CPP 32: Poster Session II

Time: Thursday 9:30–12:00 Location: P3

CPP 32.1 Thu 9:30 P3

Influence of Salt Addition on the Ionic Conductivity, Hydration Behavior, and Structure of Poly(sulfobetaine) Hydrogels for Electrolyte Applications — •Friederike Ganster[1], Marcell Wolf[2], Gilles Wittmann[2], Peter Müller-Buschbaum[1], and Lucas P. Kreuzer[2] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II), 85748 Garching, Germany

Polyzwitterionic hydrogels are promising candidates for electrolytes in aqueous solid-state batteries, such as zinc-ion batteries (ZIBs), due to their ability to retain water molecules that facilitate ionic transport. The retained water acts as a lubricant, coordinating with the charged groups of the polyzwitterion and reducing interactions with mobile Zn^{2+} ions, thereby promoting the dissociation of ions and improving ion mobility. We systematically investigate how the addition of cosmotropic $ZnSO_4$ or rather chaotropic Zn(acetate) affects the ionic conductivity of poly(sulfobetaine)-based hydrogels. Our findings reveal that while ionic conductivity is generally increased, the extent and nature of this enhancement strongly depend on the specific salt type. We attribute this to unique and salt-type sensitive structural and hydration changes. X-ray scattering techniques resolve the electrolyte structure, and FTIR and Raman spectroscopy provide insights into the altered hydration behavior. Electrochemical impedance spectroscopy correlates these structural and hydration changes with variations in ionic conductivity and ion transport efficiency.

CPP 32.2 Thu 9:30 P3

Exploring pressure effects on the coil-globule transition of a pH sensitive polymer — •Ved Mahajan, Varun Mandalaparthy, and Nico F. A. van der Vegt — Technical University, Darmstadt

Macromolecules like polymers and proteins are essential to everyday life, with their structure and function influenced by environmental changes. The coil-globule transition is ubiquitous and is influenced by factors like hydrophobic interactions. External conditions, such as pressure, impact this transition differently in proteins and thermoresponsive polymers like PNiPAM[1].

This study investigates the effect of pressure on the coil-globule transition of a pH-sensitive hydrophobic polymer using constant-pH molecular dynamics. Our Results show that both pH and pressure significantly influence the transition. While pressure and charge both cause chain swelling, charge counteracts pressure-induced chain extension at high pressure. We observe distinct water structuring around positively and negatively charged sites with consequence to the polymer's pressure response. Additionally, we explore zwitterionic polymers under pressure, providing insights into biologically relevant secondary structures.

[1] Papadakis, C. M.; Niebuur, B.-J.; Schulte, A. Thermoresponsive Polymers under Pressure with a Focus on Poly(N-isopropylacrylamide) (PNIPAM). Langmuir 2024, 40 (1), 1* 20, DOI: 10.1021/acs.langmuir.3c02398

CPP 32.3 Thu 9:30 P3

Microscopic Insights into NaTFSI Based Thermoelectric Polymer Electrolyte by Raman Spectroscopy — •Julian-Steven Schilling[1] and Jens Pflaum[1,2] — [1]University of Wuerzburg, 97074 Würzburg — [2]Center for Applied Energy Research (CAE Bayern e.V.), 97074 Würzburg

The variety of chemical components, solution-based processability, and intrinsically low thermal conductivity have positioned polymers as leading materials in the field of organic thermoelectrics. Since materials facilitating ionic transport provide significantly higher thermoelectric voltages compared to electronic ones, we have analyzed the thermoelectric transport properties of a methacrylate-based solid polymer electrolyte. This study pursued our previous work [1] on this solution processed electrolyte by revealing new insights into the interaction of the conducting NaTFSI salt and the polymer backbone on microscopic length scales. By means of Raman spectroscopy, we use e.g. the S-C stretching modes and their salt concentration dependency to identify free TSFI Ions inside the polymer matrix which are responsible for the thermoelectric properties. In addition, we highlight the concentration dependent characteristics of the liquid versus solid electrolyte phase as well as the impact of the photoinitiator used for UV-curing on the electrolyte behaviour. [1] arxiv:2403.09340

CPP 32.4 Thu 9:30 P3

Ion Transport in Block Copolymer Electrolytes: Insights from Atomistic MD Simulations — •Jignesh Dhumal[1], Diddo Diddens[2], and Andreas Heuer[3] — [1]IGS BACCARA, Universität Münster — [2]Helmholtz Institute Münster (IEK-12), Forschungszentrum Jülich GmbH — [3]Institut für physikalische Chemie, Universität Münster

Electrolytes are essential in batteries to facilitate ion transport between electrodes. Block copolymer electrolytes, have emerged as a promising class due to their high ionic conductivity and enhanced mechanical strength. However, despite several experimental and computational studies demonstrating their significance, an atomistic-level understanding of ion transport in Lithium bis(trifluoromethanesulfonyl)imide (LiTFSI)-doped polystyrene-block-poly(ethylene oxide) (PS-b-PEO) block copolymers remain limited. In this study, we employ atomistic molecular dynamics simulations over extended timescales up to a microsecond examining the structural stability of the polymeric system and determine ion co-ordination within. We also quantify ion dynamics and transport properties in the PEO bulk region and the behavior at the PS/PEO interface, providing new insights into the mechanisms governing ion transport in this material.

CPP 32.5 Thu 9:30 P3

Advanced Synchrotron Characterization of NDI based acceptor thin films — •Subhalakshmi Suresh Kumar[1,2], Eva M. Herzig[1], and Christopher R. McNeill[2] — [1]Dynamik und Strukturbildung - Herzig Group, Universität Bayreuth, Universitätsstr. 30, 95447 Bayreuth, Germany — [2]McNeill Research Group, Department of Materials Science and Engineering, Monash University, Wellington Road, Clayton, Victoria, 3800 Australia

The transition to renewable energy has brought polymer solar cells (PSCs) to the forefront due to their lightweight, flexible, and environmentally friendly properties. The alignment of conjugated polymers within PSCs is critical for improving charge transport and overall device performance. This study aims to enhance the alignment of NDI-based acceptor thin films by employing fabrication methods such as blade coating and post-treatment annealing. Thin films were methodically prepared by varying coating speeds, substrate temperatures, and annealing conditions, followed by characterization using UV-Vis spectroscopy, Near-Edge X-ray Absorption Fine Structure (NEXAFS), and Grazing Incidence Wide-Angle X-ray Scattering (GIWAXS). The analyses demonstrated a significant enhancement in molecular alignment after annealing, particularly in PNDITBT films, which showed pronounced backbone alignment. These findings highlight the potential of synchrotron-based techniques in optimizing thin-film microstructures, paving the way for the production of highly efficient laminated organic solar cells with bilayer heterojunctions.

