CPP 15: Poster Session I

Time: Monday 19:00–21:00 Location: P4

CPP 15.1 Mon 19:00 P4

Exploring Green Solvent Additives for Enhanced Solubility in Organic Photovoltaics Processing — •Leonhard Schatt, Fabian Eller, and Eva M. Herzig — Dynamik und Strukturbildung - Herzig Group, Universität Bayreuth, Universitätsstr. 30, 95447 Bayreuth, Germany

Organic Photovoltaic (OPV) devices offer the potential for low-cost production of devices that convert light into electricity. These devices are typically processed from solution, which allows for simple, scalable production methods such as printing. However, the solvents used by most research groups are halogenated aromatic solvents, as green solvents often lack good solubility for the solutes used. We are therefore experimenting with additives in green solvents as a method of tuning solubility. We monitor the solubility with in-situ solubility measurements to study the effects of additive type and volume fraction. This will allow us to map the solubility space of the high performance OPV material PM6. Our aim is to contribute to the replacement of halogenated solvents for OPV processing and to make our organic electronic material processing feasible for industrial applications.

CPP 15.2 Mon 19:00 P4

Comparing Machine Learning Force Fields for Proton Transfer Dynamics in Solid Acids — •Jules Oumard, Aaron Flötotto, and Christian Dressler — Technische Universität Ilmenau, Fakultät für Mathematik und Naturwissenschaften, Institut für Physik, Fachgebiet Theoretische Festkörperphysik, Weimarer Straße 32, 98693, Ilmenau

Solid acids are excellent water-free proton conductors and can be used in fuel cells. [1]. The rarity of long-range proton transfer events in ab initio molecular dynamic simulations makes the calculation of converged diffusion coefficients challenging. This can be overcome by accelerating these simulations with machine learning force fields (MLFF). We compare two MLFF approaches: Gaussian Approximation Potentials (GAP) with on-the-fly learning [2] and equivariant graph neural networks [3]. A protocol for fine-tuning GAP models is presented. We evaluate the calculated diffusion coefficients and explain trends in terms of jump rate functions and anion rotation rates.

[1] Mohammad, N. et al. (2016). Journal of Power Sources, 322, 77-92. doi:10.1016/j.jpowsour.2016.05.021

[2] Jinnouchi, R. et al. (2019). Physical Review B, 100(1), 014105. doi:10.1103/PhysRevB.100.014105

[3] Batatia, I., et al. (2022). Advances in Neural Information Processing Systems. https://openreview.net/forum?id=YPpSngE-ZU

CPP 15.3 Mon 19:00 P4

Towards Theoretical UV/Vis Spectra with Experimental Accuracy. Benchmarks for Spiropyran Photoswitches — •Robert Strothmann[1], Johannes T. Margraf[2], and Karsten Reuter[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]University of Bayreuth

Molecular photoswitches are molecules that undergo an isomerization upon irradiation with specific wavelengths. One key feature for understanding this process are the UV/Vis spectra of the involved species (e.g. the closed and open forms in the case of spiropyran, SP). First-principles methods like density-functional theory (DFT) allow the calculation of UV/Vis spectra within certain approximations. However, the properties of the chosen functional, the description of solvation, as well as the accuracy of conformational and vibrational sampling all contribute to discrepancies between theory and experiment. This motivates us to establish a rigorous theoretical approach to assist in the prediction and analysis of UV/Vis spectra for molecular photoswitches. As a crucial step, we here benchmark different approaches for predicting UV/Vis spectra of SP switches against experimental references. We emphasize the influence of different functional approximations and highlight the role of the conformational ensemble and molecular vibrations sampling (e.g. via by machine learning enhanced molecular dynamics simulations). The importance of these different effects is discussed, with the goal of providing best practice guidelines that enable robust predictions.

CPP 15.4 Mon 19:00 P4

Optical properties of diamondoid organotin sulfur clusters with fluorescent ligands — •Alexander Schauerte[1], Jie Wang[2], Felix Thomas[1], Irán Rojas León[2], Stefanie Dehnen[2], and Marina Gerhard[1] — [1]Faculty of Physics and Material Sciences Center, Philipps-University of Marburg, Renthof 7a, D-35032 Marburg, Germany — [2]Institute of Nanotechnology, Karlsruhe Institute of Technology, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

White light is important in our daily life as well as in technology and research. It has been shown that diamondoid organotin clusters with organic ligands emit a brilliant white light beam when pumped with an infrared laser.

We investigate the fluorescent properties of tin-sulfur/selenium clusters with three phenyl- and one tetraphenylethylene ligands using photoluminescence- and spatially resolved photoluminescenceexcitation- spectroscopy. Through temperature-dependent measurements of compounds prepared as glass and as powder, we conclude that the electron-phonon-coupling and short-range ordering seems to be reduced in a glass state compared to a powder.

Furthermore, we investigate the white light generation (WLG) and second harmonic generation of different cluster compounds, which show a dependence of the WLG-efficiency on the chemical composition. The glass has a lower excitation power threshold for WLG than the powder.

CPP 15.5 Mon 19:00 P4

Electromagnetic Compatibility Measurements of Polymers in the Automotive Industry: Shielding Effectiveness According to ASTM D 4935 — Leopold Handke, Nicola Peranio, and •Verena Cerna — Technische Hochschule Ulm, Ulm, Deutschland

Electromagnetic compatibility (EMC) is a key concern in the automotive industry due to the growing complexity of vehicle electronic systems and the need to prevent electromagnetic interference that could affect their performance and safety. Polymers used in automotive components must meet specific EMC requirements to ensure proper functioning of vehicle electronics. This study investigates the shielding effectiveness (SE) of various polymer materials using standardized measurements according to ASTM D 4935. Shielding effectiveness for both magnetic (B-field) and electric (E-field) fields was measured over a frequency range from 50 kHz to 3 GHz. SE measurements provide valuable insights into the frequency-dependent shielding properties of plastics, offering a basis for selecting appropriate materials for automotive applications to address EMC challenges.

CPP 15.6 Mon 19:00 P4

Time-resolved structure formation in biohybrid coatings revealed by in-situ GISAXS and machine learning — •Julian E. Heger[1], Shachar Dan[2], Yufeng Zhai[2], Stephan V. Roth[2,3], and Peter Müller-Buschbaum[1] — [1]1TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — [3]Department of Fibre and Polymer Technology, KTH Royal Institute of Technology, Stockholm, Sweden

Relationships between the structure and property of functional films are at the heart of material science, which makes understanding of how film morphology influences its function essential. Achieving a comprehensive and statistically relevant understanding of the film's characteristics often requires the use of indispensable tools like grazing-incidence small-angle X-ray scattering (GISAXS). GISAXS enables the exploration of the film's characteristic morphology in reciprocal space, such as characteristic size distributions. However, a challenge arises due to the loss of phase information during measurements, which inhibits a direct transformation from reciprocal space to real space via inverse Fourier transform. In addressing this obstacle neural networks (NN) emerge as promising solutions, as they offer potential ways to enable a fast transformation of GISAXS data. Here, we present the results of applying a NN which is trained on synthetic GISAXS data to evaluate the film formation of biohybrid coatings during deposition from in-situ GISAXS synchrotron data.

