CPP 17: Poster I

Focus Session: Theoretical Modeling and Simulation of Biomolecular Condensates; Hybrid, Organic and Perovskite Optoelectronics and Photovoltaics; Energy Storage Materials and Devices; French-German Session: 2D Materials, Thin Films and Interfaces; Wetting, Fluidics and Liquids at Interfaces and Surfaces

Time: Monday 19:00–21:00 Location: P5

CPP 17.1 Mon 19:00 P5

How do interfaces shape molecular conformations in condensates? — •Nora-Elen Giesinger[1] and Arash Nikoubashman[1,2] — [1]Leibnitz-Institut für Polymerforschung, Dresden, Germany — [2]Technische Universität Dresden, Dresden, Germany

The interface between biomolecular condensates and their surrounding environment plays an important role for, e.g., regulating the condensate's stability and interactions with other cellular components. These interfacial properties are primarily dictated by the density and conformation of the constituent biomolecules, but it remains experientially challenging to resolve interfacial properties on the molecular level. Further, the conformations of the constituent biomolecules are influenced by many intertwined factors like sequence patterning, electrostatics, and chain-length diversity. To understand how polymer conformations evolve from the dense condensate interior through the interfacial region into the surrounding dilute phase, we use a minimal model of fully flexible homopolymers. To disentangle effects arising from chain ends, we examine condensates formed from both linear and ring polymers. Molecular dynamics simulation show that polymers gradually collapse as they transition from the bulk-like interior of the condensate to the surrounding dilute aqueous phase. Notably, the condensate interface induces a highly non-monotonic structural crossover between the dense and dilute regions, irrespective of the polymer architecture: the side facing the interface flattens, while the inward-facing side is also compressed. As a result, the monomer cloud loses its spherical symmetry, and chains tend to align tangentially along the interface.

CPP 17.2 Mon 19:00 P5

Effects of Activity on Polymeric Condensates — •Rahul Yadav[1] and Arash Nikoubashman[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., 01069 Dresden, Germany — [2]Institut für Theoretische Physik, Technische Universität Dresden, 01069 Dresden, Germany

Biological systems are inherently out of equilibrium as external sources of energy are constantly consumed; for example, microtubules and filamentous actin seemingly move through the cytoplasmic matrix via the continuous addition and removal of subunits. At the same time, equilibrium thermodynamic properties, governed by the interactions and length scales of the (macro)molecular constituents, play a central role in phenomena such as the formation of biomolecular condensates. A central open question is whether such non-equilibrium activity enhances phase separation or, conversely, hinders it. To answer this, we performed molecular dynamics simulations of a bead-spring polymer model, systematically varying both the attrac- tion strength and activity. When the active forces act along the contour of the polymer, the miscibility gap narrows and the critical temperature decreases with increasing activity, indicat- ing that this form of activity opposes phase separation. Based on these observations, we expect that contractile active forces will instead broaden the miscibility gap and increase the critical temperature, and we plan to test this prediction in future work.

CPP 17.3 Mon 19:00 P5

Using the Patchy Particle Model to simulate Biomolecular Condensates — •Mubarrat Mursalin[1,2], Simon Dannenberg[1], and Stefan Klumpp[1,2] — [1]Georg August University Göttingen — [2]Max Planck School of Matter to Life

Biomolecular condensates are formed through liquid-liquid phase separation (LLPS) of proteins, often together with nucleic acids, typically driven by low-affinity interactions. Phase separation allows biological systems to spatially organize molecules for biological functions. Theoretical studies of LLPS are usually based on continuum descriptions of fluids, which allows access to the biologically relevant time and length scales, but neglects all molecular details of the interactions, which implements their genetic programmability and determines the local structure of the condensates. Here, we use the coarse grained patchy particles to simulate LLPS, which provides an intermediate level of description between atomistic MD and continuum descriptions, thus allowing to access systems large enough to describe droplets and still retain a coarse-grained picture of the local structure inside the condensate. We look at the effects of repulsive crowding particles on the critical values, dynamics and structures of biomolecular condensates formed by three patch patchy particles. Using NVT simulations, combined with the direct coexistance method, we study the effects of crowder concentration and size, and recreate the known depletion and excluded volume effects.

CPP 17.4 Mon 19:00 P5

Partial demixing of RNA Polymerase II condensates in transcription regulation — Arya Changiarath[1], Rosa Herrera Rodriguez[1], Jasper Michels[3], Friederike Schmid[1], Jan Padeken[2], and •Lukas Stelzl[1,2] — [1]Johannes Gutenberg University Mainz — [2]Institute of Molecular Biology (IMB) — [3]Max Planck Insitute for Polymer Research

Phase-separated condensates may spatio-temporally regulate RNA polymerase II (Pol II) during the transcription of genes. Distinct condensates may underpin the two key stages of transcription, initiation and elongation. However, it remains unclear whether these condensates mix or maintain distinct chemical environments. To investigate this, we combined multi-scale molecular dynamics simulations with experiments in C. elegans. We identified a lower critical solution temperature (LCST) behavior for Pol II, where higher temperatures promote condensation. This behavior correlates with an incremental transcriptional response to temperature but is largely uncoupled from the classical heat stress response. Our simulations demonstrate that the phosphorylation state of the disordered CTD controls the demixing of CTD and pCTD, resulting in full or partial engulfment depending on composition. Remarkably, we observe such partially-demixed of RNA polymerase II condensates by super resolution microscopy of C. elegans embryos. Overall, our results suggest that partially demixed condensates provide distinct chemical environments and binding platforms to facilitate transcription initiation and elongation.

CPP 17.5 Mon 19:00 P5

Optimization of Slot-Die Printed Organic Solar Cells — •Dinusha M. Egalla, Christoph G. Lindenmeir, and Peter Müller-Buschbaum — TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany

Organic solar cells (OSCs) are promising candidates for lightweight, flexible, and low-cost photovoltaic technologies due to their solution processability and compatibility with large-area printing. The performance and stability of printed OSCs, however, are highly influenced by the morphology and uniformity of the active layer, which are sensitive to changes in coating and processing conditions. In this work, we investigate the optimization of printed donor-acceptor active layers by systematically varying key fabrication parameters, including coating temperature, printing speed, and solution preparation. The resulting thin films are characterized using UV-Vis spectroscopy to evaluate optical absorption, and microscopy to investigate the film homogeneity, while X-ray reflectivity (XRR) is used to determine film thickness and roughness. Full devices are built and assessed through current-voltage (J-V) measurements under standard illumination to establish how different printing conditions affect active-layer morphology and overall photovoltaic performance.

CPP 17.6 Mon 19:00 P5

Tuning Two-Photon Absorption Cross Sections in Azaacene Diradicals — •Gabriel Sauter[1], Antonia Papapostolou[2], Julia Weyandt[1], Pascal Merten[3], Kerstin Brödner[3], Uwe H. F. Bunz[3], Andreas Dreuw[2], and Petra Tegeder[1] — [1]Physikalisch-Chemisches Institut — [2]Interdisziplinäres Zentrum für Wissenschaftliches Rechnen — [3]Organisch-Chemisches Institut, Universität Heidelberg

Diradical bithiophene azaacenes have been shown as an outstanding

class of nonlinear optical (NLO) materials with potential applications in bioimaging, photodynamic therapy, and 3D nanoprinting, while exhibiting exceptionally high two-photon absorption (2PA) cross sections exceeding 53000 GM [1]. Using a combined approach of experimental z-scan measurements and theoretical modeling, we analyzed the structure-property relationships governing NLO efficiency and tuning. Here especially the influence of diradical character, molecular extension, and sulfur substitution on the 2PA response was investigated. The results reveal fundamental insights into the synergy between molecular symmetry and electronic structure for optimizing the NLO responses. This enables a more targeted design of near-infrared active materials for photonic applications.
[1] G. Sauter, A. Papapostolou et al., *Angew. Chem. Int. Ed.* 2025, 64, e2503073.

CPP 17.7 Mon 19:00 P5

Long Chain, Strong Gain: How SubPC side chains control the pseudoferroelectric bulk photovoltaic effect — •Kaspar Haas[1], Sophia Klubertz[1], Victor Rodriguez[2], David González-Rodríguez[3], Miguel García Iglesias[2], and Martijn Kemerink[1] — [1]Universität Heidelberg, Heidelberg — [2]Universidad de Cantabria, Santander — [3]Universidad Autónoma de Madrid, Madrid

While most studies of the bulk photovoltaic effect (BPE) in recent years have focused on inorganic materials, this fascinating effect should also be observable in organics. In contrast to the conventional photovoltaic effect, the BPE voids the need for doping by utilizing an intrinsic symmetry breaking and could allow for wider absorption spectra while theoretically overcoming the Shockley-Queisser limit. Going organic holds the additional promise of lightweight, low-fabrication- and low-energy-cost devices, and, particularly, of a much greater tunability of the active material.