CPP 32.6 Thu 9:30 P3

Morphologies in Thin Films of Charged Pentablock Terpolymers During Solvent Vapor Annealing — •Yujia Gu[1], Constantinos Tsitsilianis[2], and Christine M. Papadakis[1] — [1]TU Munich, TUM School of Natural Sciences, Soft Matter Physics Group, Garching, Germany — [2]University of Patras, Department of Chemical Engineering, Patras, Greece

Thin films from block copolymers containing charged blocks offer enhanced possibilities for precise structural modulation. In our previous work on thin films from a symmetric ABCBA pentablock terpolymer with cationic B and C midblocks and hydrophobic end blocks A, the pH-dependent degree of ionization of the charged midblocks was found to significantly influence the thin-film morphology [1]. In this study, we explore the possibilities to tune the thin film structures during solvent vapour annealing (SVA) using the same ABCBA pentablock terpolymer. Spin-coated films are prepared at various pH values and are subjected to SVA using selective solvents. Depending on the solvent selectivity, SVA may alter the film structure, e.g. by promoting reorganization toward equilibrium morphologies. We utilize in-situ atomic force microscopy (AFM) and spectral reflectometry

(SR) to monitor structural transitions during SVA. By systematically examining the effects of pH and solvent selectivity, this study aims to provide insights into controlling nanostructure morphology in charged pentablock copolymers, with implications for advanced thin-film design.

CPP 32.7 Thu 9:30 P3

Adaptive Air-Water Interfaces with Spiropyrans and Arylazopyrazoles — •Michael Hardt[1], Javier Carrascosa-Tejedor[2], Philipp Gutfreund[2], Richard A. Campbell[3], and Björn Braunschweig[1] — [1]University of Münster (Germany) — [2]Institut Laue-Langevin (France) — [3]University of Manchester (UK)

Interfaces that can be tuned in their properties by external stimuli such as light or temperature are of great interest to drive macroscopic properties of interface-controlled soft matter materials. Using molecular switches that respond to orthogonal triggers, the properties of fluid interfaces can be preconditioned, and a low level of adaptivity can be integrated, extending the possibilities of soft matter interfaces beyond responsive functions. We explore the adaptive behaviour of air-water interfaces decorated by spiropyran (SP) and arylazopyrazole (AAP) photo-responsive surfactants. When exposed to UV light, the SP surfactants become more surface active, while the AAP surfactants undergo E/Z photoisomerization, significantly reducing their surface activity. By adjusting the intensity and duration of the UV exposure, the interfacial properties can be shifted from a simple responsive state (upon weak UV irradiation) to a more complex conditioned response (upon intense UV irradiation), accompanied by a dramatic alteration in interfacial chemistry. Vibrational sum-frequency generation (SFG) and neutron reflectometry suggest that prolonged UV exposure induces SP and AAP surfactant aggregation at the air-water interface, driving the conditioned response where thick SP layers up to 5 nm form in the presence of Z-AAP.

CPP 32.8 Thu 9:30 P3

Is Anomalous Underscreening Detectable via AFM? — •Esther Ohnesorge, Thomas Tilger, Michalis Tsintsaris, and Regine von Klitzing — Department of Physics, Technische Universität Darmstadt, Darmstadt, 64289, Germany

Since colloidal dispersions have a significant importance in our daily life, it is of special interest to gain a deeper understanding of which interfacial forces govern their stability and how this stability can be tailored.

For aqueous electrolyte solutions, the DLVO theory is a powerful and well-established framework to describe these interactions at low and intermediate ionic strengths. In contrast, the situation at high ionic strength is less understood and the main methods for direct force measurements give inconsistent results. While the surface force apparatus (SFA) provides clear evidence for a reentrant behavior of the double layer repulsion in the highly concentrated regime - termed anomalous underscreening - for a wide range of different electrolytes, similar observations weren't possible with the atomic force microscope (AFM) to date. The reason for this fundamental difference is still unclear.

To elucidate the underlying mechanism, we performed colloidal probe AFM (CP-AFM) measurements in aqueous salt solutions. We systematically varied the type of salt, the surface chemistry of the confining surfaces (silica vs mica) as well as their curvature to bridge the gap between CP-AFM and SFA.

CPP 32.9 Thu 9:30 P3

Dynamic Wetting of Adaptive Polyelectrolyte Substrates: A multiscale approach — •Mona Meltschoch, Tünde Benedek, and Regine von Klitzing — Soft Matter at Interfaces, Institute for Condensed Matter Physics, TU Darmstadt, Hochschulstraße 8, D-64289 Darmstadt, Germany

Wetting phenomena are of great importance across various scientific disciplines and the wettability dynamics of adaptive substrates, such as polyelectrolyte (PE) multilayers (PEM), have gained significant attention. An interesting property of PE substrates is their propensity to swell in a liquid environment. However, complexities like the disparity between time and length scales make experimental investigations quite challenging. We prepared PE substrates by the layer-by-layer method, with a focus on their wettability at the nanoscale. We used atomic force microscopy (AFM) as the main characterisation technique. An optical contact angle (CA) tensiometry method is used for macroscopic measurements, layer thickness is determined by ellipsometry and X-ray reflectometry (XRR). Previous results show a decrease in water CA on silicon wafers coated with polystyrene sulfonate (PSS) as outermost layer in water-saturated atmosphere. To investigate the dependence on thickness, chain length and charge of the outer layer, different PEMs were fabricated and characterised. Here, the substrates were investigated with an AFM and showed to exhibit smooth surfaces while linearly increasing in thickness. The decrease in water CA is more pronounced with an increasing thickness and differs if PSS or PAH are outermost layer.

CPP 32.10 Thu 9:30 P3

Molecular Imprinting of PEDOT in Polyelectrolyte Multilayers — •Martin Hunger, Muhammad Khurram, Sven Neuber, and Christiane A. Helm — martin.hunger@uni-greifswald.de

Electrically conductive films of Poly(3,4-ethylenedioxythiophene): poly(styrenesulfonic acid) (PEDOT:PSS) are formed by sequential adsorption of oppositely charged macromolecules. PEDOT:PSS serves as polyanion, and PDADMA is the polycation. When the top layer is PEDOT:PSS, the electrical conductivity is large (8 kS/m), when the top layer is PDADMA, the electrical conductivity is three orders of magnitude lower. In addition, vis-IR absorption spectroscopy shows that the PEDOT density in PEDOT:PSS-terminated films is high, while it is low in PDADMA-terminated films. When a PDADMA layer is adsorbed, turbidity measurements of the adsorption solution show that PEDOT diffuses out of the film. This can be explained entropically: a few PDADMA molecules with many positive charges replace many small molecules with few positive charges. Furthermore, exposure to solutions with divalent or trivalent cations reduce the conductivity of PEDOT-PSS-terminated films. We discuss whether PSS returns to previous binding sites upon adsorption of PEDOT:PSS, a behaviour that is typical for molecular imprinting.

CPP 32.11 Thu 9:30 P3

Extension of initiated chemical vapor deposition to new polymers via silylation — •Lynn Schwäke[1], Artjom Businski[2], Thomas Strunskus[1], Franz Faupel[1], Rainer Herges[2], and Stefan Schröder[1] — [1]Chair for Multicomponent Materials, Department of Materials Science, Kiel University, 24143 Kiel, Germany — [2]Otto Diels Institute of Organic Chemistry, Kiel University, 24143 Kiel, Germany

Initiated Chemical Vapor Deposition (iCVD) is a powerful technique for the solvent-free and conformal deposition of polymer thin films on sensitive substrates and complex geometries. The utilisation of a variety of monomers enables the fabrication of films with specifically tailored properties and functionalities. However, the evaporation of monomers is a prerequisite for iCVD processes. Consequently, this limits its applicability, for example, in the synthesis of hydrogels. The hydrophilic nature of potential monomers and the presence of other strong intermolecular interactions result in low vapor pressures, which in turn hinders their use in iCVD. A well-known strategy, e.g. in the context of drug detection by gas chromatography-mass spectrometry (GC-MS), is silylation, which is used to weaken inter-molecular forces. Here silylation was employed to enhance the vapor pressure of hydrophilic 2-hydroxyethyl methacrylate (HEMA), an important monomer in the synthesis of hydrogels. Consequently, silylation is proposed as a general route for the introduction of low vapor pressure monomers into iCVD systems, which would lead to a significant expansion of the available monomer toolbox.