CPP 15.7 Mon 19:00 P4

Simulation-Based Neural Network with Embedded Prior

Knowledge for Predicting Morphological Parameters in GISAXS — •Shachar Dan[1], Eldar Almamedov[2], Matthias Schwartzkopf[1], Sven-Jannik Wöhnert[1], Andre Rothkirch[1], Yufeng Zhai[1], Jose I. Robledo[4], Volker Skwarek[2], and Stephan V. Roth[3] — [1]DESY, Notkestraße 85, D-22607 Hamburg — [2]HAW, Berliner Tor 5, D-20099 Hamburg — [3]KTH, Teknikringen 56 SE-10044 Stockholm — [4]FZ-Jülich, Wilhelm-Johnen- Straße D-52428 Jülich

In-situ grazing-incidence small-angle X-ray scattering (GISAXS) is a powerful technique for analyzing nanoscale structures, yet its interpretation is challenging due to the inverse problem caused by phase information loss. Advances in simulation software and deep learning techniques have opened the door to the idea of using simulations, which can now be generated more efficiently in diverse configurations, to train neural networks (NNs). However, simulations often fail to fully represent experimental data, creating a significant sim-to-real gap. In our work, we tackle this challenge by embedding prior knowledge about the system into the NN training process. By incorporating constraints based on this knowledge, we train models on simulations and apply them to experimental data, enabling reasonable predictions of morphological parameters such as cluster radii, inter-cluster distances, and grain size distributions. This approach aims to accelerate material characterization at the nanoscale and provide a portable and efficient counterpart to traditional methods.

CPP 15.8 Mon 19:00 P4

Low-Temperature Photoluminescence Characterization of Hybrid Metal Halides — •Anton Krüger[1], Meng Yang[2], Alexander Schauerte[1], Dominik Muth[1], Johanna Heine[2], and Marina Gerhard[1] — [1]Faculty of Physics and Material Sciences Center, Philipps-Universität Marburg, Renthof 5, D-35032 Marburg, Germany — [2]Faculty of Chemistry, Philipps-Universität Marburg, Hans-Meerwein-Straße 4, D-35032 Marburg, Germany

In order to remove the toxic lead component of the otherwise promising perovskite materials, many different approaches have been pursued.
Here, the photoluminescence (PL) and absorption properties of crystalline non-toxic hybrid main group metal halide compounds, (α-Me-2-NA)$_4$E$_2$X$_{10}$ (NA=Naphthylmethylammonium, E=Sb/Bi, X=Halide) are investigated by means of time-resolved PL spectroscopy, steady-state PL spectroscopy as well as PL excitation spectroscopy.
It is shown that the absorption and PL properties of these materials depend on the metal/halide composition, giving rise to a variety of absorbers and emitters. Furthermore, temperature dependent spectroscopic experiments reveal a thermochromic behavior of the compounds.

CPP 15.9 Mon 19:00 P4

Effect of fluorinated tail groups on the properties of aromatic self-assembled monolayers — Yangbiao Liu[1], Sonja Katzbach[2], Andreas Terfort[2], and •Michael Zharnikov[1] — [1]Angewandte Physikalische Chemie, Universität Heidelberg, 69120 Heidelberg, Germany. — [2]Institut für Anorganische und Analytische Chemie, Johann Wolfgang Goethe Universität Frankfurt, 60438 Frankfurt am Main, Germany

Electric transport properties of functional self-assembled monolayers (SAMs) are important for interface engineering in organic electronics and molecular electronics. As was shown recently, substituting only one terminal hydrogen atom in SAMs with a halogen atom changes their electric conductance noticeably. In this context, we studied the respective effects in a series of non-substituted and methyl-substituted biphenylthiolate (BPT) SAMs on Au(111), exchanging the terminal hydrogen atom/atoms for fluorine/fluorines and testing not only single-component but binary SAMs as well. The gradual variation of the work function with the SAM composition was accompanied by a gradual variation of electrical conductance, decreasing, in particular, by two orders of magnitude at going from CH3-BPT to CF3-BPT SAMs. The observed behavior was tentatively explained by the higher projected density-of-states at the position of the terminal tail groups in the CH3-BPT (H-BPT) case compared to CF3-BPT (F-BPT) and by the appearance of an internal electrostatic field in the SAMs, leading to a change and renormalization of the energy level alignments within the junction upon contact of the SAMs to the top EGaIn electrode.

CPP 15.10 Mon 19:00 P4

Charge separation in a porphyrin-based metal-organic framework incorporating fullerene — •Martin Richter[1], Xiaojing Liu[2], Pavel Kolesnichenko[1], Christof Wöll[2], and Petra Tegeder[1] — [1]Physikalisch-Chemisches Institut, Universität Heidelberg, Germany — [2]Institut für Funktionelle Grenzflächen, Karlsruher Institut für Technologie, Germany

Porphyrin-based materials are attracting great interest due to their wide range of potential applications. They can be embedded into metal-organic frameworks (MOF) to manipulate and investigate the relations between function and structure. In conjunction with an electron acceptor, charge separation can be achieved, which is beneficial for applications such as solar cells or photocatalysis. Experiments on ZnTPP (Zinc 5,15-bis-(3,4,5-trimethoxyphenyl)-10,20-bis-(4-carboxyphenyl)) in a surface-anchored MOF (SURMOF) with fullerene C$_{60}$ loaded into the pores, have demonstrated that photoexcitation can enhance the conductivity by up to two orders of magnitude [1]. Here, we investigate excited states dynamics after optical excitation with transient absorption spectroscopy on the femto- to nanosecond time scale. Charge separated states can be identified, which have a lifetime of 212-360 ps. The charge separation occurs after excitation of both the Soret band and the Q band within only a few hundred femtoseconds.

References

[1] X. Liu et al., Angew. Chem. Int. Ed. 2019, 58, 9590.

CPP 15.11 Mon 19:00 P4

Structural influences on nonlinear optical activity for supercontinum generation: isolated cubane — •Alexander Kapp and Simone Sanna — Institute for Theoretical Physics, 35392 Gießen, Germany

It has been suggested that adamantane-based molecular clusters can convert a narrowband laser source into a broadband supercontinuum. Unlike thermal emitters, the resulting spectra are coherent and not constrained by Planck's law, making them highly valuable for various applications, such as high-resolution monitoring and spectroscopy.

In order to expand our library of suitable molecules, we investigate the electronic and optical properties of materials with similar symmetry. This involves performing first-principle density functional theory calculations to identify appropriate structures. Here, we focus specifically on isolated cubane (C_8H_8) molecules and their derivatives, analyzing their electronic and structural properties and their correlation with the optical response.