Here, we investigate organic molecules of the semiconducting π-conjugated SubPC-F family with the purpose of finding and quantifying a bulk photovoltaic effect. Combining electrical measurements with polarization optical microscopy (POM), XRD and AFM, we investigate the dipole alignment in these liquid crystalline materials, before assessing their photovoltaic performance under irradiation. We further build our own liquid crystal cells for measuring in out-of-plane structures to draw a connection between device thickness and performance. We also aim to quantify the influence of different side chain lengths on material properties like open-circuit voltage and photocurrent.

CPP 17.8 Mon 19:00 P5

Thin Films of Substituted Imidazoquinolines as Emitters for Blue OLED Devices — •Lasse Freitag[1], Pascal Schweitzer[1], Carina Rössiger[2], Thomas Oel[2], Richard Göttlich[2], and Derck Schlettwein[1] — [1]Justus-Liebig-Universität Gießen, Institut für Angewandte Physik, Heinrich-Buff-Ring 16, D-35392 Gießen — [2]Justus-Liebig-Universität Gießen, Institut für Organische Chemie, Heinrich-Buff-Ring 17, D-35392 Gießen

Organic semiconductors are routinely applied in microelectronics. Still challenging is the field of organic blue light emitting diodes (OLED), due to degradation of the emitters. We study the application of imidazoquinolines such as 4EstPhPh(iso)IC as emitters. Different substitutional patterns allow for tuning of their opto-electronic properties. We achieved thin films of 4EstPhPh(iso)IC via physical vapor deposition (PVD). Promising blue photo- and electroluminescence was found in solid state. Film formation at interfaces with contact materials was studied by in-situ Kelvin-probe force microscopy (KPFM). On the p-conducting poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT:PSS) we found a Stranski-Krastanov (SK) growth of the emitter. X-ray diffraction (GI-XRD) confirmed a crystalline structure in these films, in line with single crystal data. Further, the growth of n-conducting bathocuproine (BCP) on the emitter layer was monitored by KPFM, revealing SK growth followed by formation of 3D crystalline islands. As a fundamental prerequisite, morphological stability at air was confirmed by microscopy. Therefore, we built OLED with varying thickness to find the best-performing layer stack.

CPP 17.9 Mon 19:00 P5

The aggregation of DPND dyes in the solid state studied by nuclear magnetic resonance spectroscopy — •Sascha Bartosch[1], Mohamed Bouajhine[2], Łukasz Kielesiński[3], Marieta Levichkova[4], Eva Bittrich[1], Petra Uhlmann[1], Patrick Brocorens[2], Martin Pfeiffer[4], Daniel T. Gryko[3], David Beljonne[2], and Ulrich Scheler[1] — [1]Leibniz-Institut für Polymerforschung Dresden e. V. - Dresden, Germany — [2]Laboratory for Chemistry of Novel Materials, University of Mons - Mons, Belgium — [3]The Institute of Organic Chemistry of the Polish Academy of Sciences - Warsaw, Poland — [4]Heliatek GmbH - Dresden, Germany

Dipyrrolonaphthyridinediones (DNPDs) have recently been introduced as a novel class of cross-conjugated dyes. Their promising photophysical properties make them a potential candidate for various applications. Although the packing type is expected to have an influence on the performance, their aggregation remains to be studied.

Solid-state NMR 1H-1H double-quantum-single-quantum correlation experiments are suitable to probe the spatial proximity of functional groups since it is based on short-range dipolar interactions between the spins. The proximity information is used for the understanding of the packing of molecules. Signals have been assigned by comparison of the experimental to simulated chemical shifts. Strong up-field shifts of aromatic protons induced by packing effects like pi-pi-interactions were observed, consistent with predicted crystal structures. Intermolecular homo couplings were used to identify different aggregation patterns.

CPP 17.10 Mon 19:00 P5

Influence of antisolvents and interfacial layers on charge carrier dynamics of hybrid perovskite films — •Leon Weintz[1], Patrick Dörflinger[1], Volodymyr Vasylkovskyi[1], Junmo Park[2], Hobeom Kim[2], and Vladimir Dyakonov[1] — [1]Experimental Physics 6, University of Würzburg, 97074 Würzburg, Germany — [2]Department of Materials Science and Engineering, Gwangju Institute of Science and Technology, 61005, Gwang-ju, Republic of Korea

Charge carrier behavior in perovskite thin films is crucial to their optoelectronic performance; yet, the impact of antisolvents and self-assembled monolayers (SAMs) on their basic charge carrier transport properties remains not fully understood. In this work, FAPbI$_3$ and FAMACsPbBr$_3$ perovskite systems are investigated to gain a more comprehensive understanding of how processing additives influence charge generation, transport, and recombination. The mobility and lifetime of photogenerated charge carriers in perovskite layers are determined in a non-contact way using Time-Resolved Microwave conductivity (TRMC), where the interaction of an applied electro-magnetic field with the charge carriers results in a time-dependent change in conductance. Complementary time-resolved photoluminescence (trPL) measurements support the interpretation of TRMC-derived carrier dynamics. Together, TRMC and trPL provide insight into how processing additives influence charge-carrier dynamics in perovskite materials.

CPP 17.11 Mon 19:00 P5

Comparative Analysis of Excited-State Dynamics in Thiophene based D-A-Polymers — Tobias Reiker[1], Marek K Charyton[2], Liu Zitong[3], Deqing Zhang[3], Nicolas D. Boscher[2], and •Helmut Zacharias[1] — [1]Center for Soft Nanoscience, University of Münster, Germany — [2]Materials Research and Technology Department, Luxembourg Institute of Science and Technology, Esch-sur-Alzette, Luxembourg — [3]Institute of Chemistry, Chinese Academy of Science, Beijing, China

We investigate the excited state dynamics of conjugated thiophen based polymers using several kinetic models commonly discussed in the literature. These models describe scenarios in which a short lived excited state acts as a precursor for one or more long lived states and are formulated through coupled rate equations. Four representative models were fitted to the dynamics of DPP4T-1 and subsequently applied to pDPP4T, DPP DTT, pF8T2 and pTDPP to identify trends linked to structural variations within the polymer series. This analysis provides a coherent framework for comparing relaxation pathways and for assessing how precursor states influence the formation of long lived excited state populations.

CPP 17.12 Mon 19:00 P5

Tuning the switching response of purely organic photonic devices by polymer blending — •Jinghan Lin, Sebastian Schellhammer, and Sebastian Reineke — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute of Applied Physics, Technische Universität Dresden, Dresden, Germany

Programmable luminescent tags (PLTs) provide a promising photonic technology for UV sensing by utilizing the oxygen-sensitivity of room-temperature phosphorescence (RTP) from purely organic emitters [1]. In the emissive layer, the emitter molecules are diluted at low concentration in a rigid polymer host, like Polystyrene (PS) or

Poly(methyl methacrylate (PMMA), to reduce photonic loss mechanisms, e.g. triplet-triplet annihilation and non-radiative relaxation. Here, we tailor the microenvironment of RTP emitters and, thus, the photophysical characteristics of the emissive layer by blending different polymers. While the blending of PMMA550k with PS350k led to inhomogeneous films with insufficient photophysical properties, mixing of PS350k with PS40k allows the finetuning of the UV dose required to activate the RTP emission in the PLTs. By combining polymers with different physical characteristics, the local matrix rigidity, oxygen permeability, and intermolecular interactions can be varied in a controlled manner. The study demonstrates how polymer-host engineering provides a systematic route to modulate the characteristics of PLTs while maintaining their key characteristics.

[1] Gmelch et al., Science Advances 2019. aau7310

CPP 17.13 Mon 19:00 P5

Unraveling biodegradable phosphorescent emitters by combining quantum chemical simulations with photophysical spectroscopy

— •Philipp Wieland, Iuliia Malakhova, Sebastian Reineke, and Sebastian Schellhammer — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute of Applied Physics, Technische Universität Dresden

Naturally derived organic emitters are required for the design of efficient biodegradable photonic devices. For instance, quinoline alkaloids exhibit sufficient emission via room-temperature phosphorescence (RTP), enabling their successful application in programmable luminescent tags for sustainable information storage [1]. Despite minimal structural differences between specific emitters of this quinoline alkaloid material family, they result in very different device performances.