CPP 32.12 Thu 9:30 P3

In-Situ Neutron and Raman spectroscopy on polymer thin films at varying humidity — •Marcell Wolf[1], Lucas Kreuzer[1], Friederike Ganster[2], Christopher Garvey[1], and Peter Müller-Buschbaum[2] — [1]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstraße 1, 85748 Garching, Germany — [2]Lehrstuhl für Funktionelle Materialien, Physik Department, Technische Universität München, James-Frank-Straße 1, 85748 Garching, Germany

Here we present a new sample environment for in-situ neutron and Raman spectroscopy on polymer thin films at varying humidities and temperatures. The combination of in-situ Raman and neutron spectroscopy shows the advantage that no difference within the sample composition, temperatures and humidity variations at the sample can be neglected, compared to separated single measurements. The structural changes can be directly related to the dynamic changes while varying the environment. We plan to describe our setup and present the first results of this new sample environment measured at the neutron time-of-flight spectrometer FOCUS at the PSI, Switzerland. For our knowledge this is the first time, that both spectroscopy techniques in comibination with varying humidity are applied at in-situ measurements. The new sample environment will be available to all users at time-of-flight spectrometer TOFTOF at the MLZ, as soon as the reactor restarts. Different variations of the sample cell, especially designed for different neutron experiments are available at other neutron instruments at the MLZ.

CPP 32.13 Thu 9:30 P3

Second order nonlinear optical properties of hexagonal boron nitride nanosheets h-BNNs — •Dina Atwa Khalil and G. Omar — Laser Institute for Research and Applications, Beni-Suef University, Egypt

The superior optical characteristics of hexagonal boron nitride nanosheets (h-BNNs) have been drawing more attention in the past few years. However, scientists have not yet thoroughly studied the nonlinear optical (NLO) properties of such innovative material. Here, NLO characteristics of h-BNNs are investigated for the first time utilizing the Z-scan approach that had been irradiated with 100 fs laser pulses using different excitation wavelengths that started from 740 to 820 nm at a constant incident power of 1 W. The studied 2D nanomaterial was prepared by a straightforward and effective technique for producing (h-BNNs), which is mechanical exfoliation. Their morphology and crystal structure have been investigated using different techniques, including UV-vis spectroscopy, scanning electron microscopy (SEM), transmission electron microscopy (TEM), and Raman spectroscopy. The measurements of nonlinearity show that by increasing the excitation wavelength, the nonlinear absorption coefficient decreases in a linear trend. The as prepared h-BNNs performed fascinating optical limiting with excellent two-photon absorption. This innovative optical nanomaterial makes them promise for sensitive optical components and laser protection applications.

CPP 32.14 Thu 9:30 P3

Highly oxidized Graphene Oxide as a Drug Delivery platform: Functional Group Interactions and Controlled Release Mechanisms — •Codrut Costinas[1], Liviu Cosmin Cotet[2], Monica Baia[1], Klara Magyari[3], and Lucian Baia[1] — [1]Faculty of Physics, Babes-Bolyai University, Cluj-Napoca, Romania — [2]Faculty of Chemistry and Chemical Engineering, Babes-Bolyai University, Cluj-Napoca, Romania — [3]Interdisciplinary Research Institute on Bio-Nano-Sciences, Babes-Bolyai University, Cluj-Napoca, Romania

Graphene oxide (GO) presents a promising platform for drug delivery, given its versatile surface chemistry and high surface area that enable effective drug loading and controlled release. Our study investigates the capabilities of an in-house produced, highly oxidized GO as a carrier by examining its interactions with two model compounds: methylene blue and methyl orange, as well as two drugs: doxorubicin and gentamicin sulfate. Through spectroscopic investigations (UV-VIS, FT-IR, and Raman), potentiometric titrations, and drug loading and release experiments we successfully identify the functional groups and bond types involved in drug-GO interactions in different pH media, most notably hydrogen bonding, electrostatic interactions, and π-π stacking. Furthermore, by taking into consideration the pKa values between GO acidic groups and the drugs ionizable groups, we can estimate both loading and pH-responsive release behavior in simulated physiological pH conditions. These findings highlight the flexibility of GO as a drug carrier, supporting its application in the development of customizable drug delivery systems for various therapeutic needs.

CPP 32.15 Thu 9:30 P3

Electronic Properties of a Naphthalene Diimide (NDI)-based Covalent Organic Framework (COF) — •Johann Olbrich[1], Laura Fuchs[1], Bibhuti Bhusan Rath[2], Bettina V. Lotsch[2], and Frank Ortmann[1] — [1]TUM School of Natural Sciences, Technische Universität München, Germany — [2]Nanochemistry Department, Max-Planck-Institute for Solid State Research, Stuttgart, Germany

Covalent organic frameworks (COFs) are a versatile class of porous polymers that exhibit exceptional tunability and electronic properties, making them attractive for various applications including water splitting [1], solar batteries [2] or other optoelectronic applications. We investigated the electronic properties of a naphthalene diimide (NDI)-based COF, which demonstrates robust photoinduced charge separation in aqueous environments, by using density functional theory (DFT) calculations. We provide theoretical insights into the stability of the charges in NDI-based COFs under hydrated conditions, highlighting their potential for advanced electronic and material applications. For this, we determined the formation of a stable radical on the NDI unit through the addition of a hydrogen atom. Further modeling of interactions of small water clusters with the COF indicated the emergence of a radical anion on the NDI, accompanied by the stabilization of H+ in an H2O cluster.

[1] K. Gottschling, G. Savasci, H. Vignolo-González, S. Schmidt, C. Ochsenfeld, and B. V. Lotsch, J. Am. Chem. Soc. 2020, 142, 12146.

[2] Y. Wang, Y. T. Chan, T. Oshima, V. Duppel, B. V. Lotsch, J. Am. Chem. Soc. 2024, 146(37), 25467-25476.

CPP 32.16 Thu 9:30 P3

Lithium Distribution Heterogeneity in the Graphite Anode of 21700-Type Cylindrical Li-Ion Cells during Aging — Dominik Petz[1,2], •Peter Müller-Buschbaum[2], and Anatoliy Senyshyn[1] — [1]Heinz Maier-Leibnitz-Zentrum (MLZ), 85748 Garching, Germany — [2]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany

Electrochemical cycling in lithium-ion batteries involves an active exchange of lithium ions and electrons between the cathode and anode materials. In addition to material properties, this exchange is influenced by cell parameters such as electrode dimensions and geometry, current density, temperature, pressure, reaction rate, and others. These parameters are generally neither uniformly distributed nor static, thereby contributing to the stabilization of heterogeneous states in Li-ion batteries, typically seen in the lithium concentration distribution across the electrodes.

Previous studies have shown that, with cell aging, the distribution of lithium ions in the graphite anode of 18650-type lithium-ion batteries shifts over time. In this study, the heterogeneity of a fresh and an aged 21700-type Li-ion battery was examined using multiple diffraction techniques with both synchrotron and neutron radiation. Laboratory-based techniques such as SEM and incremental capacity analysis were also employed. The findings revealed a notable lithium distribution after cell aging, prompting the question of how cell format impacts cell aging behavior.