CPP 15.12 Mon 19:00 P4

Impact of Classical and Quantum Light on Donor-Acceptor-Donor Molecules — •Haraprasad Mandal[1,2], Sajal Kumar Giri[3], Sara Jovanovski[1], Oleg Varnavski[1], Malgorzata Zagorska[4], Roman Ganczarczyk[4], Tse-Min Chiang[3], George C. Schatz[3], and Theodore Goodson III[1] — [1]Department of Chemistry, University of Michigan, Ann Arbor, Michigan 48109, United States — [2]Department of Chemistry, University of Graz, Heinrichstrasse 28, 8010 Graz, Austria — [3]Department of Chemistry, Northwestern University, Evanston, Illinois 60208, United States — [4]Faculty of Chemistry, Warsaw University of Technology, Noakowskiego 3, 00-664 Warsaw, Poland

Investigations of entangled and classical two-photon absorption have been carried out for six donor (D)-acceptor (A)-donor (D) compounds containing the dithieno pyrrole (DTP) unit as donor and acceptors with systematically varied electronic properties. Comparing ETPA (quantum) and TPA (classical) results reveals that the ETPA cross section decreases with increasing TPA cross section for molecules with highly off-resonant excited states for single-photon excitation. Theory (TDDFT) results are in semiquantitative agreement with this anticorrelated behavior due to the dependence of the ETPA cross section but not TPA on the two-photon excited state lifetime. The largest cross section is found for a DTP derivative that has a single photon excitation energy closest to resonance with half the two-photon excitation energy. These results are important for the possible use of quantum light for low-intensity energy-conversion applications

CPP 15.13 Mon 19:00 P4

Correlating molecular properties to the SHG response: Prerequisites for white light generation. — •Ferdinand Ziese and Simone Sanna — Institut für Theoretische Physik and Center for Materials Research (LaMa), Justus-Liebig-Universität Gießen, 35392 Gießen, Germany

Recent studies have demonstrated white light generation from molecular clusters with adamantane-like cores and different substituents [1,2]. Systematic investigations further our understanding of the origin of this behavior, we have investigated structural, electronic, and (nonlinear) optical properties from first principles for isolated molecules [3].

Core modifications mostly change the characteristic of the response in a more subtle manner while the exchange of substituents exhibit a greater impact. Distinct changes to the intensity, energy, and characteristic can be observed. The presented results provide a theoretical foundation for the design of tailored nonlinear optical sources.

[1] N. W. Rosemann, J. P. Eußner, A. Beyer, S. W. Koch, K. Volz, S. Dehnen, S. Chatterjee, Science 2016, 352, 1301

[2] N. W. Rosemann, J. P. Eußner, E. Dornsiepen, S. Chatterjee, S. Dehnen, J. Am. Chem. Soc. 2016 138 (50), 16224-16227

[3] Ziese, F., Wang, J., Rojas León, I., Dehnen, S., Sanna, S., 2024. J. Phys. Chem. A 128, 8360-8372

CPP 15.14 Mon 19:00 P4

Effect of Deposition Rates on the Morphology and Efficiency of Blue TADF OLEDs — •Tolga Durmus, Marius Schnapp, Ahmed Mohamed, Vladimir Dyakonov, and Andreas Sperlich — Experimental Physics 6, University of Würzburg, 97074 Würzburg, Germany

The efficiency and stability of blue thermally activated delayed fluorescence (TADF) OLEDs are strongly influenced by the structural properties of their active layers. In this study, we investigate the impact of varying deposition rates on the morphology of these layers, focusing on their amorphous or crystalline nature. Atomic force microscopy (AFM) is used to analyze the surface morphology of the deposited layers and we aim to establish a correlation between the deposition conditions, the structural properties of the layers, and the efficiency of the OLEDs. These investigations are expected to provide valuable insights into optimizing fabrication parameters for improved blue TADF-OLEDs.

CPP 15.15 Mon 19:00 P4

Temperature-dependent Transient Electroluminescence of Blue TADF OLEDs — •Klara-Maria Bögle, Felix Kübert, Ahmed Mohamed, Vladimir Dyakonov, and Andreas Sperlich — Experimental Physics 6, Julius-Maximilians-Universität Würzburg, 97074 Würzburg, Germany

Third generation OLEDs use, in contrast to first and second generation OLEDs, ambient thermal energy to increase fluorescence, so-called Thermally-Activated Delayed Fluorescence (TADF). This is achieved via reverse inter-system crossing (*rISC*), which means that non-radiative triplet excitons are up-converted to radiative singlet excitons. This process significantly increases the internal quantum efficiency, up to 100%. In this study, OLEDs with the multiple resonance blue TADF emitter ν-DABNA embedded in an mCP matrix are investigated. Transient electroluminescence (EL) reveals a strong temperature dependence, which we model with rate equations to better understand the TADF process in an OLED under operating conditions. The rate equations describe the population densities of the triplets, singlets and charge carriers using the different rates of *(r)ISC*, triplet-triplet annihilation (*TTA*), triplet-polaron annihilation (*TPA*) as well as the (non-) radiative singlet/triplet decay rates. Traditionally, such analysis is often based on transient photoluminescence at room temperature, which also lacks charge carrier contributions and is thus inconclusive. We therefore aim to get a full picture of *all* population densities and recombination mechanisms to better understand efficiency limiting processes.

CPP 15.16 Mon 19:00 P4

Porous poly(ethylene glycol) films as a versatile platform for ssDNA immobilization and hybridization — Zhiyong Zhao and •Michael Zharnikov — Angewandte Physikalische Chemie, Universität Heidelberg, 69120 Heidelberg, Germany

Poly(ethylene glycol) (PEG) films, fabricated by thermally induced crosslinking of amine and epoxy-terminated four-arm STAR-PEG precursors, were used as porous and bioinert matrix for single-stranded DNA (ssDNA) immobilization and hybridization. The immobilization relied on either the reaction between the amine groups in the PEG matrix and N-hydroxy succinimide (NHS) ester groups of the NHS-ester-decorated ssDNA or the reaction between the epoxy groups in the matrix and thiol groups of the respectively substituted ssDNA. The mixing ratio of the precursors was varied to tune the density of the amine and epoxy groups available for the immobilization. Spectroscopic and electrochemical data confirmed the successful immobilization of the ssDNA probes into the PEG matrix as well as the high hybridization efficiency, selectivity, and sensitivity of the resulting DNA sensors. Whereas these sensors were equivalent to the direct ssDNA assembly in terms of efficiency, they exhibited better selectivity and bioinert properties because of the bioinert character of the PEG matrix. The above findings place PEG films as a promising platform for highly selective ssDNA sensing, leveraging their flexible chemistry, 3D character, and bioinert properties.