In this work we present a combined experimental and computational characterization of RTP-active quinoline alkaloids, aiming to improve the understanding of their structure-property relationship. Photoluminescence analysis of quinine and cinchonine shows that phosphorescence dominates as the radiation process in cinchonine, whereas fluorescence is much more pronounced in quinine. To understand the origin of these differences, Density Functional Theory simulations are conducted. Conventional modelling approaches typically rely on static descriptions, which, while efficient, fail to capture the behavior of highly dynamic molecules. To overcome this limitation, we explicitly incorporate Molecular Dynamics into the screening of excited state properties. [1] Thomas et al. Adv. Mater. 2024, 36, 2310674.

CPP 17.14 Mon 19:00 P5

Stabilization via Confinement of Halide Perovskites

— •Marius Kaiser[1], Osama Alsheika[2], Helen Grüninger[2], and Eva M. Herzig[1] — [1]Dynamik- und Strukturbildung - Herzig Group, University of Bayreuth, Germany — [2]Bavarian Center for Battery Technology (BayBatt) and Inorganic Chemistry, University of Bayreuth

The practical use of halide perovskites (HPs) for optoelectronic applications is severely limited by degradation caused by intense light exposure, heat, and unintended ion transport under external electric fields [1]. Key challenges in this field include understanding the underlying mechanisms, stabilizing the semiconductor, and achieving controlled electron and ion transport.

Methylammonium lead bromide (MAPbBr3) is used as a model system, and its lattice parameters are systematically investigated in both bulk form and when confined within SBA-15 silica nanopores (average diameter ~8.4 nm), across a range of temperatures and pore loadings.

Furthermore, we examine thermal expansion behaviour of the materials and evaluate the effect of surface functionalization.

These results provide valuable insights for the development of more stable HP-based optoelectronic devices with directionally controlled charge transport.

[1] Greve, C. et al. To Stop or to Shuttle Halides? The Role of an Ionic Liquid in Thermal Halide Mixing of Hybrid Perovskites. ACS Energy Lett. 8 (2023).

CPP 17.15 Mon 19:00 P5

Early-Stage Growth and Morphological Evolution of Ag Electrodes during Sputter Deposition on PDINN

— •Doan Duy Ky Le[1], Kristian Reck[2], Benedikt Sochor[3], Thomas Strunskus[2], Jungui Zhou[3], Anuragk Keloth[3], Lyuyang Cheng[1], Sarathal Koyiloth Vayalil[3], Stephan V. Roth[3], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]CAU, Kiel, Germany — [3]DESY, Hamburg, Germany

The integration of sputtered metal electrodes with organic interlayers remains a key challenge for the scalable fabrication of organic solar cells (OSCs). PDINN is an efficient cathode interlayer, yet its behavior under sputter deposition is not well understood. Here, we use *in situ* GISAXS to resolve the nanoscale morphological evolution of Ag during direct-current magnetron sputtering (DCMS) onto PDINN thin films. Time-resolved scattering reveals distinct early-stage growth regimes, including the nucleation of small Ag clusters, their coalescence into medium-sized species, and the formation of laterally connected domains. Compared to thermally evaporated Ag, sputtered Ag achieves continuous coverage at significantly reduced thickness. These findings confirm the feasibility of sputter-deposited Ag/PDINN interfaces and establish a foundation for scalable electrode fabrication in next-generation OSCs.

CPP 17.16 Mon 19:00 P5

Spin-Sensitive Spectroscopy of TADF OLEDs

— •Andreas Kohrmann, Ahmed Mohamed, Vladimir Dyakonov, and Andreas Sperlich — Experimental Physics 6, University of Würzburg, 97074 Würzburg, Germany

The performance of the blue emitter ν-DABNA in thermally activated delayed fluorescence (TADF) organic light-emitting diodes (OLEDs) is closely related to the dynamics of triplet excitons. In optically excited host-guest thin films, triplet states are generated and evolve through the intricate interplay of triplet diffusion, triplet recombination, and triplet-triplet annihilation (TTA). Thereby TTA and triplet diffusion are inherently host-dependent. Consequently, the host environment exerts a pivotal influence on exciton loss and delayed emission pathways. We used spin-sensitive optical spectroscopy, specifically photoluminescence-detected magnetic resonance (PLDMR) to examine the spin nature of the singlet-triplet interaction in optically excited host-guest thin films. Correlating these with exciton kinetics from transient photoluminescence (trPL) yields insights on the luminescence as well as the formation, diffusion, and annihilation of triplet excitons. The findings of this study offer a more profound understanding of the triplet harvesting mechanisms in TADF emitters. Additionally, they offer guidance for host selection strategies that are intended to enhance the efficiency and stability of the devices.

CPP 17.17 Mon 19:00 P5

Excimers in carbazole-substituted 4NICz TADF emitters: from frozen solution to films.

— •Anatolii Kuimov[1], Oliver Lee[2], Eli Zysman-Colman[2], and Anna Köhler[1] — [1]Soft Matter Optoelectronics, University of Bayreuth, 95440 Bayreuth, Germany. — [2]Organic Semiconductor Centre, EaStCHEM School of Chemistry, University of St Andrews, St Andrews, UK, KY16 9ST

To obtain high brightnesses in OLEDs, emitters need to be packed sufficiently densely for good charge transport. However, too close a proximity between chromophores can lead to the formation of excimers. We investigate under which conditions such excimers are formed in carbazole-substituted 4NICz blue emitters and how this formation can be controlled. In dilute solution at room temperature, we see only emission from non-interacting molecules, whereas in frozen glass a weak red-shifted emission band appears that grows with laser intensity. A similar increase is observed in films. We attribute excimer formation in the glass and in films to structural reorganization after local heating that results from the absorption of the laser pulses.

CPP 17.18 Mon 19:00 P5

Bulk-Heterojunction Morphology Engineering in D18:Y6 Solar Cells

— •Dennis Straub, Lixing Li, and Peter Müller-Buschbaum — TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany

Organic solar cells based on non-fullerene acceptors have attracted considerable interest due to their favourable optoelectronic properties and compatibility with low-temperature solution processing. In this work, the D18 polymer donor and the non-fullerene acceptor Y6 (BTP-4F) are used as the active layer materials. The study investigates how variations in fabrication parameters influence the evolution of the bulk-heterojunction morphology and the resulting photovoltaic behaviour. Key factors examined include solvent choice, wet-film formation, drying kinetics, and thermal treatment, which govern phase separation, domain purity, and molecular ordering within the active layer.

To further explore morphology control, selected additives are introduced that may affect miscibility, aggregation, and domain formation. Their influence on the structural organisation of the D18:Y6 blend is analysed to determine how additive-induced morphological changes impact charge generation, transport pathways, and recombination processes. By correlating structural characteristics with device performance, this work aims to clarify how processing and material modification shape the efficiency and reproducibility of D18:Y6 organic solar cells and to provide guidance for future optimisation.

CPP 17.19 Mon 19:00 P5

Spray Engineering for High-Efficiency Organic Solar Cells — •Xinyu Jiang[1], Kang An[2], Nadja Koelpin[1], Ning Li[2], and Stephan V. Roth[1,3] — [1]Deutsches Elektronen-Synchrotron DESY, Notkestraße 85, 22607 Hamburg — [2]Institute of PolymerOptoelectronic Materials and Devices, State Key Laboratory of Luminescent Materials and Devices, South China University of Technology (SCUT), Guangzhou, Guangdong 510641, China — [3]Department of Fibre and Polymer Technology, KTH Royal Institute of Technology,Teknikringen 56-58, SE-100 44 Stockholm, Sweden

Spray coating has emerged as a powerful and scalable technique for fabricating high-performance organic solar cells (OSCs), offering precise control over ink deposition and rapid compatibility with large-area manufacturing. Compared with conventional solution-processing methods, spray deposition enables fine tuning of droplet dynamics, solvent evaporation, and wet-film thickness, which are critical for achieving optimal phase separation and molecular ordering in the active layer. In this work, we demonstrate that rational engineering of spray parameters such as atomization rate, nozzle substrate distance, carrier-gas flow, and solvent volatility significantly improves film uniformity and reduces morphological defects, leading to enhanced charge transport and suppressed recombination losses. By integrating these optimized spray processes, the resulting OSCs exhibit markedly improved device efficiency and excellent reproducibility across enlarged areas. These results highlight spray coating as a highly efficient and industry-ready pathway for the scalable integration of organic solar cells.