CPP 32.17 Thu 9:30 P3

Steering sulfur reduction kinetics of lithium-sulfur batteries by interfacial microenvironment modulation — •Cheng Yuan[1,2], Liang Zhang[2], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]Institute of Functional Nano & Soft Materials (FUNSOM), Soochow University, Suzhou 215123, China

Catalytic conversion of lithium polysulfides (LiPSs) is considered as an effective avenue to suppress the shuttle effect of lithium-sulfur (Li-S) batteries, for which the interfacial microenvironment constructed by the interaction between electrocatalysts and LiPSs plays a pivotal role in modulating the sulfur reduction kinetics. However, most of previous reports mainly focused on modulating the band structure of electrocatalysts or LiPSs alone to enhance the catalytic activity rather than considering the interfacial microenvironment as a whole. Herein, we propose a binary descriptor composed of the energy difference between d-band of electrocatalysts and p-band of LiPSs ($\Delta\epsilon$M-S) and the antibonding filling degree (ϵABF), which capture the energy band contributions from both electrocatalysts and LiPSs, to reveal the influence of interfacial microenvironment on sulfur reduction kinetics. Among different designed electrocatalysts, NiO presents a moderate LiPSs anchoring capacity and rapid electron transfer kinetics owing to the optimal $\Delta\epsilon$M-S and decreased ϵABF after interacting with LiPSs, which lead to a robust interfacial microenvironment and thus guarantee a continuous catalytic conversion of LiPSs in the long-term cycling.

CPP 32.18 Thu 9:30 P3

Polymer of intrinsic microporosity as the silicon-based anode electrode additive — •Ming Yang[1], Ruoxuan Qi[1], Ya-Jun Cheng[2], Yonggao Xia[2], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]Ningbo Institute of Materials Technology & Engineering, Chinese Academy of Sciences, 1219 Zhongguan West Rd, Ningbo, 315201, Zhejiang Province, P. R. China

Silicon-based anodes are promising alternatives due to their high theoretical specific capacity and low voltage platform to traditional graphite anodes for high-energy-density lithium-ion batteries (LIBs). However, their performance is significantly hindered by silicon's substantial volume expansion during cycling, which often leads to electrode degradation. Therefore, it is crucial to design a robust electrode structure and establish a stable solid electrolyte interface (SEI) to address these challenges. Herein, an intrinsic microporosity polymer PIM-COOH is prepared, which has good compatibility with the polyacrylic acid (PAA) binder as a silicon-based anode additive. The microporous structure of the PIM-COOH molecule can effectively improve the transport of lithium ions and improve the electrochemical kinetics. In addition, due to the inherent microporous properties of PIM-COOH additives, the affinity between the electrode and the electrolyte is enhanced. As a result, good lithium-ion transport and mechanical integrity are maintained, resulting in improved long-term stability and high-rate performance.

CPP 32.19 Thu 9:30 P3

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, 85748 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 film 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 32.20 Thu 9:30 P3

Ionic transport race between lithium and sodium in non-aqueous electrolytes — •Chinwendu Nancy Anabaraonye[1,2], Diddo Diddens[3], and Andreas Heuer[1,3] — [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]Helmholtz Institute Mnster (IEK-12),Forschungszentrum Jülich GmbH, 48149 Münster,Germany;

The need to meet the storage requirements of energy systems safely and efficiently has led to research into electrolytes other than the commonly used lithium-ion batteries. While the lithium-ion battery is the clear market leader, there is increasing interest in sodium-ion batteries, which are cheaper and more abundant. The present work is a comparative study of the transport properties of lithium hexafluorophosphate ($LiPF_6$) and sodium hexafluorophosphate ($NaPF_6$) in carbonate electrolytes consisting of ethylene carbonate (EC) and ethyl methyl carbonate (EMC). Using molecular dynamics simulations, we analyse the influence of EC ratio and salt concentrations on the solvation structure and how this affects the ionic transport properties such as diffusivity and ionic conductivity of the system. Our results show higher conductivity and diffusivity of Na compared to Li for the analysed systems. Optimal ionic conductivity for Na was achieved above 1 M concentration, in contrast to Li. Overall, we observed differences in the coordination and mobilities of lithium and sodium cations.

CPP 32.21 Thu 9:30 P3

3D Electrodeposition of Porous Cu for long-cycling Lithium-Metal Batteries — •Lyuyang Cheng[1], Zhuijun Xu[1], Tianle Zheng[1], Yingying Yan[1], Fabian Apfelbeck[1], Yuxin Liang[1], 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

Lithium (Li) metal is the ultimate anode for rechargeable batteries. Its high specific capacity (3860) and low voltage (3.04 V vs standard hydrogen electrode) warrant optimal cell energy density. However, these anodes rely on repeated plating and stripping of Li, which leads to consumption of Li inventory and the growth of dendrites that can lead to self-discharge and safety issues. To address these issues and problems related to the volume change of these anodes, 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 show 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 32.22 Thu 9:30 P3

Operando study on structure-activity relationship between electrolyte components and electrochemical performance for all-solid-state lithium batteries — •Yingying Yan[1], Liangzhen Liu[2], Yuxin Liang[1], Fabian A.C. Apfelbeck[1], Guangjiu Pan[1], Lyuyang Cheng[1], Roland A. Fischer[2], and Peter Müller-buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]TUM School of Natural Sciences, Chair of Inorganic and Metal-Organic Chemistry, 85748 Garching, Germany

All-solid-state lithium-ion batteries (ASSLIBs) are the most promising power sources for high-safety and high-energy-density energy storage devices. However, the practical application of ASSLBs has been hindered by poor interfacial stability and inferior ionic conductivity. Herein, a layered-double-hydroxide (LDH) reinforced poly(ethylene oxide) (PEO) composite polymer electrolyte is designed, which delivers a wide electrochemical window, high ionic conductivity, and superior Li+ transference number with a low LDH loading. The Li symmetric cells show ultra-long cycling stability at 0.1 mAh/cm2. The all-solid-state Li//LiFePO4 exhibits an excellent cycling stability with a high capacity retention of 90.1% at 0.1 C over 250 cycles. Furthermore, the structure-activity relationship between the component structure of the electrolyte and the electrochemical performance was elucidated by operando nanofocus wide-angle X-ray scattering (nWAXS).

CPP 32.23 Thu 9:30 P3

Organic polyaniline-based cathode materials — •Meriem N. Boudjenane[1], Friederike Ganster[2], Sebastian Mühlbauer[1], and Lucas P. Kreuzer[1] — [1]Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II), 85748 Garching, Germany — [2]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany

Organic cathode materials feature tuneable structures, abundant active sites, and compatibility with multivalent charge carriers, thereby allowing to overcome challenges typically faced in inorganic cathode systems such as structural instability, and environmental hazards. We focus on the development of polyaniline (PANI) based cathodes. PANI, a conductive polymer, has demonstrated high capacity, excellent rate capability and fast ionic diffusion. Cellulose-based materials such as carboxymethyl cellulose (CMC) are used as binders and enhance the overall stability and electrochemical performance. By tuning parameters such as material composition, ionic strength, water content, and temperature, we elucidate how the conductivity and electrochemical stability of the PANI-based cathode can be optimized. Advanced techniques like X-ray diffraction, scanning and transmission electron microscopy, and electrochemical analysis provide deep insights into the structure-function relationship of the cathode materials while operando Raman spectroscopy will give insights into the charge/discharge mechanism and respective redox reactions, guiding the development of high-performance organic cathodes.