CPP 15.17 Mon 19:00 P4

The effect of spherical nanoceria on the anionic polysaccharides and in vitro behavior as a wound dressing — •Alexandra Feraru[1,2], Zsejke-Réka Tóth[2], Klára Magyari[2,3], Monica Baia[4,5], Tamás Gyulavári[6], Emoke Páll[7], Emilia Licarete[8], Codrut Costinas[1,5], Oana Cadar[9], Ionel Papuc[7], and Lucian Baia[2,4,5] — [1]Doctoral School of Physics, Babes-Bolyai University, M. Kogălniceanu 1, 400084 Cluj-Napoca, Romania — [2]Nanostructured Materials and Bio-Nano-Interfaces Center, Interdisciplinary Research Institute on Bio-Nano-Sciences, Babes-Bolyai University, T. Laurian 42, 400271 Cluj-Napoca, Romania — [3]INSPIRE Research Platform, Babes Bolyai University, 400084, Cluj-Napoca, Romania — [4]Faculty of Physics, Babes-Bolyai University, M. Kogălniceanu 1, 400084 Cluj-Napoca, Romania — [5]Institute for Research-Development-Innovation in Applied Natural Sciences, Babes-Bolyai University, Fântânele 30, 400294, Cluj-Napoca, Romania — [6]Department of Applied and Environmental Chemistry, University of Szeged, Rerrich B. sqr. 1, Szeged 6720, Hungary — [7]Faculty of Veterinary Medicine, University of Agricultural Science and Veterinary Medicine, 400372 Cluj-Napoca, Romania — [8]Faculty of Biology and Geology, Babes-Bolyai University, 400015 Cluj-Napoca, Romania — [9]INCDO-INOE 2000, Research Institute for Analytical Instrumentation, 67 Donath Street, 400293 Cluj-Napoca, Romania

In this study, we aimed to enhance the understanding of how chemical bonds form when sodium alginate and gum arabic interact with nanoceria nanoparticles.

CPP 15.18 Mon 19:00 P4

Programming fibril alignment and mechanical response in electron beam-modified collagen type I fibers — •Friedrich Schütte[1,2], Anastassiya Bublikova[1,2], and Stefan G. Mayr[1,2] — [1]Division of Surface Physics, Department of Physics and Earth System Sciences, University of Leipzig, Linnéstr. 5, 04103 Leipzig — [2]Leibniz Institute of Surface Engineering (IOM), Permoserstr. 15, 04318 Leipzig, Germany

Modifying collagenous systems for tendon and tissue replacements in a controlled manner to produce biomimetic implants has a high potential for future biomedical applications. As a polymeric biomaterial, abundant in human bodies and influencing cellular morphology, collagen type I provides structural integrity and strength to tissues. However, applications are limited because even in crosslinked cases, the biomechanical properties of collagen networks can differ by several orders of magnitude in terms of both elasticity and load capacity. The widely used crosslinker glutaraldehyde has been the subject of controversy due to cytotoxic effects. In contrast, electron-beam-treatment allows reagent free control over a rapid and sterilizing crosslinking method in a non-cytotoxical biomimetic manner, resulting in improved mechanical properties due to high penetration depth and sufficiently high irradiation-induced doses. Subsequently, the modification of collagen type I fibers by energetic electron-beam-treatment during prestrain induced alignment of the inner filaments is shown to achieve and imprint network anisotropies resulting in mechanical properties with Young's moduli bridging orders of magnitude from a kPa range to a MPa range.

CPP 15.19 Mon 19:00 P4

Biopolymer-Templated Deposition of Hierarchical 3D-Structured Graphene Oxide/Gold Nanoparticle Hybrids for Surface-Enhanced Raman Scattering — •Yingjian Guo[1,2], Jungui Zhou[1], Constantin Harder[1,2], Guangjiu Pan[1], Yusuf Bulut[1,2], Gergely Nemeth[3], Ferenc Borondics[3], Benedikt Sochor[1], Sarathlal K. Vayalil[1], Daniel Söderberg[4], Peter Müller-Buschbaum[2], and Stephan V. Roth[1,4] — [1]Deutsches Elektronen-Synchrotron, 22607 Hamburg, Germany — [2]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [3]Synchrotron SOLEIL, Saint-Aubin, France — [4]KTH Royal Institute of Technology, Stockholm, Sweden

Cellulose has emerged as a promising bio-based template for sensors, smart windows, and bioelectronics. Typically, Surface Enhanced Raman Scattering (SERS), an advantageous analytical technique, allows for the rapid detection and structural analysis of chemical compounds through their spectral patterns in nanotechnology. Crucial for SERS is fabricating the substrates with strong enhancements of the Raman signal over large areas. Herein, we present a straightforward approach utilizing the layer-by-layer spray coating method to fabricate films loaded with gold nanoparticles and graphene oxide to serve as SERS substrates. GISAXS combined with nano-FTIR spectroscopy was used to confirm a synergistic Raman enhancement mechanism of localized surface plasmon resonance and interface charge transfer. Our approach provides a reference for facile and scalable production of SERS substrates.

CPP 15.20 Mon 19:00 P4

Analysis of folding/unfolding behavior of micro and nano collagen fibers by SFTIRM — •Selcuk Kaan Haciosmanoglu[1], Gihan Kamel[2,3], and Murat Kazanci[1,4] — [1]Nanoscience and Nanoengineering Program, Graduate School, Istanbul Medeniyet University, Istanbul, Turkey — [2]SESAME (Synchrotron-light for Experimental Science and Applications in the Middle East), Allan, Jordan — [3]Department of Physics, Faculty of Science, Helwan University, Cairo, Egypt — [4]Biomedical Engineering Department, School of Engineering and Natural Sciences, Istanbul Medeniyet University, Istanbul, Turkey

Collagen nanofibers are essential extracellular matrix (ECM) components widely used in regenerative medicine. While both electrospinning and wet-spinning techniques can produce anisotropic collagen micro- and nanofibers from dissolved collagen solutions, electrospun fibers require crosslinking to maintain water stability for cell culture applications. This study investigates in-situ crosslinking during electrospinning using chemical agents and physical methods. Synchrotron Fourier-Transform Infrared Microspectroscopy (sFTIRM) analysis revealed distinct molecular structural changes in the collagen nanofibers based on processing methods. Protein band positions shifted according to the extraction methods employed. Notably, electrospinning inhibited collagen molecule self-assembly, resulting in lower band positions compared to wet-spun fibers. The choice of crosslinking agent significantly influenced collagen's secondary structure, with genipin-mediated in-situ crosslinking better preserving the native structure of electrospun collagen nanofibers compared to UV crosslinking.

CPP 15.21 Mon 19:00 P4

Enhancing Endothelial Cell Attachment on PNIPAM-Based Microgel Coatings with RGD Ligand Functionalization — •Leonie Beer, Souraj Mandal, and Regine von Klitzing — Soft Matter at Interfaces, Department of Physics, Technical University of Darmstadt, Darmstadt 64289, Germany

Endothelial cell (EC) attachment is crucial for capillary formation and the success of artificial vascular networks in tissue engineering. Poly(N-isopropylacrylamide) (PNIPAM) microgels offer a promising platform for this application due to their tunable mechanical properties and ability to incorporate bioactive ligands. This study investigates the use of PNIPAM-based microgel coatings functionalized with the integrin-binding peptide sequence arginine-glycine-aspartate (RGD) to enhance EC adhesion. Successful conjugation of RGD peptides was confirmed using infrared spectroscopy and fluorescence microscopy. To evaluate the impact of ligand configuration, we compared three variations of RGD based peptides. The results reveal that increasing the anchor length significantly improves HUVEC recognition of the ligands, resulting in enhanced cell attachment and proliferation. These findings highlight the critical role of ligand design in optimizing biofunctional coatings. This work presents a straightforward chemical strategy for improving endothelial cell adhesion on PNIPAM-based microgel surfaces, paving the way for advanced artificial vascular networks in tissue engineering and regenerative medicine.