CPP 17.20 Mon 19:00 P5

Narrowband organic Photodetectors with J-Aggregate materials — •Angelina Stoer[1], Jakob Wolansky[1], Matthias Stolte[2], Frank Würthner[2], Karl Leo[1], and Johannes Benduhn[1] — [1]Institut für Angewandte Physik und Photonik, TU Dresden — [2]Institut für Organische Chemie, Universität Würzburg

With the development of organic photodetectors, new opportunities for narrowband photodetection have emerged. Instead of relying on costly and unwieldy optical filters, the molecular structure of organic materials can be chemically tailored to tune their absorption range. Recently, the material class of merocyanine dyes has been investigated as a promising candidate for this purpose, exhibiting favorable absorption properties. By post-annealing these dyes, the molecules can rearrange and form J-aggregated thin films, resulting in a narrowband absorption spectrum due to the intermolecular interactions.

In this work, the merocyanine dye 1(Hex) is used in fully vapor-deposited organic photodetectors. Narrowband detection with a FWHM as low as 15 nm could be realized at a center wavelength of 755 nm. Through careful optimization of the heating conditions and device structure, a notable external quantum efficiency was achieved, accompanied by very low noise at zero voltage. Based on this, the resulting specific detectivity exceeds 10^{12} Jones. The comprehensive photodetector characterization is complemented by an in-depth analysis of changes in the thin film‘s morphology and energetics induced by the J-aggregation formation process.

CPP 17.21 Mon 19:00 P5

Nanoscale Structural and Electronic Characterization of the DTDCPB:C70 donor-acceptor system for vacuum-deposited organic solar cells — •Milena Merkel[1,2], Jan ter Glane[1,2], and Harry Mönig[1,2] — [1]Institute of Physics, University of Münster, Münster, Germany — [2]Center for Nanotechnology (CeNTech), Münster, Germany

The active layer of organic solar cells is produced either by solution-processing or vacuum thermal evaporation. While solution-processed cells have achieved higher efficiencies to date, vacuum-deposited cells exhibit higher morphological stability and thus a longer durability. For a future commercialization of organic solar cells, where both efficiency and durability are crucial, understanding the current limitations of vacuum-deposited cells is thus of major interest.

Cells based on an active layer made of the DTDCPB:C70 donor-acceptor system have so far achieved one of the highest efficiencies in the group of vacuum-deposited organic solar cells, while also exhibiting high durability [1,2]. We used a combined approach of high-resolution scanning tunneling microscopy and spectroscopy to investigate the structural and electronic properties of assemblies of these donor and acceptor molecules deposited on single-crystalline substrates, as well as of their lateral and vertical interfaces.

[1] Griffith et al., Phys. Rev. B 92, 085404 (2015)
[2] Zou et al., J. Mater. Chem. A 2, 12397 (2014)

CPP 17.22 Mon 19:00 P5

Interfacial modification of transport layers for enhancing the performance and stability of organic solar cells — •Saib Jahan Qazi[1,2], Md. Moidul Islam[1,2], Md. Zobaer Ahmed Rahat[1,2], Md. Farhatul Hassan[1,2], Ulrich S. Schubert[1,2], and Harald Hoppe[1,2] — [1]Laboratory of Organic and Macromolecular Chemistry (IOMC Jena), Friedrich Schiller- University Jena, Jena, Germany — [2]Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich-Schiller-University Jena, Jena, Germany

Organic solar cells are emerging as promising prospects in the field of solar energy technology due to their low-cost, lightweight and simple roll to roll fabrication properties. A record power conversion efficiency above 19% has already been reported. However, long-term stability is still the main obstacle for commercialization due to inherent instability particularly at the interfaces. In this study, we demonstrate solution processed interfacial modification of zinc oxide (ZnO). ZnO is widely used in organic solar cells for electron extraction, but it brings performance and lifetime limitations due to surface defects and photochemical reactions under UV exposure, which generates radicals resulting into accelerated degradation of the photoactive layer in the device. Here we compare approaches using organic acids with polysilazane, for successful ZnO passivation.

CPP 17.23 Mon 19:00 P5

Simulation of Pump-Probe Spectra Including Linear Vibronic Coupling – A Study on Naphthalene Diimide — •Matthias Knechtges, Maximilian F. X. Dorfner, and Frank Ortmann — Department of Chemistry, TUM School of Natural Sciences, and Atomistic Modeling Center, Munich Data Science Institute, Technical University of Munich, München, Germany

Non-linear optical techniques such as pump-probe spectroscopy provide insight into the dynamical processes governing excited-state evolution, which are often influenced by electron-vibrational interactions. The theoretical computation of pump-probe spectra remains an open research field [1] due to the complicated treatment of coupled electronic and nuclear dynamics, which require feasible but accurate approximations [2]. In particular, including the full quantum nature of the nuclei remains a major challenge.

In this contribution, we present a framework for calculating pump-probe spectra of molecules based on an analytic linear electron-vibrational coupling model. Evaluating the third-order response function in the Franck-Condon approximation and including vibrational transitions enables us to predict the pump-probe signal in the infrared region as well. We apply this to the Naphthalene Diimide molecule, a building block for a prospective solar cell material.

[1] Gelin, M., et al., Comp. Mol. Sc. (2025); [2] Park, J. W., et al., J. Chem. Theory Comput. (2017)

CPP 17.24 Mon 19:00 P5

QD-based hybrid organic photo detectors for narrowband IR sensing — •Johann Demel[1], Louis Conrad Winkler[1,3], Andrey Iodchik[2], Moritz Flemming[1], Tobias Antrack[1], Karl Leo[1], and Johannes Benduhn[1,3] — [1]IAP, TU Dresden — [2]Chemistry, TU Dresden — [3]German Center for Astrophysics

The ability to detect infrared radiation is relevant across a multitude of fields. Autonomous driving and deep space exploration utilize its ability to propagate long distances with little absorption losses. While, e.g., medical diagnostics can profit from its penetration depth into biological tissue. Organic materials have proven to be a viable platform for photo detection, with advantages such as low-cost fabrication, flexible devices, and tunable absorption; however, their IR absorption capabilities are limited.

This work presents a hybrid structure combining organic transport layers and PbS nanoparticles into optical microcavities. Based on transfer-matrix simulations, the resonance wavelength of the stack can be precisely predicted and tuned by adjusting the thickness of the organic transport layers. By combining precise thermal evaporation of the organic layers with interface assembly to incorporate nanoparticle layers into the stack, wavelength-selective devices are achieved whose resonance feature can be tuned from 750 nm up to 1800 nm. This expands the advantageous properties of the organic device framework by the wavelength-tunable IR absorption capabilities of semiconductor nanoparticles, leading to devices with specific detectivity values D^* of $10^{11}\ cm \cdot \sqrt{Hz} \cdot W^{-1}$ (based on noise measurements).

CPP 17.25 Mon 19:00 P5

Heat induced morphological changes in P3HT:PCBM solar cells — •Jose Prince Madalaimuthu[1,2], Edward Wijaya[1,2,3], Ulrich S Schubert[1,2], and Harald Hoppe[1,2] — [1]Laboratory of Organic and Macromolecular Chemistry (IOMC Jena), Friedrich-Schiller-Universität Jena, Germany — [2]Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich-Schiller-Universität Jena, Germany — [3]Department of Chemical Engineering, Swiss German University, 15143 Tangerang, Indonesia

Organic solar cells are becoming an important technology for next-generation energy applications since they can be made into flexible and lightweight devices. However, attaining thermal stability remains a significant challenge for its actual deployment. Heat-induced morphological alterations within the photoactive layer typically led to considerable performance reductions. It's interesting to note that this effect may be reversed in some circumstances. Our investigations on P3HT:PCBM solar cells show that devices subjected to high-temperature exposure (up to 250°C) demonstrated substantial performance recovery upon cooling. Thermally driven and reversible morphological change in the active layer was demonstrated by photoluminescence analysis.

CPP 17.26 Mon 19:00 P5

Trace Intrinsically Microporous Polymer Additives Induce LiF-Rich SEI for Enhanced Performance of Silicon-Based Lithium-Ion Batteries — •Ming Yang[1], Ruoxuan Qi[1], Ya-Jun Cheng[2], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]College of Renewable Energy, Hohai University, Changzhou, Jiangsu Province, P. R. China

Silicon-carbon (Si/C) composite anodes are promising candidates for high-energy-density lithium-ion batteries due to the high theoretical capacity of silicon. However, their practical application is hindered by severe volume expansion and unstable solid electrolyte interphase (SEI) formation during cycling. Fluoroethylene carbonate (FEC) is commonly used to improve interfacial stability, but its effectiveness is limited by concentration sensitivity and uncontrollable side reactions. This study introduced carboxyl-functionalised intrinsically microporous polymer (PIM-COOH) as a functional additive, achieving dual regulation of electrode structural evolution and interfacial chemistry. Only 0.5wt% PIM-COOH is required to achieve these effects. The Si/C@PIM||Li half-cell retains 90% of its capacity after 300 cycles at 1.0 C, demonstrating excellent long-term stability. The utilisation of 1Ah NCM811-Si/C pouch cells demonstrates its commercial potential. These results demonstrate a scalable and effective strategy for stabilizing silicon-based anodes, offering valuable insight into the design of next-generation lithium-ion batteries with both high energy density and long cycle life.

