Li-ion batteries. High concentrated lithium oxalyldifluoroborate (LiODFB) is selected as the lithium salt with a carefully designed high thermal stability solvent group. As a result, this unique high-concentration electrolyte can promote to form a stable and inorganic solid electrolyte interface layer on the electrode at elevated temperature, leading to improved performance in MCMB/Li and lithium iron phosphate (LFP)/Li half-cells, and achieve reversible capacities of 160 and 350 mA h/g, respectively, with Coulombic efficiencies > 99.3%. Subsequently, we further investigate the mechanism of high concentration LiODFB electrolytes by molecular dynamics simulations and XPS characterization techniques, exploring a new way for future high-temperature electrolytes.

CPP 17.51 Mon 18:00 P3

Morphology Control of Titanium Thin Films in a Low Temperature Process — •GUANGJIU PAN¹, SHANSHAN YIN¹, LINUS F. HUBER¹, CAROLINE EHGARTNER², NICOLA HÜSING², MATTHIAS SCHWARTZKOPF³, STEPHAN V. ROTH^{3,4}, and PETER MÜLLER-BUSCHBAUM^{1,5} — ¹TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — ²Universität Salzburg, 5020 Salzburg, Austria — ³DESY, 22607 Hamburg, Germany — ⁴KTH Royal Institute of Technology, SE 100 44 Stockholm, Sweden — ⁵TUM, MLZ, 85748 Garching, Germany

A low-temperature routine to realize inorganic hole-blocking layers (HBLs) is important for the commercialization of perovskite solar cells. Fabricating HBLs at low temperature is energy-saving and compatible with flexible substrates. In this work, titania thin films are synthesized at low temperature (below 100 Celsius degree) with a polymer template sol-gel method based on the amphiphilic diblock copolymer polystyrene-*b*-polyethylene oxide (PS-*b*-PEO), in combination with selective incorporation of the titanium precursor ethylene glycol-modified titanate (EGMT). A joint process of UV treatment and water-vapor treatment is introduced to substitute the traditional high-temperature calcination. Morphology tailoring of titania thin films in the low-temperature process is achieved by managing phase separation of the polymer template. The surface morphologies of titania films are probed via scanning electron microscopy and GISAXS. The optical properties are examined with ultraviolet-visible spectroscopy and photoluminescence spectra.

CPP 17.52 Mon 18:00 P3

Bilayer formation in liquid-processed mono-functionalized BTBT films — TIM HAWLY, •ANDREAS SPÄTH, MANUEL JOHNSON, MARCUS HALIK, MINGJIAN WU, ERDMANN SPIECKER, and RAINER H. FINK — FAU Erlangen-Nürnberg, Erlangen, Germany

Two-dimensionally (2D) extended thin films of the p-type organic

semiconductor C13-BTBT were fabricated by self-controlled growth at the water-toluene interface. Depicting a compound class originally developed for further functionalization and subsequent realization of self-assembled monolayers (SAMs) or their implementation into SAM-based organic field-effect transistors, the potent BTBT core unit commonly excels in high-quality structure formation as well as charge-transport characteristics. Utilizing various spectromicroscopic tools, we observe extraordinarily crystalline C13-BTBT films with a close to upright standing configuration of the BTBT backbone accounting for superior intermolecular orbital overlap. The well-defined morphology and internal structure of the film are underpinned by superior charge-transport parameters in corresponding OFETs. The inherently favorable membrane-like bilayer molecular arrangement is confirmed by the unambiguous representation of the unit cell as derived from STEM tomography. This study has been funded by the DFG within GRK 1896, the BMBF (contract 05K19WE2) and the Bavarian SolTECH initiative. [1] T. Hawly et al., ACS Adv. Energy Mat.(2022)/doi:10.1021/acsaelm.2c01095

CPP 17.53 Mon 18:00 P3

Characterization of pure DbSeQ thin films and their multilayers with different semiconductor materials — •ANTON PYLYPENKO, ELENA CHULANOVA, ALEXANDER GERLACH, and FRANK SCHREIBER — Universität Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany

Organic semiconductor thin films are widely used in different areas of science and industry, especially for the manufacturing of organic optoelectronic devices. Bilayers of organic semiconductors are of high interest for research due to the possibility of increasing the advantages of blended materials [1]. Prospective candidates for these applications are derivatives of 2,1,3-benzothiadiazole, especially Dibenzoselenadiazoloquinoline (DbSeQ). The heavy atom has a strong impact on the spin-orbit coupling and thus the optical properties of the film. Understanding and investigating mechanisms of growth behavior is a key requirement for optimizing films.