CPP 15.22 Mon 19:00 P4

Green plastics: Direct production from grocery wastes and characterization by using S-FTIR — •Onur Aras[1], Gihan Kamel[2,3], and Murat Kazanci[4,5] — [1]Istanbul Medeniyet University, Nanoscience and Nanoengineering Program, Graduate School, 34700 Istanbul, Turkey — [2]SESAME Synchrotron (Synchrotron-light for Experimental Science and Applications in the Middle East), 19252 Allan, Jordan — [3]Department of Physics, Faculty of Science, Helwan University, Cairo, Egypt — [4]Istanbul Medeniyet University, School of Engineering and Natural Sciences, Department of Biomedical Engineering, Istanbul, Turkey — [5]Istanbul Medeniyet University, Science and Advanced Technologies Research

This study investigates the production of cellulosic bioplastics from four green waste sources: hemp, parsley stem, pineapple leaves, and walnut shell, using either trifluoroacetic acid (TFA) or water as solvents. Synchrotron FTIR Microspectroscopy (SR-*FTIR) was employed to analyze structural modifications during biofilm formation and regeneration.Water-based biofilms retained their native cellulose, hemicellulose, and lignin components. In contrast, TFA-dissolved samples exhibited additional spectral bands in the hemicellulose region, attributed to ester bond hydrolysis and subsequent carboxylic acid formation. Principal component analysis revealed distinct groupings based on solvent type and polymer addition.

CPP 15.23 Mon 19:00 P4

How do stiffness patterns, with no topographical or chemical cues, influence cellular and tissue contact guidance? — •Mathis Grelier[1], Carlos Urena Martin[2], Mark Schvartzman[2], and Ana Suncana smith[1,3] — [1]Puls Group, Institute for Theoretical Physics and Interdisciplinary Center for Nanostructured Films (IZNF), Friedrich-Alexander Universität Erlangen-Nürnberg (FAU), 91058 Erlangen, Germany — [2]Department of Materials Engineering and Ilse Katz Institute for Nanoscale Science and Technology, Ben-Gurion University of the Negev, Beer-Sheva, Israel — [3]Group of Computational Life Sciences, Division of Physical Chemistry, Rudjer Bošković Institut, 10000 Zagreb, Croatia

While current systems cannot disentangle the effects of topography and stiffness contrasts, our study overcomes this challenge by investigating cell and tissue behavior on substrates with only alternating stiffness stripes. Our experiments and model reveal that wider stripes enhance alignment along stiffer or softer regions due to the higher energy cost of traversing softer substrates. At the cellular level, we employ a stochastic model based on Boltzmann weights applied to possible cell shapes, integrating energy contributions that govern movement across stiffness boundaries. For tissues, we extend this framework using a dissipative particle model to capture collective dynamics and mechanical interactions. To further explore these effects, we applied a Globalized Bounded Nelder-Mead optimization, enabling the efficient recovery of key physical parameters, such as stiffness and contractility, under both untreated and treated conditions.

CPP 15.24 Mon 19:00 P4

Latex film formation investigated by GISAXS and spectral reflectance — •Simon Schraad[1,2], Helder Marques Salvador[4], Nadja Kölpin[1], Nicolae Tomozeiu[4], Peter Müller-Buschbaum[2], and Stephan Volkher Roth[1,3] — [1]Deutsches Elektronen Synchrotron, Notkestraße 85, 22607 Hamburg — [2]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [3]Department of Fibre and Polymer Technology, KTH Royal Institute of Technology, Teknikringen 56, 100 44 Stockholm, Sweden — [4]Canon Production Printing Netherlands B.V., Van der Grintenstraat 10, 5914 HH Venlo, Niederlande

The film formation of latex inks on nanoporous substrates is of high interest for scientific and industrial applications. Inks are multi-component, complex fluids and consist of colloids, pigments and solvents. The film formation is a multistage process. After deposition, solvent begins to evaporate and finally nanoparticles self assembly. To quantitatively analyze latex film formation a combination of in-situ grazing incidence small angle scattering (GISAXS) and light scattering will be employed. Here structural changes during the deformation and coalescence phase of latex colloids will result in changes in the scattering patterns. We present a design of an experimental spray chamber to allow in-situ GISAXS and the spectral reflectance during spray deposition of latex inks to be used at synchrotron facilities.

CPP 15.25 Mon 19:00 P4

Dynamic magnetic response of multicore particles: the role of grain magnetic anisotropy and intergrain interactions — •Ekaterina Novak[1], Elena Pyanzina[1], Andrey Kuznetsov[2], and Sofia Kantorovich[2] — [1]Ekaterinburg, Russia — [2]University of Vienna, Vienna, Austria

This study examines the magnetic properties of multicore magnetic nanoparticles (MMNPs) utilizing Brownian dynamics simulations in conjunction with the Landau-Lifshitz-Gilbert equation. We demonstrate that the magnetic responses of MMNPs, both static and dynamic, are governed by a complex interplay between the cores magnetic anisotropy and the strength of inter-core magnetic interactions. These insights are crucial for refining the design of multicore magnetic particles in various applications, including magnetic hyperthermia, data storage, and targeted drug delivery, where accurate control over magnetic characteristics is vital.

CPP 15.26 Mon 19:00 P4

Kinetics of nanostructure and interface evolution induced by photopolymerization — •Shouzheng Chen[1,2,3], Yufeng Zhai[2], Jungui Zhou[2], Guangjiu Pan[1], Sarathlal Koyiloth Vayalil[2], Rolf A.T.M. van Benthem[4], Johan F.G.A Janssen[5], Mats K. G. Johansson[6], Peter Müller-Buschbaum[1], and Stephan V. Roth[2,6] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]DESY, Notkestraße 85, 22607 Hamburg, Germany — [3]FRM II, Lichtenbergstraße 1, 85748 Garching, Germany — [4]Eindhoven University of Technology, Groene Loper 5, 5600, MB, Eindhoven, the Netherlands — [5]Covestro (Netherlands) B.V., Urmonderbaan 22, 6167, RD, Geleen, the Netherlands — [6]Department of Fibre and Polymer Technology, KTH Royal Institute of Technology, Teknikringen 56, SE-100 44 Stockholm, Sweden

Photopolymerization offers spatial resolution, low energy consumption, and high curing speeds, making it a widely used technology in additive manufacturing. The kinetics of the physical transformation of the resin from liquid to solid (cross-linked) state induced by photopolymerization and the kinetics of the solid-liquid interface formation of resin multilayer are the key to achieving controllable high-precision manufacturing. By modulating precursor resin components and combining grazing incidence small angle X-ray scattering (GISAXS), the UV-curing induced nanostructure and the buried interface of resin multilayer are probed. We reveal how solvents and additive monomers determine in nanostructure and multilayer interface formation during photopolymerization.