CPP 17.27 Mon 19:00 P5

In-situ WAXS observation of 3D porous electrodeposition Cu in lithium-metal batteries — •Lyuyang Cheng[1], Zhuijun Xu[1], Yingying Yan[1], Fabian Apfelbeck[1], Yuxin Liang[1], Anton Davydok[3], Christina Krywka[3], Yajun Cheng[2], and Peter Müller-buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]Hohai University, 213022 Changzhou, China — [3]Helmholtz-Zentrum Hereon, 21502 Geesthacht, Germany

Lithium (Li) metal is the ultimate anode for rechargeable batteries. Its high specific capacity (3860 mAh/kg) and low voltage warrant optimal cell energy density. However, these anodes rely on repeated plating and stripping of Li, which leads to consumption of Li and the growth of dendrites that can lead to self-discharge and safety issues. To address these issues and problems, a number of different porous conductive scaffolds have been reported to create high surface area electrodes on which Li can be plated reliably. While impressive results have been reported in literature, current processes typically rely on either expensive or poorly scalable techniques. Herein, we report a scalable fabrication method to create porous Cu anodes using a one-step electrodeposition process. The areal loading, pore structure, and electrode thickness can be tuned by changing the electrodeposition parameters, and we illustrate the in-situ nano WAXS images with lithium growth, which can help to explain the mechanism. We also provide a feasible method to fabricate the porous Cu cathodes with different electrodeposition solution concentrations.

CPP 17.28 Mon 19:00 P5

Ionic-Liquid-Regulated PVC-Based Solid Polymer Electrolyte for High-Performance Lithium Metal Batteries — •Jiaqi Ding and Peter Müller-Buschbaum — TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany

Lithium metal batteries (LMBs) are regarded as one of the most promising next-generation energy-storage systems owing to their ultrahigh theoretical capacity. However, the safety issues associated with conventional liquid electrolytes, including dendrite-induced short circuits and interfacial instability, severely hinder their practical application. Solid polymer electrolytes (SPEs) offer a potential pathway to address these challenges. In this work, we develop a poly(vinyl carbonate) (PVC)-based solid polymer electrolyte incorporating the ionic liquid [EMI][TFSI] to enhance both ion transport and mechanical integrity. Structural and electrochemical characterizations show that the ionic liquid effectively regulates ion transport within the polymer matrix, enabling the formation of continuous Li ion conduction pathways and improving the compatibility of the electrolyte with lithium metal. This tailored ion-transport behavior leads to enhanced ionic conductivity, mitigated interfacial degradation, and significantly extended cycling stability in LMBs. The results highlight the critical role of ionic-liquid modification in tuning transport properties of polymer electrolytes and provide a viable materials strategy for high-performance lithium metal batteries.

CPP 17.29 Mon 19:00 P5

Investigation of the Effects of LiDFOB Salt Concentration on the Fast-Charging Performance of LiCoO2 Cathodes — •Yifeng Liu, Ming Yang, and Peter Müller-Buschbaum — TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany

Fast-charging lithium-ion batteries have drawn increasing interest, yet lithium cobalt oxide ($LiCoO_2$) paired with commercial electrolytes generally suffers from severe capacity fading and limited cycle life at high charging rates. This study aims to explore strategies for improving capacity retention of $LiCoO_2$-based lithium-ion batteries under fast-charging conditions. We employ boron-containing lithium salt LiDFOB as an electrolyte additive and systematically investigate its concentration-dependent effects on the capacity retention of LCO cells under fast-charging operation. Interfacial stability and charge-transfer kinetics associated with different LiDFOB levels are evaluated through cyclic voltammetry (CV), linear sweep voltammetry (LSV), Tafel analysis, and chronoamperometry (CA). The results show that the concentration of LiDFOB has a pronounced influence on the cycling performance. In particular, the optimized LiDFOB concentration enables the LCO cells to stably cycle for over 1000 cycles at 1C and 3C, benefiting from the improved interfacial stability and enhanced Li^+ transference number. Morphological and material characterizations further reveal that different LiDFOB concentrations generate SEI films with distinct compositions and structures, which account for the disparities in fast-charging capacity retention.

CPP 17.30 Mon 19:00 P5

High-Power Continuous Laser-Guided Synthesis of Bimetallic Metal-Organic Framework (NiCoMOF) Structures and Their Composites: Photophysical, Photochemical, and Electrical Characterization — •Saliha MUTLU[1,2], Bülend ORTAÇ[2], Ali KARATUTLU[2,3], Nergis ARSU[4], and Sevil SAVAŞKAN YILMAZ[1,2] — [1]Karadeniz Technical University Chemistry Department, Trabzon, Türkiye — [2]Bilkent University, Institute of Materials Science Nanotechnology and National Nanotechnology Research Center (UNAM), Ankara, 06800 Turkey — [3]Sivas University of Science and Technology, Department of Engineering Basic Sciences, Sivas, 58100 Turkey — [4]Department of Chemistry, Yildiz Technical University, Davutpasa Campus, Istanbul 34210, Turkey;

Metal-organic frameworks (MOFs) are among the most innovative breakthroughs in chemistry and materials science. In this study, the first bimetallic synthesis of MOFs was achieved using the high-power laser-induced rapid synthesis (LIRS) method via two different ligand and metal salt combinations with different π-conjugated linkers. The synthesis of NiCo-MOF structures (in 1:2 and 2:1 ratios) was completed in just 70 minutes using the LIRS method. Furthermore, the synthesis of MOF composites (rGO/MOF) containing reduced graphene oxide (rGO) was also achieved for the first time. On top of these, the electrical properties of the epoxy acrylate-based MOF and rGO@MOF composites prepared by in situ photopolymerization were investigated in detail. This study was supported by TÜBITAK-BIDEB 2211-A National PhD Scholarship Programs.

CPP 17.31 Mon 19:00 P5

A gel polymer electrolyte interface layer-amphiphilic polymer/salt composite nanoarray for lithium metal batteries — •Thomas Bullinger, Ming Yang, and Peter Müller-Buschbaum — TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany

Research on lithium-ion batteries has been focused on improving energy density, which is mainly limited by conventional graphite anodes. Therefore, lithium metal has emerged as a desirable anode material due to its high energy density. However, it easily reacts during cycling, thus forming lithium dendrites, which can lead to short-circuiting of the battery. As liquid electrolytes cannot solve this problem, solid-state polymer electrolytes have shown promise as an alternative, but their ionic conductivity at room temperature limits their practical use, leading to the compromise of gel polymer electrolytes. In this project the block copolymer P2VP-b-PEO together with the lithium salt lithium nitrate, both dissolved in tetrahydrofuran (THF), surprisingly lead to the solvent phase changing to a gel polymer, which was then used as the electrolyte in coin cells. For the cycling and rate performance tests, Li||LFP batteries were investigated. Further experiments include cycling voltammetry (CV), linear sweep voltammetry (LSV), Tafel curves and impedance spectroscopy.

CPP 17.32 Mon 19:00 P5

In-situ interface film forming on the high-voltage LiCoO2 cathode by a tiny amount of nanoporous polymer additives — •Ruoxuan Qi[1], Ming Yang[1], Tianle Zheng[1], Xingchen Liu[2], Yonggao Xia[2], Ya-Jun Cheng[2,3], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]NIMTE, CAS, Zhejiang Province, P. R. China — [3]College of Renewable Energy, Hohai University, Jiangsu Province, P. R. China

The LiCoO2 (LCO) cathode has been foreseen for extensive commercial applications owing to its high specific capacity and stability. Therefore, there has been considerable interest in further enhancing its specific capacity by increasing the charging voltage. However, single-crystal LCO suffers from a significant capacity degradation when charged to 4.5 V due to the irreversible phase transition and unstable structure. Herein, an ultra-small amount (0.5 wt% in the electrode) of multi-functional PIM-1 (a polymer with intrinsic microporosity) additive is utilized to prepare a kind of binder-free electrode. PIM-1 modulates the solvation structure of LiPF6 due to its unique structure, which helps to form a stable, robust, and inorganic-rich CEI layer on the surface of LCO at a high voltage of 4.5 V. This reduces the irreversible phase transition of LCO, thereby enhancing the cyclic stability and improving the rate performance, providing new perspectives for the electrodes fabrication and improving LCO-based high-energy-density cathodes.