CPP 32.24 Thu 9:30 P3

Consistent Electrostatics in Bottom-Up Modeling of Electrode-Fluid Systems: Determining the Capacity from Ab-Initio to Continuum Models — •Philipp Stärk[1,2], Henrik Stooss[3], Philip Loche[4], and Alexander Schlaich[3] — [1]Stuttgart Center for Simulation Science (SC SimTech), University of Stuttgart, 70569 Stuttgart, Germany — [2]Institute for Computational Physics, University of Stuttgart, 70569 — [3]Institute for Atomistic Modeling of Materials in Aqueous Media, Hamburg University of Technology, 1073 Hamburg, Germany — [4]Laboratory of Computational Science and Modeling, IMX, Ecole Polytechnique Federale de Lausanne,1015 Lausanne, Switzerland

Detailed understanding of electro-catalysis, batteries and supercapacitors, often requires modeling these systems on an atomistic scale. However, at this length scale and level of detail, most continuum assumptions about electrodes are clearly no longer valid. This is problematic for physical models and methods of analysis which rely on concepts from continuum electrostatics. We demonstrate in this work that a realistic Constant Potential Method model based on DFT data for gold can still consistently be described by concepts of continuum electrostatics, provided the electrostatic boundary condition is modeled correctly. Furthermore, we apply this description to determine the dielectric behavior of water in nanoporous gold. We systematically investigate the difference between conducting and inert confinement on the static dielectric response.

CPP 32.25 Thu 9:30 P3

Evaluating the Impact of Electrode Defects on PEMFC Performance and Durability — •Faezeh Mehdizadeh siahroudi[1], Sebastian Prass[1], and Andreas Bett[2] — [1]Division Hydrogen Technologies Department Fuel Cell Fraunhofer Institute for Solar Energy Systems ISE 79110 Freiburg, Germany — [2]Fraunhofer-Institut für Solare Energiesysteme ISE

According to previous research, imperfect membrane electrode assembly (MEA) manufacturing processes can lead to catalyst layer and membrane defects. Therefore, we have decided to investigate the impact of missing areas in cathode and anode electrodes on the performance and durability of polymer electrolyte fuel cell (PEMFC). Missing areas with varied sizes and configurations are used to determine a threshold at which a missing area can be considered as a crucial defect that degrades MEA components. In our work, several in-situ electrochemical techniques were used, including polarization curves, linear sweep voltammetry (LSV), cyclic voltammetry (CV), and electrochemical impedance spectroscopy (EIS) experiments. The structural changes in the electrodes and the membrane are visualized through SEM cross-sectional imaging.

CPP 32.26 Thu 9:30 P3

Hybrid electrolyte LLZO/PEO-systems: Impact of salt concentration and temperature on the structural properties close to the interface — •Laura Hölzer[1], Melania Kozdra[2], Daniel Brandell[2], and Andreas Heuer[1] — [1]Institut für physikalische Chemie, Universität Münster, Corrensstr. 28-30, 48149 Münster, Germany — [2]Department of Chemistry - Ångström Laboratory, Uppsala University, Box 538, 75121 Uppsala, Sweden

Composite electrolytes are an opportunity for creating new and improved materials as ideally they combine the advantages of different types of electrolytes. One example for this being the LLZO/PEO-system. Insights into the properties and dynamics at and around the interface can be gained by looking at the system with atomistic simulations. Previously it could be seen that over the course of a simulation there is a movement of the Li^+ ions into the crystal.[1] Here, we analyse under which conditions equilibration is possible on the simulation time scales. Molecular dynamic simulations are performed. Three different concentrations and temperatures between 400K and 700K are studied. One could see the formation of a well-defined structure around the interface, which includes an additional layer of Li ions on both sides of the crystal that in equilibrium at 700K is independent of concentration, indicating structure formation via strong enthalpic driving forces. Furthermore, interesting insight into the reorganization of the polymer and the salt due to the presence of the LLZO can be gained.

[1] Kozdra, M.; Brandell, D.; Araujo, C. M. G.; Mace, A. Physical Chemistry Chemical Physics 2024, 26, 6216-6227.

CPP 32.27 Thu 9:30 P3

Structural investigation of lithium deficient metal chlorides solid electrolytes — •Francesco Falsina — TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany

The strong demand for new and emerging sustainable energy solutions to address climate change and the requirements for increased high energy and power density have positioned solid-state batteries as a key research area. Lithium metal chlorides (LiMCl) are considered as promising candidates for next-generation batteries due to their high ionic conductivity, thermodynamic stability, and favourable mechanical properties. In this study, we investigated Li(3-3x) M(1+x)Cl6 compounds with M = Dy, Ho, Tb, and Tm using X-ray diffraction (XRD), confirming that all samples crystallize in the space group P3m1, though exhibiting partial crystallinity and high disorder without post-synthesis annealing. The effect of lithium deficiency was explored on the ionic conductivity employing Electrochemical Impedance Spectroscopy (EIS), offering further insights into their potential for solid-state battery applications.

CPP 32.28 Thu 9:30 P3

Morphology and intracrystalline dynamics of semicrystalline polyester Poly(3-hydroxy-2,2-dimethylbutyrate) — •Johann C. Holz[1], Arman Edalat[1], Kay Saalwächter[1], Thomas Thurn-Albrecht[1], and Eugene Chen[2] — [1]Martin-Luther-University, Halle, GER — [2]Colorado State University, Fort Collins, USA

Semicrystalline polymers are classified as crystal-fixed (non-diffusive) or crystal-mobile (diffusive) based on polymer chain mobility within the crystal. Crystal-fixed polymers exhibit lower crystallinity, thinner lamellae ($d_a > d_c$), and less variation in thickness ($\sigma_a > \sigma_c$). Finding a biodegradable alternative for crystal-mobile polyethylene (PE) remains a priority for sustainable research. Poly(3-hydroxybutyrate) (P3HB), a biodegradable polyester, was recently found to be crystal-mobile, but suffers from poor mechanical properties.

We here study Poly(3-hydroxy-2,2-dimethylbutyrate) (P3H$(Me)_2$B), a structurally similar polyester with methyl-groups substituted for the two α-hydrogens, to improve mechanical toughness, thermal stability, and recyclability. Our analysis of P3H$(Me)_2$B by Small-Angle X-ray Scattering (SAXS) revealed that it crystallizes in a crystal-fixed mode. This finding contrasts with the crystal-mobile behavior observed in P3HB. Wide-Angle X-ray Scattering (WAXS) corroborated the crystal structure that has already been described in literature, while also revealing previously undetected diffraction peaks. Furthermore, Nuclear Magnetic Resonance (NMR) spectroscopy enabled precise quantification of the polymer's crystallinity, facilitating accurate determination of the melting enthalpy H_f for a 100% crystalline sample.