We have investigated thin film growth and templating effects for various bilayers like DbSeQ:PIC or DbSeQ:DIP. The binary thin films are prepared by consistent evaporation of DbSeQ, DIP, and PIC on weakly interacting substrates under ultra-high vacuum conditions. Using ex-situ AFM, UV-VIS, and photoluminescence spectroscopies, X-ray reflectometry, and grazing-incidence wide-angle X-ray scattering, we have observed the morphology, structure, and crystallinity of bilayer films.

[1] A. Hinderhofer, F.Schreiber Chem Phys Chem (2012) 13 628

CPP 17.54 Mon 18:00 P3

Tunable morphologies in charged multiblock terpolymers in thin film geometry: effect of solvent vapor annealing — •BAHAR YAZDANSHENAS¹, FLORIAN A. JUNG¹, TIM BOHNEN¹, SINA ARIAE², DORTHE POSSELT², HEINZ AMENITSCH³, CONSTANTINOS TSITSILIANIS⁴, and CHRISTINE M. PAPADAKIS¹ — ¹Technische Universität München, TUM School of Natural Sciences, Soft Matter Physics group, Garching, Germany — ²Roskilde University, Department of Science and Environment, Roskilde, Denmark — ³Graz University of Technology, Institute of Inorganic Chemistry, Graz, Austria — ⁴University of Patras, Department of Chemical Engineering, Patras, Greece

Thin films of a pentablock terpolymer with an ABCBA architecture of two types of pH-responsive midblocks and short hydrophobic end blocks are investigated. As-prepared spin-coated films from different pH-values have previously shown highly tunable and non-monotonous behavior of the lateral structure sizes, based on the charge [1]. Here, we investigate further accessible morphologies by swelling the films in the vapors of solvents having different selectivity. Results from spectral reflectance, atomic force microscopy, and grazing-incidence small-angle X-ray scattering suggest that a solvent selective for the pH-responsive blocks leaves the nanostructures intact, while a nonselective solvent enables reorganization. Their vapor mixtures are also studied to potentially access further orientations and morphologies. In addition, an ABA triblock copolymer is investigated as a reference. [1] F. A. Jung, C. M. Papadakis et al., Adv. Funct. Mater. 2021, 31, 2102905.

CPP 17.55 Mon 18:00 P3

Computer simulations of liquids in extreme Confinement — •LUCIA MUIGG¹, GERHARD JUNG², THOMAS FRANOSCH¹, and ROLF SCHILLING³ — ¹Institute for Theoretical physics, Universität Innsbruck, Innsbruck, Austria. — ²Laboratoire Charles Coulomb (L2C),

Université de Montpellier, CNRS, 34095 Montpellier, France. —
³Institut für Physik, Johannes Gutenberg-Universität Mainz, Germany.

Computer simulations of a monodisperse hard-sphere liquid confined between two parallel hard walls of accessible width L are performed. By reducing the distance between the walls the two-dimensional limit $L \rightarrow 0$ is approached. An analysis of structural properties, such as the structure factor and the radial distribution function shows convergence to their two-dimensional counterparts, which is in agreement to the theoretical predictions. Furthermore an isobaric-like ensemble, with the slit width as an additional degree of freedom is introduced to study the behavior of the compressibility.

CPP 17.56 Mon 18:00 P3

Exploring the deposition conditions for formation of larger homogeneous colloidal arrays — ●JOANNE NEUMANN, JAN RUBECK, ANDREI CHUMAKOV, and MATTHIAS SCHWARTZKOPF — DESY, Photon Science, Notkestr. 85, D-22607 Hamburg

Installing regular arrays on mesoscopic length scales plays an important role in nanotechnology to create uniform templates for sputter deposition or plasma treatments. Different techniques of self-assembly via solvent evaporation out of dispersions have been used to obtain highly ordered colloidal structures. We used spin-coating, Langmuir-Blodgett (LB) technique and spray-deposition, representing the most attractive tools for the formation of larger homogeneous colloidal arrays on plain substrates. Due to their different deposition and boundary conditions, the assembly behaviour of polystyrene nanoparticles varies, resulting in two-dimensional layers with LB-technique and a large variety of pattern by spray deposition. We present our first results from atomic force microscopy and microbeam grazing incidence small-angle x-ray scattering (GISAXS).

CPP 17.57 Mon 18:00 P3

Incorporation of Nanomaterials to Form Electrically Conductive Multilayers with the Layer-by-Layer Technique — ●MUHAMMAD KHURRAM¹, SVEN NEUBER², ANNEKATRIN SILL³, and CHRISTIANE A. HELM⁴ — ¹muhammad.khurram@uni-greifswald.de — ²sven.neuber@uni-greifswald.de — ³annekatrin.sill@uni-greifswald.de — ⁴helm@uni-greifswald.de