CPP 17.33 Mon 19:00 P5

Effects of differently sized and shaped active and passive Filler for PVDF-HFP CPEs in All Solid-State Lithium-Ion Batteries — •Daniel Karlinger, Yuxin Liang, and Peter Müller-Buschbaum — TUM School of Natural Sciences, Chair for Functional Materials, Graching, Germany

All-solid-state lithium-ion batteries are regarded as highly promising due to their enhanced safety and potentially higher energy density compared to conventional cells with liquid electrolytes. In this project, solid polymer electrolytes based on PVDF-HFP are investigated with the aim of improving ionic conductivity and overall electrochemical performance. The approach is to incorporate combinations of ac tive and passive fillers to tailor the material properties. Conductivity and mechanical stability will be systematically examined with cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS), X ray diffraction (XRD) and other methods, in order to identify opti mized compositions for solid-state battery applications.

CPP 17.34 Mon 19:00 P5

Tracing the Path from Solvation to Transport in Lithium and Sodium Electrolytes — •Chinwendu Nancy Anabaraonye[1,2], Diddo Diddens[3], and Andreas Heuer[1,2] — [1]Institute of Physical Chemistry, University of Münster, Corrensstraße 28/30, 48149 Münster, Germany — [2]International Graduate School for Battery Chemistry, Characterization, Analysis, Recycling and Application (BACCARA), University of Münster, Corrensstr. 40, 48149 Münster, Germany — [3]Forschungszentrum Jülich GmbH, Helmholtz-Institute Münster (IMD-4), Corrensstraße 48, 48149 Münster, Germany

Advancing technology continues to increase demands on energy storage devices and their performance requirements. Over the years, lithium-ion batteries have consistently remained the market leader. However, their long-term sustainability remains questionable due to the limited lithium reserves. Therefore, there is need for increased research toward alternative battery chemistries, among which are sodium-ion batteries. The present work is a comparative study of the transport properties of lithium hexafluorophosphate (LiPF6) and sodium hexafluorophosphate (NaPF6) in carbonate electrolytes consisting of ethylene carbonate (EC) and ethyl methyl carbonate (EMC). Based on molecular dynamics simulations, we analyse the influence of EC ratio and salt concentrations on the solvation structure with particular focus on the formation of contact ion pairs (CIP), solvent-seperated ion pairs (SSIP) and ion aggregates and how this correlates with the ionic transports within the systems.

CPP 17.35 Mon 19:00 P5

Modeling Electron Transfer at Electrode-Electrolyte Interfaces — •Joshua Krieger[1,2,3], Johannes Tölle[4,5,3], Diddo Diddens[2,6], and Andreas Heuer[2,6] — [1]International Graduate School BACCARA, University of Münster, 48149 Münster, Germany — [2]Institute for Physical Chemistry, University of Münster, Münster, Germany, 48149 Münster, Germany — [3]Center for Multiscale Theory and Computation (CMTC), University of Münster, 48149 Münster, Germany — [4]Department of Chemistry, University of Hamburg, 22761 Hamburg, Germany — [5]The Hamburg Centre for Ultrafast Imaging (CUI), 22761 Hamburg, Germany — [6]Helmholtz Institute Münster - Forschungszentrum Jülich GmbH (IEK 12), 48149 Münster, Germany

The solid electrolyte interphase (SEI) is an important component in rechargeable battery performance and lifetime, but the complex mechanisms behind its formation are still not yet fully understood. Accurate electron-transfer (ET) rates are important for simulating SEI growth, e.g. using reactive molecular dynamics simulations that require electrolyte reduction rates. To obtain the ET rates, we investigate a simplified Anderson impurity-type model designed to describe non-equilibrium electron transfer between an electrode and the redox-active species under an applied potential. This framework enables systematic exploration of how molecular distance, electronic coupling, as well as solvent interactions and reorganization effects influence electron-transfer dynamics. The resulting insights provide a foundation for constructing more reliable, physics-based rate expressions that can be integrated into large-scale SEI formation simulations.

CPP 17.36 Mon 19:00 P5

Toward Improved Lithium Batteries: Performance of Magnetron-Sputtered Silicon Anodes — •Thomas Köhler[1], Christian Ludt[1], Tina Weigel[1], Marc Ferch[2], Robert Hahn[2], Annekatrin Delan[3], Charaf Cherkouk[4], Hartmut Stöcker[1], and Dirk C. Meyer[1] — [1]TU Bergakademie Freiberg, 09599 Freiberg, Germany — [2]Fraunhofer IZM, 13355 Berlin, Germany — [3]Fraunhofer IZM-ASSID, 01468 Moritzburg, Germany — [4]Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany

Silicon is considered one of the most promising anode materials for lithium-ion batteries due to its high theoretical specific capacity of 3590 mAh/g in the $Li_{3.73}Si$ phase at room temperature and its broad availability. However, its practical application remains limited because i) significant volume changes occur during cycling, ii) its intrinsic electronic conductivity is low, and iii) the stability of the solid-electrolyte interphase is insufficient.

In this work, silicon thin-film anodes were fabricated by magnetron sputtering onto copper foil. The electrodes were thoroughly characterized regarding their chemical composition and surface morphology. Scanning electron microscopy was used to evaluate the structural stability of the silicon layers in contact with a polymer-based solid electrolyte and to compare their degradation behavior with that in conventional liquid electrolyte. Electrochemical testing with the polymer electrolyte shows promising cycling performance; the reduced surface degradation observed in SEM correlates with improved long-term stability of the cell system.

CPP 17.37 Mon 19:00 P5

Structural and Ionic Transport Properties of Li3-3xDy1+xCl6 Solid Electrolytes — •Francesco Falsina[1,2], Peter Müller-Buschbaum[1], and Anatoliy Senyshyn[2] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]MLZ, TUM, Garching, Germany

Ternary lithium lanthanide chlorides, Li_3RCl_6 (R = rare earth), have recently emerged as promising solid electrolytes. Although initially thought to exhibit low ionic conductivity, later studies showed that ball milling synthesis, by leading to microstructure modification, can raise conductivity to $\sim 10^{-3}$ S·cm^{-1}. In this work we studied the $Li_{3-3x}Dy_{1+x}Cl_6$ system (x = −0.1 to 0.1). For $x = 0$, we assessed how annealing conditions affect structure and conductivity. Ionic transport was measured using isostatically pressed, gold-sputtered pellets and broadband impedance spectroscopy. XRD, DSC, and EIS analyses of as-milled, annealed, and melt-synthesized samples show that conductivity decreases by nearly an order of magnitude after annealing, while over-lithiated compositions consistently display higher conductivity, highlighting the impact of lithium retention. DSC and XRD also reveal an orthorhombic-to-trigonal transition with increasing lithium content. Overall, these results clarify how composition and disorder govern ionic transport in the Li_3MCl_6 electrolyte family.

CPP 17.38 Mon 19:00 P5

Investigating the Interfacial Impedance Characteristics of Composite Materials — •Janne Mattis König[1,2], Felix Schug[1,2], Christian Heiliger[1,2], and Janis K. Eckhardt[1,2,3] — [1]Institute of Theoretical Physics, Justus-Liebig-University Giessen, 35392 Giessen, Germany — [2]Center of Material Research (ZfM), Justus-Liebig-University Giessen, 35392 Giessen, Germany — [3]Institute of Physical Chemistry, Justus-Liebig-University Giessen, 35392 Giessen, Germany

All-solid-state batteries (ASSBs) are a promising alternative to conventional lithium-ion batteries, offering high energy and power densities, long-term stability, and fast-charging capability. Consequently, significant effort is focused on identifying suitable materials. Electrochemical impedance spectroscopy (EIS) is a key characterization technique, but interpreting spectra from realistic composite systems remains challenging. In this work, we investigate interfacial impedance in simplified composite microstructures using a 3D electrical network model. The simulations reveal that high charge-transfer resistances lead to geometric constriction effects, producing an impedance signature that closely resembles a migration process or a charge-transfer reaction. This constriction impedance is strongly influenced by the composite microstructure. Furthermore, increased conductivity along the interface introduces a characteristic deformation in the impedance spectrum shape. Overall, these findings clarify the origin of interfacial impedance features in composite materials and support more informed interpretation of EIS measurements in ASSB research.