CPP 32.29 Thu 9:30 P3

Optical properties of biosynthesized nanoscaled Eu_2O_3 for red luminescence and potential antidiabetic applications — •Hamza Mohamed — iThemba LABS, Cape Town, South Africa

This contribution reports on the optical properties of biosynthesised Eu_2O_3 nanoparticles bioengineered for the first time by a green and cost effective method using aqueous fruit extracts of Hyphaene thebaica as an effective chelating and capping agent. The morphological, structural, and optical properties of the samples annealed at 500°C were confirmed by using a high-resolution transmission electron microscope (HR-TEM), x-ray diffrac tion analysis (XRD), UV-Vis spectrocopy, and photoluminescence spectrometer. The XRD results confirmed the characteristic body-centered cubic (bcc) structure of Eu_2O_3 nanoparticles with an average size of 20 nm. HRTEM revealed square type morphology with an average size of ≈6 nm. Electron dispersion energy dispersive x-ray spectroscopy spectrum confirmed the elemental single phase nature of pure Eu_2O_3. Furthuremore, the Fourier transformed infrared spectroscopy revealed the intrinsic characteristic peaks of Eu-O bond stretching vibrations. UV-Vis reflectance proved that Eu_2O_3 absorbs in a wide range of the solar spectrum from the VUV-UV region with a bandgap of 5.1 eV. The luminescence properties of such cubic structures were characterized by an intense red emission centered at 614 nm. It was observed that the biosynthesized Eu_2O_3 nanoparticles exhibit an efficient red-luminescence and hence a potential material as red phosphor.

CPP 32.30 Thu 9:30 P3

Green synthesis of nanocellulose for archaeological wood preservation: a case study of cheops' second solar boat — •Ihab Abdelbaki — Cairo University, Egypt

The preservation of ancient wooden artifacts presents significant challenges due to environmental degradation and biological deterioration. This study addresses these challenges through the development of an eco-friendly nanocellulose-based preservation method, specifically targeting the deterioration observed in the second solar boat of king khufu (cheops), one of egypt's most significant archaeological wooden artifacts. Nanocellulose was synthesized via a green approach using controlled acid hydrolysis of agricultural waste cellulose, followed by mechanical ultrasonication. the degradation assessment of the second solar boat revealed severe biological infestation, structural weakening, and dimensional instability, particularly in areas exposed to fluctuating humidity levels. The prepared nanocellulose, characterized by TEM, FTIR and XRD, exhibited crystallite sizes of 20-30 nm and a crystallinity index of 82%. when applied to degraded wood samples from similar archaeological contexts, the nanocellulose treatment demonstrated significant improvements in mechanical strength (40% increase), dimensional stability (65% reduction in swelling), and biological resistance. Importantly, the treatment maintained the artifact's aesthetic and historical integrity while providing a sustainable, reversible preservation solution. this study presents a promising green approach for the conservation of ancient wooden artifacts, offering implications for cultural heritage preservation worldwide.

CPP 32.31 Thu 9:30 P3

Investigation of photoelectrochemically induced degradation of III-V nanowires — •Chris Y. Bohlemann, Juliane Koch, David Ostheimer, Peter Kleinschmidt, and Thomas Hannappel — Technische Universität Ilmenau, Faculty of Mathematics and Natural Sciences, Fundamentals of Energy Materials, Gustav-Kirchhoff-Str. 5, 98693 Ilmenau

Over the past two decades, nanoscale structures like III-V nanowires (NWs) have become versatile components in electronic and photonic applications [1]. The large surface-to-volume ratio of NWs enhances reaction efficiency by providing more active sites for light-driven processes. To explore NWs' potential in photoelectrochemical solar energy conversion, we investigated their optoelectronic behavior. First, GaAs NWs were grown via Vapor-Liquid-Solid growth mode using Metal-Organic Vapor Phase Epitaxy. We performed Linear Sweep Voltammetry measurements where the III-V sample was brought into direct contact with the electrolyte. However, a major challenge is the degradation in performance due to the limited durability of NWs in electrolytes compared to planar surfaces. To evaluate the corrosion of NWs in electrolytes, we analyzed the NW structures before and after two hours of stability testing measurements by Scanning Electron Microscopy. Our results indicate that under continuous illumination no significant degradation besides surface roughening is observed while samples under chopped illumination, are nearly completely etched, with few or no NWs remaining intact.

[1] J. Koch et al., Adv. Mater. Interfaces 9, 2200948, 2022.

CPP 32.32 Thu 9:30 P3

Fabrication of Gas Sensors with High Sensitivity to NO_2 Based on Photoactivation of Porous Carbon Materials — •Laura Pascual[1], Berta Pérez-Román[2], Jesús López-Sánchez[2], M. Alejandra Mazo[2], Álvaro Peña[3], David G. Calatayud[4], Daniel Matatagui[3], and Fernando Rubio-Marcos[2] — [1]Instituto de Catálisis y Petroleoquímica (ICP-CSIC), Madrid, España — [2]Instituto de Cerámica y Vidrio (ICV-CSIC), Madrid, España — [3]Instituto de Magnetismo Aplicado, (IMA-UCM-ADIF), Madrid, España — [4]Departamento de Química Inorgánica, Universidad Autónoma de Madrid (UAM), Madrid, España

The rise in gas emissions harms public health, with nitrogen dioxide (NO_2) being particularly dangerous due to its impact on the lungs and respiratory conditions. This emphasizes the need for highly selective gas sensors capable of detecting concentrations below 1 ppm in real time, while being miniaturised and operable at room temperature (RT).

Carbon-derived materials from carbides (CDC) are created through high-temperature chlorination, achieving surface areas over 2000 m^2/g. These materials feature hierarchical porosity (micro- to mesopores) and abundant active sites that support redox reactions for NO_2 detection. Incorporating heteroatoms improves charge transfer and electron-hole trap formation. The results show exceptional selectivity and sensitivity to NO_2, with detection below 1 ppm and room temperature operation using UV excitation (275 nm).

CPP 32.33 Thu 9:30 P3

Bimetallic Core-Shell-Nanoparticles for enhanced Raman spectroscopy — •Moritz Willems[1], Steffi Stumpf[1,2], and Stephanie Hoeppener[1,2] — [1]Jena Center for Soft Matter (JCSM) — [2]Institute of Organic and Macromolecular Chemistry (IOMC)

Bimetallic Core-Shell-Nanoparticles have emerged as a versatile tool for advanced sensing applications, particularly in surface-enhanced Raman spectroscopy and tip-enhanced Raman spectroscopy. The combination of two metals in a Core-Shell configuration enhances the plasmonic properties and allows for extended plasmonic bandwidths, as well as superior electromagnetic field amplification in comparison to the monometallic nanoparticles. Silver nanoparticles have been demonstrated to offer effective enhancements for Raman spectroscopy. However, they do present certain challenges, including a narrow spectral range, poor chemical stability, and a relatively short lifespan. The coating of silver nanoparticles with a thin gold shell promises precise control over localised surface plasmon resonance, expanding spectral ranges for Raman spectroscopy measurements, especially between the peaks of gold and silver, by changing the relative thickness of the shell. Furthermore, the gold coating allows for measurements in water, while also providing a prolonged lifespan. The synthesis of these nanoparticles utilizes chemical reduction by microwave irradiation, providing fast, energy efficient and uniform heating. Various methods have been tested to overcome the problems of synthesising a gold shell on silver, and detailed transmission electron microscopy and UV-Vis spectroscopy analysis complement the Raman spectroscopy results.