CPP 15.27 Mon 19:00 P4

Effect of grafting density on particle distribution in polymer brush/gold nanoparticle composite materials — •Elias Hallenbach, Hayden Robertson, and Regine von Klitzing — Institute for Condensed Matter Physics, Technical University of Darmstadt, Germany

Metal/polymer nanocomposites are versatile hybrid materials and find use in many fields such as photonics, biomedical engineering and catalysis. A promising realization of this type of hybrid material is the controlled self-assembly of gold nanoparticles (AuNPs) inside a polymer brush, which induces color changes upon exposure to environmental changes enabling sensor applications.

The polymer brushes serve as a matrix for the immobilization of AuNPs. Particle uptake into the brush matrix is affected by parameters such as thickness, particle size and the grafting density. Polymer brushes with varying grafting densities are synthesized by a controlled polymerization (SI-ARGET ATRP) directly from a silicon substrate. The nanocomposite materials are fabricated by dip-coating of polymer brushes into a AuNP dispersion. Characterization of the nanocomposites is performed by (in situ) spectroscopic ellipsometry, atomic force microscopy and (in situ) X-ray reflectometry (XRR).

Uptake of nanoparticles has proven to be highest at intermediate grafting densities. I will discuss the influence of particle distribution inside the brush on particle uptake, which can be yielded by XRR measurements.

CPP 15.28 Mon 19:00 P4

Multi-material filament fabrication for 3D printing photoelectrocatalytic carbon nitride composites — •Timo Uhlein and Siowwoon Ng — FAU Erlangen-Nürnberg, Erlangen, Germany

Additive manufacturing of electrochemically active 3D structures is of rising interest. In particular, using fused deposition modeling (FDM) based on filament extrusion concept to produce carbon-polymer-based 3D structures offers several advantages, such as accessibility, low-cost and ease of use. Nevertheless, carbon-based filaments are limited with their applications. Therefore, incorporating additional materials to produce a multi-material filament is of interest, to create 3D-printed electrodes with new or targeted functional properties. In this project, we fabricated a multi-material filament consists of carbon nitride, C3N4, and carbon nanotubes, CNTs, for its photocatalytic properties and high conductivity, respectively, and polymer as the backbone of a FDM filament. We examined the performance of the composite C3N4-CNT electrodes for hydrogen evolution and the photocatalytic degradation of a dye. We indicate that further advancements can be achieved by developing multi-material filaments in order to use them for further electrochemical applications.

CPP 15.29 Mon 19:00 P4

Mechanochemical Behavior and Flow Dynamics of Glycerol Aqueous Solutions Confined between Ferrous Surfaces: Atomic-scale Insights from Reactive Molecular Dynamics Simulations — •Vahid Fadaei Naeini[1,2], Andreas Larsson[1], and Roland Larsson[2] — [1]Applied Physics, Division of Materials Science, Department of Engineering Sciences and Mathematics, Luleå University of Technology, Sweden. — [2]Machine Elements, Division of Machine Elements, Department of Engineering Sciences and Mathematics, Luleå University of Technology, Sweden.

This study explores the tribochemical behavior of glycerol and its aqueous solutions confined between ferrous surfaces using reactive non-equilibrium molecular dynamics simulations. Results show that glycerol reduces friction effectively, with viscosity decreasing as water content increases. Pure glycerol achieves lower friction but exhibits significant wall slip and deviations from a linear velocity profile near the surfaces. Glycerol dissociation, influenced by shear stress and pressure, produces water and organic acid by-products, with dissociation rates decreasing at higher water concentrations. Atomic-scale analysis reveals increased surface wear and iron atom dissociation under elevated stresses. These findings highlight the balance between friction reduction, viscosity, and tribochemical reactivity in glycerol-water mixtures, offering insights for sustainable lubricant design under extreme conditions.

CPP 15.30 Mon 19:00 P4

Evaluating the Properties of Nafion PEMFC Membrane via MD Simulations — •Mateja Jovanović[1], Matthias Baldofski[1], Igor Stanković[2], Marcin Rybicki[1], and Miljan Dašić[2] — [1]Freudenberg Technology Innovation SE & Co. KG, Hoehnerweg 2-4, 69469 Weinheim, Germany — [2]Scientific Computing Laboratory, Center for the Study of Complex Systems, Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Zemun, Serbia

Understanding the nanoscale interactions within Nafion membranes is crucial for optimizing their performance in Proton Exchange Membrane Fuel Cells (PEMFC). In present a molecular dynamics study of the structural and dynamic properties of Nafion-water systems under varying hydration levels using molecular dynamics simulations. The density of the Nafion-water system is examined to identify deviations from the ideal additivity rule, providing insights into molecular interactions and structural rearrangements. The radial pair distribution function, radius of gyration, pore-water contact surface, and diffusion coefficients for water and hydronium ions are analyzed to reveal the local organization, solvation quality, porosity, and transport properties within the hydrated Nafion membrane. The methodology used to obtain properties of the Nafion-water mixture builds on techniques previously developed for the study of ionic liquids [1].

[1] I. Stanković, M. Dašić, M. Jovanović, A. Martini, Langmuir 2024, 40(17), 9049-9058, doi:10.1021/acs.langmuir.4c00372

CPP 15.31 Mon 19:00 P4

Exploring Polymer Aging: Microscopy and Thermal Analysis — •Judith Bünte, Laila Bondzio, Karsten Rott, and Andreas Hütten — Universität Bielefeld, Dünne Schichten und Physik der Nanostrukturen, Universitätsstr. 25, 33615 Bielefeld

The analysis of polymers and their additives is essential for understanding material performance and longevity, particularly in the context of aging processes. This work emphasizes the synergistic application of advanced microscopy and thermal analysis techniques to investigate polymer composition, structure, and degradation behavior.

Transmission Electron Microscopy (TEM) and Scanning Electron Microscopy (SEM) were utilized to visualize the microstructural features of polymer matrices, as well as the distribution of particles within the polymer. TEM offered high-resolution imaging to reveal morphological details, while SEM enabled surface characterization. These imaging techniques were further augmented by Differential Scanning Calorimetry to analyze thermal properties.

Polymer aging was studied under controlled conditions to evaluate structural and compositional degradation over time. Changes in microstructure and thermal properties were correlated with aging-related alterations.

The integration of these analytical techniques establishes a robust framework for characterizing polymers and their additives. This approach yields valuable insights into the stabilizing role of additives, such as TiO_2, in protecting polymers against environmental and thermal stressors.