CPP 17.39 Mon 19:00 P5

Aluminium-Polymer Batteries as a viable Post-Lithium Technology — •Oliver Schmidt[1,2], Amir Mohammad[1,2], Shuvrodev Biswas[1,2], Mostafizar Rahman[1,2], Nathan Leubner[1,2], Thomas Köhler[1,2], Hartmut Stöcker[1,2], and Dirk C. Meyer[1,2] — [1]TU Bergakademie Freiberg, Institute of Experimental Physics, Leipziger Str. 23, 09599 Freiberg — [2]Zentrum für effiziente Hochtemperatur-Stoffwandlung, Winklerstr. 5, 09599 Freiberg

One of the key challenges of the energy transition is the rising demand for lithium. In the future, there will be a supply gap, even taking into account recycling and the development of new mining areas. In addition to the limited availability, safety risks such as fire hazards make lithium-ion batteries less suitable for the long-term requirements of the energy transition.

Here, we present the aluminium-polymer battery as a novel technology adressing these issues. Aluminium is the most abundant metal in the Earth's crust and therefore inexpensive. It is available in Europe and is highly recyclable. The battery cells are free of toxic or critical raw materials and eliminate the risk of fire.

Pouch cells consisting of a simple 3-layer setup have been developed: aluminium anode, polymer electrolyte (consisting of $AlCl_3$, Et_3NHCl and PAN) and graphite cathode. Capacity, safety and recycling tests show promising results. Remaining challenges are tackling the self-discharge and scaling up the cell fabrication. The future goal is making large-scale storage systems cost-effective, efficient and safe.

CPP 17.40 Mon 19:00 P5

Microstructure-Resolved Impedance Modeling of Cathode Composite Electrodes for Solid-State Batteries — •Matthias Braun[1,2], Felix Schug[1,2], Christian Heiliger[1,2], and Janis K. Eckhardt[1,2,3] — [1]Institute for Theoretical Physics, Justus-Liebig-University Giessen, Germany — [2]Center for Materials Research (ZfM), Justus-Liebig-University Giessen, Germany — [3]Institute of Physical Chemistry, Justus-Liebig-University Giessen, Germany

Solid-state batteries (SSBs) rely on composite cathodes whose complex microstructures critically influence ionic and electronic transport. Electrochemical impedance spectroscopy (EIS) is widely used to probe these transport processes. The impedance behavior of mixed ionic electronic conductors is commonly interpreted using transmission-line models (TLMs). However, the extent to which composite microstructure governs impedance features and the validity of TLM-based interpretations remains insufficiently understood. In this work, we employ microstructure-resolved impedance simulations to investigate how key structural characteristics of cathode composites shape their impedance response. We demonstrate that interface morphology and porosity significantly modulate the spectra, giving rise to microstructure-specific features that conventional TLMs fail to capture. In particular, geometric current-constriction effects at the cathode active material/solid-electrolyte interface emerge as dominant contributors to impedance behavior. These findings provide a deeper mechanistic understanding of microstructure-induced impedance signatures and offer practical guidance for interpreting EIS data in composite electrodes for SSBs.

CPP 17.41 Mon 19:00 P5

Optimization in Fabrication Process and Understanding the Impact of Crystal Size and Growth in RbCsMAFA Perovskite Solar Cells — •Bashudev Bhandari[1,2,3], Sai Durga Prasad Sudana[1,2], Chikezie Williams Ugokwe[1,2], Ulrich S Schubert[1,2], and Harald Hoppe[1,2] — [1]Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich-Schiller-University Jena, Germany — [2]Laboratory of Organic and Macromolecular Chemistry (IOMC Jena), Friedrich-Schiller- University Jena, Germany — [3]Faculty of Physics and Astronomy, Friedrich-Schiller- University Jena, Germany

Perovskite solar cells (PSCs) emerged as remarkable and promising cutting-edge clean and green energy sources. Recent breakthroughs in their performance attract researcher's interest. Despite its promising performance, degradation issues and defects are critical obstacles to overcome. Our work explores different mechanisms to suppress defects and improve stability via improved crystallization. We have systematically optimized different processing parameters such as annealing time, antisolvent dropping time, hot casting, etc., and introduced additives like different phosphonium salts and PEAI for passivation and seeding for perovskite growth. Different Characterization and imaging techniques illustrate improved crystalline and opto-electronic properties of the perovskite film and solar cells.

CPP 17.42 Mon 19:00 P5

In Situ Investigation of Ag Sputter Deposition on a Zwitterionic Polymer Film — •Georgios Panagiotidis[1], Christoph Lindenmeir[1], Grace Leone[2], Lixing Li[1], Lyuyang Cheng[1], Doan Le[1], Yufeng Zhai[3], Kristian Reck[4], Benedikt Sochor[3], Matthias Schwartzkorpf[3], Anurag Keloth[5], Sarathlal Vayalil[3,5], Todd Emrick[2], Thomas Russell[2,6], Stephan V. Roth[3,7], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]UMass Amherst, Massachusetts, United States — [3]DESY, Hamburg — [4]CAU, Kiel, Germany — [5]UPES, Dehradun, India — [6]LBNL, Berkeley — [7]KTH, Stockholm, Sweden

While organic electronic devices mainly use organic or organic-inorganic hybrid materials, many electrodes still rely on pure metals due to their unparalleled electrical conductivity. Thus, the polymer-metal interface is crucial to device performance. Studies have demonstrated the use of ultrathin metal electrodes for (semi)transparent organic solar cells, and the quality of the interface influences the formation of structural defects, which can increase resistance and the likelihood of a short circuit. These metal contacts are typically deposited through lab-scale methods such as thermal evaporation, while industrial manufacturing prefers large-scale sputter deposition. Moreover, zwitterionic polymers can reduce the work function of metals and serve as interlayers in inverted organic solar cells. Therefore, understanding the growth behavior of sputtered silver on zwitterionic polymer surfaces is critical.

CPP 17.43 Mon 19:00 P5

Probing the Distribution of Residual Stresses in Thin Polymer Films Using Mechanochromic Molecular Springs — •Meirui Fu[1], Raphael Hertel[2], Bence Dajka[3], Michael Walter[3], Michael Sommer[2], and Günter Reiter[1] — [1]Institute of Physics, University of Freiburg, Germany — [2]Institute for Chemistry, Chemnitz University of Technology, Germany — [3]FIT Freiburg, University of Freiburg, Germany

Polymer thin films prepared rapidly from solution by spin coating often retain residual stresses originating on a molecular level. However, typically these stresses are probed on a macroscopic level, yielding spatially averaged responses, but do not resolve forces acting on individual chains. Here, we employed mechanochromophores, covalently integrated along the backbone of a glassy polymer, as optical reporters whose emission response varies continuously with the applied force. By combining optical microscopy and spectroscopy, we were able to measure the sum of the forces acting on individual chains with high spatial resolution. In particular, we investigated the distribution of forces acting on non-equilibrated polymer chains. Samples prepared under different spin coating conditions exhibited systematic variations in the emission spectra, which reflect differences in the distribution of the sum of forces acting on individual chains. We distinguish contributions from polymers experiencing low and high forces, respectively, which exhibited opposite trends with preparation conditions. We tentatively relate the heterogeneity of the acting forces to differences in conformation of the non-equilibrated polymer chains.

CPP 17.44 Mon 19:00 P5

Real Time Spectroscopy of Plasmonic Core-Shell Microgels during Compression at Air/Water Interfaces — •Matthias Karg and Déborah Feller — Martin Luther University Halle-Wittenberg, Halle, Germany

Plasmon resonance coupling is strongly distance-dependent. In contrast to near-field coupling of plasmonic nanoparticles in close proximity, periodic superstructures support plasmonic-diffractive coupling. The resulting surface lattice resonances are interesting for their narrow linewidth and sensitivity to refractive index environment and lattice periodicity. Typically studied periodic arrays are (solid) substrate-supported and thus structurally fixed unless elastic substrates are used. Seeking an alternative approach, we demonstrate the large dynamic control of periodic plasmonic lattices using soft and deformable core-shell microgels self-assembled at air/water interfaces. Using microgels with gold cores and sufficiently thick microgel shells, we realized periodic monolayers where the periodicity can be controlled by compression using a Langmuir trough. The implementation of an extinction spectrometer setup was used to probe the optical response of the monolayer in situ during continuous reduction of the available area, in real time. We monitor plasmon resonance coupling with a never before reported stepsize in interparticle spacing by following peak position, width and intensity. The observed spectral changes support recent findings that confined microgel monolayers at fluid interfaces show a continuous reduction in spacing when uniaxially compressed opposed to the cluster formation that is observed after drying on solid substrates.