Surface modification of an implant provides an adequate bio-interface and determines which promotes cell adhesion and proliferation. To promote healing, the coating should be electrically conductive. The Layer-by-Layer (LbL) method * sequential adsorption of oppositely charged macromolecules or nanoparticles - has become prominent in coating and functionalizing a surface. Polyelectrolytes show poor charge transfer capabilities; therefore, electrically conductive nanoparticles are essential. MXene nanoparticles are investigated. The MXene contains a high aspect ratio, functional groups, and good electrical conductivity. LbL films are built from polyanion MXene and polycation poly-diallyldimethylammonium (PDADMA). In addition, the conductive and conjugated polymers poly(3,4-ethylene dioxythiophene):poly(styrene sulfonate) (PEDOT:PSS) is used because of their promising electrical properties. PDADMA is again the polycation. With the Atomic Force Microscope (AFM) film morphology and roughness are determined. Layer growth is monitored by UV-Vis Spectroscopy and ellipsometry. The electrical conductivity is determined with the two-point method.

CPP 17.58 Mon 18:00 P3

Band Gap Modification of 2D Covalent-Organic Frameworks (COFs) with Electron Rich and Electron Deficient Molecules — ●LAURA FUCHS, KONRAD MERKEL, and FRANK ORTMANN — School of Natural Sciences, Technische Universität München

A new type of porous materials are covalent-organic frameworks (COFs), which are suitable candidates as active substances for solar cells due to their highly tunable physical and electronic properties.

Introducing electron rich (donor) and electron deficient (acceptor) regions to the molecular structure of 2D-COFs has a significant influence on the energetic levels of the highest occupied (HOMOs) and lowest unoccupied molecular orbitals (LUMOs). We provide insights to construction principles for band gap modifications by comparing the nature of the effect of widely-known electron acceptor and donor molecules[1] on the frontier electronic levels, as well as their impact on the charge density distribution using ab initio calculations within the density functional theory (DFT).

[1]Chua, M. H., Zhu, Q., Tang, T., Shah, K. W., & Xu, J. (2019). Diversity of electron acceptor groups in donor-acceptor type electrochromic conjugated polymers. *Solar Energy Materials and Solar Cells*, 197, 32-75.

CPP 17.59 Mon 18:00 P3

From a Completely Different Angle: Exploring Twistronics in Layered Materials with Atomic Force Microscopy — ●ALEXANDER KLASSEN¹ and JAMES KERFOOT² — ¹Park Systems Europe GmbH Schildkroetstrasse 15,68199 Mannheim, Germany — ²Park Systems UK Limited, MediCity Nottingham Thane Road NG90 8BH, Nottingham, UK

Single atomic layer-based systems emerged as a promising class of materials with unique optical, mechanical, and electronic properties that could provide a pathway to novel applications.^{1,2} Their two-dimensional nature gives rise to a wide range of tunability since their functional properties do not only depend on the type of atoms and bonds within one plane but also on the strain, local defects, and interplay between adjacent layers.^{3,4} Here, we present Atomic Force Microscopy (AFM) based approaches as an ideal toolbox to map various functional properties of 2D materials and heterostructures on a nanometer scale. More specifically, by deterministically breaking and re-stacking single flakes of layered materials, we form homostructures of both hexagonal boron nitride (hBN) and molybdenum disulfide (MoS₂) Investigating ferroelectric superlattices on a hexagonal boron nitride bilayer on a graphene single layer, we can induce domain switching when applying a constant DC potential and study them via Piezoelectric Force Microscopy.^{5,6} We will show how conductive AFM (C-AFM) and Lateral Force Microscopy (LFM) allow imaging strain variations as distorted domains in both the current channel and the lateral force channel.

CPP 17.60 Mon 18:00 P3

Lieb lattice embedded in square polymer — ●YINGYING ZHANG, MIROSLAV POLOŽIJ, and THOMAS HEINE — Faculty of Chemistry and Food Chemistry, TU Dresden, Dresden, Germany

Dirac cone and flat band are exotic band features, which attracted much attention in these years, in which the movement of charge carriers is massless fermions, leading to ultra-high carrier mobility and various quantum Hall effects. Structure in lieb lattice owns these two intriguing bands simultaneously, characterized by one dispersive Dirac band inserted with a flat band, which may give rise to many exotic quantum phenomena such as ferromagnetism, topological states, or superconductivity.

The theoretical TB model predicted that the idea lieb band requires rigorous lattice symmetry and zero next-nearest neighbor (NNN) hopping, making the lieb band rarely found in real materials except widely studied via TB model or photonic and cold-atom. There are only two synthesized structures with lieb band were reported.

Therefore, I studied a systematic square phthalocyanine COF with a defined length of linkers, showing that the lieb band is embedded in square polymer. The Pc-xBz COFs show how the band evolution between square and lieb is based on a series of structures with extending linkers. The band structure and charge density distribution are analyzed to further study the electronic properties. We also show that, by charge doping and atom replacement, the fermi level can be tailored to the lieb band position, making the structure intriguing and potential.