CPP 15.32 Mon 19:00 P4

Atomistic simulations of PEDOT:PSS — •Richard Schömig[1,2], Annalena Riffelt[2], and Alexander Schlaich[1] — [1]Institute for Atomistic Modeling of Materials in Aqueous Media, Hamburg University of Technology, Hamburg — [2]SC SimTech, University of Stuttgart, Stuttgart

PEDOT:PSS is by far the best known conjugated polymer with a broad application in e.g. bioelectronics, energy storing devices or neuromorphic computing due to its electrolyte-dependent swelling behavior and extraordinary conductance in the doped (oxidized) state. However, the insolubility of its films once their dried hinders classic experimental studies, thus making molecular dynamics simulations an indispensable tool to understand its electronic and mechanical behavior on an atomic scale. Here, we employ different established force fields to study the influence of a set of parameters such as different water models, dissociation degrees, partial charges and simulation protocols on the structural changes and polymer physics by water uptake for both the PEDOT and the PSS part. We test the validity of these force fields by benchmarking them against ab-initio MD and experimental results.

CPP 15.33 Mon 19:00 P4

Analysis of the Reciprocity Theorem in the DWBA — •Reinhard Sigel — Independent Scientist, D-88677 Markdorf, Germany

The Distorted Wave Born Approximation (DWBA) is a favored theory among X-ray scientists for the analysis of interface scattering experiments [1,2]. Unfortunately, there is no proper clarification which X-ray specific aspects and approximations enter the DWBA and what is the difference to interface scattering of coherent visible laser light. Based on the differing refractive index approaches for X-rays and for visible light, we identify the spot where an X-ray specific equation enters the derivation [1] of the so-called reciprocity theorem. It involves an intermixing of microscopic and macroscopic Maxwell equations. A much simpler correct derivation valid for both wavelength ranges is discussed.
[1] Daillant, Gibaud, *X-ray and Neutron Reflectivity*, Springer 2009.
[2] Renaud, Lazzari, Leroy, Surf. Sci. Reports 64, 255–380 (2009).

CPP 15.34 Mon 19:00 P4

Dynamic Polarization and Electrostriction of PVDF-Based Copolymer Films as Measured with Double-Modulated Interferometry — Marvin Malchau[1], Philipp Ramming[2], and •Lothar Kador[1] — [1]University of Bayreuth, Institute of Physics and BIMF, 95440 Bayreuth, Germany — [2]University of Bayreuth, Experimental Physics II, 95440 Bayreuth, Germany

Thin films of a ferroelectric copolymer based on polyvinylidene fluoride (PVDF) were exposed to electric ac fields with amplitudes up to 115 MV/m and frequencies between 5 and 100 Hz. The electrical polarization of the material was calculated by integrating the current flow, and the electric-field-induced thickness change (electrostriction) was measured with double-modulated interferometry. Thickness changes up to 60 nm were observed in an 8 μm thick film. The polarization shows a hysteresis loop typical for ferroelectric materials; it is independent of frequency in the investigated frequency range. The electrostriction exhibits a different type of hysteresis with strong frequency dependence. This indicates that the mechanical relaxation of the polymer film is independent of the electric dipole orientation.

CPP 15.35 Mon 19:00 P4

Ternary Organic Solar Cells For Space Applications — •Ivonne A. Zitzmann, Lukas V. Spanier, and Peter Müller-Buschbaum — TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany

It has been demonstrated that organic solar cells (OSC) are capable of achieving high gravimetric power density, making them suitable for space applications. However, they still exhibit insufficient long-term stability, and there are few studies on their performance under space-like conditions. Here we investigate the ternary OSC system PBDB-T-2F:BTP-eC9:$PC_{71}BM$ by optimizing its efficiency and studying its structure and degradation by optical measurements and grazing incidence wide and small angle X-ray scattering. Space conditions were simulated with AM0 illumination. Further, the OSCs were exposed to temperature cycling to assess their stability in a space environment, subject to rapidly changing temperatures. In addition, data from a suborbital rocket flight was examined for performance and degradation of the solar cells. These results may allow for the furthering of our understanding of photovoltaic power generation in harsh environments.

CPP 15.36 Mon 19:00 P4

Degradation of Printed Organic Solar Cells at High Temperatures — •Christoph G. Lindenmeir[1], Simon A. Wegener[1], Christopher R. Everett[1], Julian E. Heger[1], Sigrid Bernstorff[2], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]Elettra, 34149 Basovizza, Trieste, Italy

Organic solar cells (OSCs) have gained significant attention recently due to their non-toxicity, short energy payback times, and fast efficiency improvements. Their high absorbance, potentially flexible design, and easy solution-based manufacturing make them particularly promising. Especially slot-die printing, a fast and low-waste fabrication method, enhances their scalability and potential for various applications, including space use. OSCs are particularly suited for space as their thin, lightweight structure provides a higher power-to-weight ratio than traditionally used solar cells, lowering production and launch costs. However, space conditions like extreme temperatures, high vacuum, and radiation accelerate degradation. This study focuses on the impact of extreme temperature variations on printed OSCs. We optimized their printing process and analyzed their degradation using operando grazing incidence small-angle X-ray scattering (GISAXS), a nondestructive method for studying thin-film morphology. Additionally, we monitored their electrical performance under high vacuum to simulate space conditions.

CPP 15.37 Mon 19:00 P4

Modulate Pre-aggregation to Optimize the Morphology in Organic Solar Cells — •Tim Bohnen, Jinsheng Zhang, and Peter Müller-Buschbaum — TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany

Morphology optimization has emerged as a key strategy to effectively improve device performance and stability in organic solar cells. Due to the solution-processing method, the selection of solvents for precursor solutions is crucial, as it directly affects the ultimate the morphology of active layer. Recent research demonstrates that donor and acceptor molecules form aggregates of varying sizes in precursor solutions, subsequently inducing different phase separation and crystallization behavior during drying process. However, the detailed correlation between pre-aggregation behavior and final morphology has yet to be fully elucidated. In this study, the active layer is composed of PBDB-TF-TTz acting as the donor and BTP-4F-24 as the non-fullerene acceptor. Next, we characterize the resulting morphology using atomic force microscopy (AFM) and grazing incidence small- and wide-angle X-ray scattering (GIWAXS and GISAXS).

CPP 15.38 Mon 19:00 P4

Investigation of quenching in exciplex OLEDs under variation of the giant surface potential — •Clarisse Henriques, Albin Cakaj, Alexander Hofmann, and Wolfgang Brütting — Institut für Physik, University of Augsburg, Augsburg, Germany

An exciplex is a short-lived excited charge transfer state formed between donor and acceptor molecules of different species, in which under radiative decay a photon is emitted. They can either function as efficient host for emitters or directly as emitter because of their apparent thermally activated delayed fluorescence characteristics. Especially the electron accepting materials tend to show a macroscopic film polarization, which is also referred to as giant surface potential (GSP). The presence of GSP in an organic light emitting diode (OLED) promotes charge injection in the electron transport layer (ETL), but causes the accumulation of holes, which can result in exciton quenching. Consequently, studying the impact on the device is of crucial importance. The main interest lies now on the tunability of this parameter by using the material as a co-host or directly as emitter. We investigate OLEDs with different film thickness of the ETL and emission layer. Additionally, devices of donor and acceptor with different mixing ratios were prepared. The major focus is now on studying these systems by current density-voltage-luminance, photoluminescence (PL) and electroluminescence spectra, impedance spectroscopy and their PL quenching under different bias voltages. Such studies are fundamental to understand the impact of SOP in OLEDs for further improvement.