CPP 17.45 Mon 19:00 P5

In-situ FTIR spectroscopy on organic semiconductor electric double-layer transistors — •Marvin Schmidt[1], Pushi Wang[2], Jun Takeya[2,3], and Martin Dressel[1] — [1]1. Physikalisches Institut, Universität Stuttgart, Germany — [2]Graduate School of Frontier Sciences, The University of Tokyo, Kashiwa, Japan — [3]Research Center for Materials Nanoarchitectonics, National Institute for Materials Science, Tsukuba, Japan

The field of organic electronics is ever-growing due to the enormous range of unique properties and possible applications exhibited by organic molecules. Electric double-layer transistors (EDLTs) consisting of the organic semiconductor 3,11-dinonyldinaphtho[2,3-*d*:2′,3′-*d*′]benzo[1,2-*b*:4,5-*b*′]dithiophene (C_9-DNBDT-NW) have recently attracted attention because they are highly processable and, thus, allow for the fabrication of large-scale single-crystal transistors with excellent crystallinity and high mobility. Furthermore, Hall effect measurements indicate the emergence of a metallic phase with strong correlations upon doping.

Here, we performed, for the first time, in-situ Fourier-transform infrared spectroscopy on EDLTs composed of C_9-DNBDT-NW single crystals for different sheet conductivities and temperatures down to 6K in the mid and far infrared regions. Our results give insights into how thermal fluctuations are suppressed with decreasing temperature and increasing electrostatic doping concentration, which manifests itself in the behavior of the displaced Drude peak.

CPP 17.46 Mon 19:00 P5

Measurement of photon antibunching of organic molecules by substrate scanning — •Janne Oskar Becker, Robert Schmidt, Steffen Michaelis de Vasconcellos, and Rudolf Bratschitsch — Institute of Physics, University of Münster

Single-molecule photoluminescence spectroscopy is often performed in solution, with molecules drifting in and out of a stationary focus. To immobilize single molecules, they are typically diluted in a solvent and spin-coated on a substrate. However, bleaching processes lead to decreasing photoluminescence count rates when illuminating isolated single-molecules over time, making photon antibunching measurements extremely challenging. To circumvent this, we measure multiple molecules sequentially by spatially scanning the spin-coated surface and accumulating photons of multiple single-molecules. In that way, we are able to measure photon antibunching Si/SiO_2 substrate.

CPP 17.47 Mon 19:00 P5

Large-Area Semiconducting 2D Imine-COF Polymer Films on Dielectric Glass for Electronic Applications — •Diksha Srivastava[1], Vipin Mishra[2], Showkat H. Mir[3], Jyotirban Dey[1], Jayant k. Singh[1], Manabendra Chandra[1], and Thiruvancheril g. Gopakumar[1] — [1]Indian Institute of Technology Kanpur, Kanpur 208016, India — [2]Vellore Institute of Technology, Vellore, Tamil Nadu 632014, India — [3]University of Kashmir, Hazratbal, Srinagar 190006, Jammu and Kashmir, India

Two-dimensional imine-based covalent organic frameworks (2D COFs) are a growing class of crystalline π-conjugated organic polymers with strong potential in thin-film electronics and optoelectronics. We present a scalable and reproducible strategy for producing 2D imine-COF-based polymer thin films through a quasi-equilibrium Schiff-base reaction between p-phenylenediamine (PDA) and benzene-1,3,5-tricarboxaldehyde (TCA). This method enables the growth of large-area polymer films (up to 2 cm) on dielectric substrates with controlled thickness. SEM, TEM, and AFM confirmed the layered and crystalline morphology of the films. Optical absorption and scattering measurements revealed a semiconducting band gap consistent with the DFT-calculated band structures, indicating the presence of delocalized states suitable for charge transport. To probe intrinsic electrical behaviour, COF polymer films were integrated into Ag/COF/Glass devices. The I-V curves revealed semiconducting behaviour with low current density and field-assisted conduction limited by electrode-COF injection barriers.

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Designing functional polymer surfaces by initiated chemical vapor deposition — •Stefan Schröder, Lynn Schwäke, Tobias Giez, Thomas Strunskus, Franz Faupel, and Tayebeh Ameri — Kiel University, Kiel, Germany

Polymer thin films and organic surfaces have attracted significant interest across diverse application areas, ranging from wearable electronics to biomedicine and encapsulation. The demand for new functional surfaces, combined with ongoing device miniaturization, requires defect-free nanoscale polymer films with precise control over thickness and chemistry. Chemical vapor deposition (CVD) of polymer surfaces addresses these challenges by eliminating the dewetting and surface tension effects commonly encountered in conventional solution-based thin film fabrication. In particular, initiated chemical vapor deposition (iCVD) enables the fabrication of conformal polymer coatings with nanoscale precision on large-area substrates as well as on complex geometries. Moreover, iCVD allows for room-temperature deposition on delicate substrates, including flexible organic materials, copy paper, and biomedical patches. This contribution presents the fundamentals of the iCVD process and highlights selected application examples.

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Controlling Surface Wetting through Light- and Electric-Fields — •Billura Shakhayeva[1], Bas ter Beest[2], Frieder Mugele[2], and Björn Braunschweig[1] — [1]University of Münster, Institute of Physical Chemistry, Germany — [2]University of Twente, Physics of Complex Fluids

Electro-dewetting (EDeW) enables reversible control of surface wettability using ionic surfactants. Using dodecyl tetraethyl ammonium bromide (DTAB) as a cationic surfactant, previous studies achieved a change in the apparent contact angle (CA) of up to 30°. We used vibrational sum-frequency generation (SFG) spectroscopy and ellipsometry to probe the molecular structure close to the three-phase contact line under initial and EDeW conditions. Using 0.15 mM DTAB we observed the largest changes in contact angle and observed spreading of surfactant even at larger distances from the contact line. Further, we extended this approach from DTAB to photoswitchable arylazopyrazole triethylammonium bromide (AAP-TB) surfactants. AAP-TB can undergo E/Z photoisomerization and allows to change the surface activity through the choice of the configurational isomer with the Z being less surface active compared to the E. We demonstrate that EDeW with AAP-TB surfactants is possible similar to DTAB, but with a smaller maximum change in contact of about 13° once a potential of +3 V is applied. In addition, photo-isomerization of AAP-TB allows to further finetune the CA reversibly by about 4°.

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Dynamic wetting of mixed rod-sphere suspensions and its relation to the suspension rheology — •Reza Azizmalayeri and Günter Auernhammer — Leibniz-Institut für Polymerforschung Dresden e. V.

In this study, we examine dynamic wetting of mixed rod-sphere suspensions near the advancing contact line. We compare pure spherical suspensions with 98:2 sphere-rod mixtures. Using a pinned droplet and moving substrate geometry on an inverted microscope, we achieve a locally stable contact line. Astigmatism Particle Tracking Velocimetry (APTV) measures the trajectories of tracer particles within the refractive index-matched suspension. Pinch-off experiments conducted via the Dripping-onto-Substrate (DoS) method provide Protorheology insights into shear and extensional viscosities. We analyse rod dynamics and orientation as they approach the advancing contact line, interact with the substrate, and re-enter the bulk suspension. In purely spherical suspensions, tracer trajectories near the advancing contact line deviate significantly from hydrodynamic model predictions. Conversely, mixed rod-sphere suspensions exhibit minimal deviations. Rod inclusion reduces effective viscosity during pinch-off, promoting deformation and thread thinning. This effect is amplified by rod-induced polydispersity and the disruption of spherical contact structures, weakening resistance to flow and altering rheology. Visualizations reveal that rods align parallel to the contact line, then rotate 90 degrees to align with the substrate.

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Statics and dynamics of drops on liquid infused surfaces — Hossein Abdolnezhad[1], •Martin Brinkmann[2], Ralf Seemann[2], and Ciro Semprebon[1] — [1]Department of Mathematics, Physics and Electrical Engineering, Northumbria University, Newcastle, UK — [2]Zentrum für Biophysik, Universität des Saarlandes, Saarbrücken, Germany

Slippery liquid-infused porous surfaces (SLIPS), inspired by the slippery properties of the Nepenthes pitcher plant, have been introduced to increase the mobility of wetting drops by minimizing the liquid-solid contact. Preparation of these surfaces involves infusing a lubricating liquid into a porous or textured surface, creating a thin liquid layer on top of the surface resulting in high drop mobility as well as unique properties such as anti-corrosion, self-cleaning, heat transfer enhancing, anti-fouling and anti-icing, water harvesting properties with a broad potential for application in industry.

The complex relationship between lubricant properties and retention mechanisms in liquid-infused surface, particularly the role of the lubrication ridge forming around the drop causing depletion of the lubricant over time brings up the questions of whether the lubricant ridge can be effectively controlled as well as whether there is an optimal size in relation to the volume of the drop sliding over liquid-infused surface. Recent experiments elucidate the role of the lubricant ridge in the dynamics of drops on liquid-infused surfaces, and led to the development of a theoretical understanding of the experimental observations combining finite-element and analytical modeling approaches.