CPP 32.34 Thu 9:30 P3

Classical simulation studies of dissociation equilibria in nanoconfined systems — •Kira Fischer, Henrik Stooss, and Alexander Schlaich — Institute for Atomistic Modeling of Materials in Aqueous Media, Hamburg University of Technology, Germany

Dissociation equilibria in nanoconfinement are relevant to the chemistry of nanostructured catalysts, aerosols and protein pockets. Experiments indicate that nanoconfinement affects the dissociation of water, however to date a comprehensive understanding is still lacking. Here, we investigate dissociation equilibria in nanoconfinement from a classically. Using molecular dynamics and free energy methods we study hydrochloric acid in diamond nanoconfinement in the dilute limit at ambient conditions.

Our studies reveal a depletion of hydrochloric acid in nanoconfinement, with a negative excess by up to a factor of 100. The negative excess is attributed to the balance between hydronium adsorption and chloride depletion at the interface. Additionally, we propose that hydronium is adsorbed to the diamond interface by dipole orientation within a local electric field. Notably, in the smallest pore, the $\mathrm{p}K_\mathrm{a}$ is increased by 1. We also introduce useful concepts for analysing dissociation equilibria in confinement. This includes the chemical potential in confinement, which enables quantification of ionic excess in the dilute limit. Furthermore, we demonstrate how to derive the chemical potential from the potential of mean force, thereby decomposing the different energetic contributions to the excess chemical potential.

CPP 32.35 Thu 9:30 P3

Gas quenching under ambient conditions for efficient and stable inverted perovskite solar cells with surface treatment — •Zhaonan Jin, Xiongzhuo Jiang, Zerui Li, Xiaojing Ci, Guangjiu Pan, Kun Sun, and Peter Müller-Buschbaum — TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany

Inverted perovskite solar cells have gained significant attention due to their potential for high efficiency and stability. In the process, the active layer fabrication plays a key role in determining the performance of the solar cells. Gas quenching is an important technique in the preparation of perovskite solar cells as it enhances the film quality and solar cell performance by precisely controlling the crystal growth and minimizing defects. As for the post-treatment of the active layer, surface passivation plays a crucial role in enhancing the performance of perovskite solar cells by reducing surface defects of perovskite interfaces. This study explores the influence of different passivation materials on the morphology of perovskite films and the performance of gas-quenching assisted FA0.8Cs0.2Pb(I0.6Br0.4)3 solar cells. This work provides a practical solution for the production of low-cost and high-performance inverted perovskite solar cells while maintaining operational stability in real-world environments.

CPP 32.36 Thu 9:30 P3

Facet-dependent photovoltaic efficiency and stability variations in mixed Sn-Pb perovskite solar cells — •Xiaojing Ci, Xiongzhuo Jiang, Guangjiu Pan, Jinsheng Zhang, Zerui Li, Kun Sun, and Peter Müller-Buschbaum — TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany

Since the first breakthrough of perovskite solar cells using a solid-state structure, the solar cell power conversion efficiency has increased from 9.7% to 26%. These exciting improvements are mainly attributed to achieving a pinhole-free thin film at the beginning and an increased understanding of microstructures on perovskite thin films. In addition, the rapid PCE improvement has been accompanied by an increased understanding of microstructures on perovskite thin films. The photovoltaic performance of PSCs has been found to correlate strongly with their facet orientations. For example, the charge carrier lifetime, open-circuit voltage deficit and device hysteresis of PSCs are related to the structure and density in (111) crystal facets of perovskite. Besides, different crystal facets have different atomic arrangements and coordination, which lead to different atomic potential landscapes and, subsequently, to different electronic, physical, and chemical properties. Nevertheless, the deep understanding of perovskite thin films, especially the crystal facets of the thin film, still lags behind that of single-crystal samples or other inorganic thin films. In this work, we prepare the mixed tin-lead perovskite film with different orientations according to the facet engineering. We research the role of the different perovskite crystal facets in stability and optoelectronic properties.

CPP 32.37 Thu 9:30 P3

Processing-property relationships in printed hybrid halide perovskites — •Manuel Lippert[1], Meike Kuhn[1], Maximilian Spies[2], Anna Köhler[2], and Eva M. Herzig[1] — [1]Dynamik und Strukturbildung - Herzig Group, Universität Bayreuth, Universitätsstr. 30, 95447 Bayreuth, Germany — [2]Optoelektronik weicher Materie, Universität Bayreuth, Universitätsstr. 30, 95447 Bayreuth, Germany

Solution processable hybrid halide perovskites solar cells have been extensively studied over the last ten years and great advances in efficiency have been achieved. An important factor for the performance of the final solar cell is the morphology of the perovskite layer. Therefore, control of structure formation mechanisms is highly desirable. [1] We investigate systematically the processing of the active layer to determine processing parameters that are decisive for structure formation. To reliably study the effect of time relevant processing steps on the perovskite layer, we use automated processing. Applying photoluminescence, optical microscopy and grazing incidence wide angle X-ray scattering (GIWAXS) allows us to determine the morphology on the nano and micron scale and detect the correlations between processing and efficiency.

[1] Meike Kuhn, Felix A. Wenzel, Christopher Greve, Klaus Kreger, Matthias Schwartzkopf, Hans-Werner Schmidt, Helen Grüninger, Eva M. Herzig, Tailored Supramolecular Additives to Control the Crystallization Process and Morphology of MAPbI3, *submitted*

CPP 32.38 Thu 9:30 P3

Simulating light induced phase separation in $\mathbf{MAPbBr_{1.8}I_{1.2}}$ perovskites — •Sebastian Schwartzkopff, Ivan Zaluzhnyy, Ekaterina Kneschaurek, Paul Zimmermann, Dmitry Lapkin, Hans Mauser, Alexander Hinderhofer, and Frank Schreiber — University of Tübingen

By changing the ratio of halides within mixed organic halide perovskites, such as $MAPbBr_{1.8}I_{1.2}$ (MA -methylammonium), one can adjust the band gap. This is quite desirable for solar cell applications where precisely tunable bandgaps enable the creation of high efficiency solar cells. However, when illuminated with visible light, these materials undergo a phase separation into Br-rich and I-rich phases, which destroys the tuned band gap. To better understand; and hopefully control this process, we utilize phenomenological approaches, such as Cahn-Hilliard and Monte Carlo models, to simulate the light-induced phase separation. We compared the results of our simulations with the experimental diffraction data. Cahn-Hilliard simulations presented quite a few difficulties in replicating the observations. The Monte Carlo simulations on the other hand allow us to investigate the influence of various material parameters on the phase separation, such as iodine-to-bromine ratio, charge carrier density and intensity of illumination. In general, we found that Monte Carlo simulations with the right choice of model parameters are quite capable of reproducing the experimental observations.

CPP 32.39 Thu 9:30 P3

Enhanced Stability of Perovskite Solar Cells via Double-End Coupling Silane — •Xinwei Tian, Xiongzhuo Jiang, and Peter Müller-Buschbaum — TUM School of Natural Science, Chair for Functional Materials, 85748 Garching, Germany

Containing reactive triethoxysilyl groups, 1,4-bis(triethoxysilyl)benzol (BTEB) has high thermal stability by forming robust siloxane networks through hydrolysis and condensation reaction. Besides, BTEB has good hydrophobicity, so it can function as a protective barrier to prevent moisture ingression into the sample, which ensures long-term operation of the perovskite solar cells (PSCs). BTEB can also passivate the interface defect, thus reducing non-radiative recombination. On the other hand, because of the surface passivation effect of BTEB, a smoother and more uniform film layer can be obtained, which can enhance light absorption and reduce scattering loss effectively. In this way, the power conversion efficiency (PCE) can also be improved. In our work, we aim to apply BTEB as the interface modification material, ethyl acetate as antisolvent, to construct inverted perovskite solar cells with higher efficiency and stability.

CPP 32.40 Thu 9:30 P3

Morphology Control and Optical Modelling of $\mathbf{CsPbBr_3}$ Nanocrystal Films for Emission Orientation Studies — •Lea Kolb, Roshini Jayabalan, and Wolfgang Brütting — Universität Augsburg, 86135 Augsburg, Germany

The remarkable properties of $CsPbBr_3$ perovskite nanocrystals, exhibiting a high photoluminescence quantum yield (PLQY) and a narrow emission linewidth with size- and composition-tunable bandgap, render them promising for the application as emitters in light-emitting diodes (LEDs). While PLQY and charge carrier transport for perovskite LEDs have been in the focus of extensive studies, the orientation of the emissive transition dipole moment (TDM) has not been investigated thoroughly yet. However, for TDM analysis, determining the complex refractive index of the nanocrystal films is crucial. In this work, variable angle spectroscopic ellipsometry (VASE) was used to obtain the optical constants of various samples containing $CsPbBr_3$ nanocrystals. To avoid scattering effects, VASE measurements require homogeneous films with minimal roughness. For this reason, the substrates on which the nanocrystal films were spin-coated had to be modified and the sample fabrication process was optimized. In order to describe the measured data accurately with optical fit models, the morphology and thickness of the films were studied comprehensively by atomic force microscopy (AFM). Finally, angular dependent photoluminescence (ADPL) measurements have been performed and modelled in order to obtain information about the TDM-orientation.

CPP 32.41 Thu 9:30 P3

PIN-type perovskite solar cells for space applications — •Ruodong Yang, Simon A. Wegener, and Peter Müller-Buschbaum — TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany

Perovskite solar cells have advantages such as low costs and high power-to-weight ratio, which render them to be promising candidates for space applications, where the mass is crucial for launch costs. In this study PIN-type solar cells are investigated. With its inverted p- and n-type structure, it has great research potential. However, solar cells in space also face challenges, such as vacuum, extreme temperature fluctuations during each orbit, and high radiation levels. The purpose of this study is to optimize the manufacturing procedure of PIN-type perovskite solar cells to address these challenges. We investigate the power conversion efficiency of the solar cells under similar environmental conditions to the low Earth orbit with illumination from an AM0 light source and thermal cycling by using optical microscopy to observe the structural changes during the operation. With the results of the measurements, the manufacturing procedure will be optimized, to determine the key factors to improve the performance and efficiency of PIN-type cells under space conditions.

CPP 32.42 Thu 9:30 P3

Perovskite solar cells temperature dependence under space-like conditions — •Anthony Vizcaino, Simon Alexander Wegener, and Peter Müller-Buschbaum — TUM School of Natural Sciences, Chair of Functional Materials, 85748 Garching, Germany

In recent years, perovskites have attracted the scientific community's attention due to their properties and possible applications, making their use in solar cells one of the most relevant. Their high-power conversion efficiency, power-to-weight ratio, and manufacturing compared to the to-date used multi-junction devices make them a promising device for space applications, where it is possible to take advantage of all the intensity of sunlight that at the Earth*s surface is lost by absorption or scattering by the atmosphere. However, in this scenario, radiation and high temperatures would affect the solar cell. This study focuses on one of these problems and tries to understand how extreme temperatures and thermocycling through large periods of heating and cooling encountered in low Earth*s orbit affect perovskite solar cell performance and degradation. Operando studies allow to simulate thermal cycling conditions and measure the transmittance of solar cells, which combined with electrical characteristics from I-V measurements and active layer morphology from GIWAXS give us a robust knowledge of the temperature dependence of perovskite-based solar cells.

CPP 32.43 Thu 9:30 P3

In-situ Monitoring for Optimizing Perovskite Solar Cell Fabrication: Correlating Process Parameters with Power Conversion Efficiency — •Yuxin Liu, Alexander Tarasov, Maxim Simmonds, and Eva Unger — Department Solution Processing of Hybrid Materials and Devices, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, 12489 Berlin, Germany

Halide perovskite solar cells need dependable, reproducible production to reach commercialization. For stable perovskite photovoltaic manufacture and research, deposition processes must be monitored. In-situ photoluminescence (PL) monitoring compares the PL during spin-coating and annealing with absolute PL measurements obtained after annealing of the sample. Examples demonstrating how process conditions and variables like anti-solvent type and drip timing significantly influence PL signatures. We demonstrate that insight during processing can serve as feedback to stabilize the perovskite solar cell fabrication. In-situ PL monitoring shows two distinct peaks within one second of anti-solvent treatment, revealing perovskite nucleation and growth mechanism. All Helmholtz association perovskite PV research uses a standard operating procedure (SOP) for solar cell samples. Absolute PL measurements for thin-film samples quantify Quasi-Fermi Level Splitting, reflecting the opto-electronic quality of the absorber and losses at selective contacts. The absolute PL is correlated to the in-situ PL to establish how far in-situ PL during processing can predict solar cell performance. This study highlights the potential of optical process monitoring to enhance material and interface quality.

CPP 32.44 Thu 9:30 P3

The Construction of Temperature Gradient during Annealing to Guide Crystallization Direction — •Yiran Shi — Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany

Perovskite solar cells have gained significant attention as promising candidates for next-generation photovoltaics due to their outstanding advantages. The quality of the perovskite layer is a crucial determinant of the efficiency and stability of photovoltaic devices. As a polycrystalline thin film, the size and compactness of crystals are key quality metrics, closely linked to the annealing process. Conventional annealing typically involves placing the thin film, post-nucleation, on a fixed-temperature heating platform for crystal growth. Without external guidance, crystallization usually progresses top-down, preferentially completing at the upper surface. This sequence often traps solvents within the film, hindering evaporation and leading to void formation, which negatively affects film quality and device performance. To address this issue, we propose an improved annealing strategy by introducing a vertical thermal gradient to guide a bottom-up crystallization process. This approach aims to delay top-surface crystallization, allowing solvents to escape more effectively and reducing void formation. From the results about SEM and GIWAX, it is improved film quality, with enhanced structural integrity and reduced defects, offering a pathway to optimize perovskite photovoltaic performance.

CPP 32.45 Thu 9:30 P3

Optimizing RbCsFAMA perovskite solar cells with piperazine-inspired passivation technique — •Bashudev Bhandari[1,2,3], Zekarias Teklu Gebremichael[1,2], Niklas Manikowsky[2,3], 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 — [2]Faculty of Physics and Astronomy, Friedrich-Schiller- University Jena, Jena, Germany — [3]Laboratory of Organic and Macromolecular Chemistry (IOMC Jena), Friedrich-Schiller- University Jena, Jena, Germany

Perovskite solar cells (PSCs) have emerged as a promising photovoltaic technology, with extraordinary optoelectronic properties. However, stability and defects are the challenges of perovskite solar cells. This work explores the role of piperazine as a novel passivating agent to address these limitations. Piperazine's bifunctional structure enables effective defect passivation at the grain boundaries and interfaces of RbCsFAMA perovskite films, significantly reducing non-radiative recombination losses. Different characterization and imaging techniques photoluminescence spectroscopy, X-ray diffraction and scanning electron microscopy demonstrate improved crystallinity and electronic properties of the RbCsFAMA perovskite films after passivation. This improvement is shown to be transferred into solar cell devices.