CPP 15.39 Mon 19:00 P4

Tracking degradation of non-fullerene organic solar cells under dynamic environmental conditions — •Lixing Li, Lukas Spanier, Zhaonan Jin, Linus Huber, Guangjiu Pan, and Peter Müller-Buschbaum — TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany

The power conversion efficiency (PCE) of non-fullerene organic solar cells (OSCs) has already approached 20%, but stability and environmental degradation issues have always been one of the biggest challenges limiting their application. Considerable research has been conducted to understand the degradation mechanisms in OSCs, especially under extreme environmental conditions like high and low temperatures. While these studies offer valuable insights, they do not fully represent the dynamic conditions that most organic solar cells face in real-world environments. In practical scenarios, environmental factors such as temperature, humidity, and light fluctuate over time rather than remaining constant. Therefore, it is crucial to investigate how OSCs degrade not only under steady stress but also when exposed to varying environmental conditions. This study explores the degradation of BTP-4F non-fullerene organic solar cells subjected to multiple environmental cycles. Advanced characterization methods, including grazing-incidence X-ray scattering (GIXS) and atomic force microscopy (AFM), are used to monitor both in-situ and ex-situ structural changes in the active layer of OSCs, offering deeper insights into the underlying degradation mechanisms.

CPP 15.40 Mon 19:00 P4

Revealing the Effect of Solvent Vapor Annealing on the Morphology of Non-Fullerene Organic Solar Cells — •Liansong Chu — TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany

Solvent vapor annealing (SVA), as an effective post-treatment technique, has been widely used to optimize the morphology in organic solar cells (OSCs). When exposed to the specific solvent atmosphere, the swelling effect induced by solvent vapor facilitates molecular mobility of both donor and acceptor molecules, leading to modifications in crystallinity and phase separation. Hence, the selection of solvent and annealing duration for SVA is critical for the morphology, which ultimately determines the power conversion efficiency and stability. However, fundamental understanding of solvent selection criteria and the associated kinetic processes during treatment remains unknown. In this work, we systemically investigates the impact of different solvents for SVA on the morphological properties of non-fullerene OSCs (PBDB-TF-TTz as the donor and BTP-4F-24 as the acceptor) using atomic force microscopy (AFM), grazing incidence small- and wide-angle X-ray scattering (GISAXS and GIWAXS). Furthermore, we provide real-time insights into the morphological evolution during SVA through in situ UV-Vis absorption spectroscopy and photoluminescence measurements.

CPP 15.41 Mon 19:00 P4

Impact of the electrode area on the local J-V curves of organic photovoltaics — •Paul Schwanitz[1], Fabian Eller[1], Carsten Deibel[2], and Eva M. Herzig[1] — [1]Dynamik und Strukturbildung - Herzig Group, Universität Bayreuth, Universitätsstr. 30, 95447 Bayreuth, Germany — [2]Institut für Physik, Technische Universität Chemnitz, 09126 Chemnitz, Germany

Organic photovoltaics (OPV) are promising candidates for flexible solar cells, which may be more cost efficient to produce than their silicon counterparts. The organic semiconductor materials can be dissolved and printed on large scale, with the attractive advantage that the geometry of the OPV devices can be chosen on demand. The aim here is to analyze the influence of the top and bottom size of the electrodes on the J-V curve measurements. If the active areas are too small, fluctuations in the performance can occur, which are caused by inhomogeneities in the film. As the active area increases, performance is expected to stabilize as it is averaged over a larger area [1]. The different sizes of the anode and cathode also enable in-line measurements during production. The sizes of the electrodes are systematically varied to estimate the influence on the measurements, to interpret the J-V curves correctly and to account for the dark currents.

[1] Herzig, E. M., Gao, F., Bergqvist, J., Loi, M. A., & Meier, S. B. Harmonizing organic photovoltaics research and development among academia and industry. Joule, 8, 2171 (2024). https://doi.org/10.1016/j.joule.2024.07.015

CPP 15.42 Mon 19:00 P4

Thin Films of Substituted Benzo[*b*]fluorenes as Emitting Layers for Blue OLED Devices — •Pascal Schweitzer[1], Christopher M. Leonhardt[2], Cazibe Arslan[1], Hermann A. Wegner[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 light emitting diodes (OLED), despite widespread application in displays, still exhibit major challenges: The search for stable and efficient blue-emitting molecules continues, as these often suffer from degradation. Here we study substituted benzo[*b*]fluorenes (BF) as an alternative for such emitters. Their modular structure allows for tuning opto-electronic properties. Thin films of different BF were prepared by solution-based methods or physical vapor deposition (PVD). Significant blue emission was found by photoluminescence spectroscopy in solid state. Film growth at device interfaces was studied. In-situ Kelvin-probe force microscopy (KPFM) gave insight into electrical contact formation to typical transport materials: Stranski-Krastanov growth was found in PVD onto hole-conducting poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT:PSS), accompanied by the formation of an interface dipole. On the electron-conducting side, a pronounced Volmer-Weber growth of bathocuproine (BCP) on the emissive layer demands a high film thickness for pinhole-free contacts. Finally, based on these findings, we show a working prototype of a blue OLED based on a substituted BF.

CPP 15.43 Mon 19:00 P4

Excimer as intermediate in singlet fission process for Polydiketopyrrollopyrole based materials — •Sruthy Asa Rajan, Sergey Bagnich, and Anna Köhler — University of Bayreuth, Bayreuth, Germany

Photovoltaics are essential for renewable energy generation, but the efficiency of conventional solar cells is constrained by the Shockley-Queisser limit, which arises from fundamental and practical losses such as thermalisation loss. Singlet fission (SF), a carrier multiplication process, offers a promising pathway to surpass this efficiency limit. However, a key challenge lies in identifying SF molecules with triplet energy levels that align with the silicon band gap, enabling the efficient formation of correlated triplet pairs, 1(TT) and their subsequent separation into individual triplets.

Polydiketopyrrollopyrole (PDPP) is a molecule with a comparable triplet energy to the silicon bandgap. We investigate the influence of solvent properties on the optical behaviour of N-substituted pyrene-bridged PDPPs. We employ temperature-dependent steady-state and time-resolved photoluminescence studies on N-substituted pyrene-bridged PDPPs in protic polar and aprotic polar solvents to study the evolution of different species. We observe excimer emission at intermediate temperature and 1(TT) emission at lower temperature. This observation supports the notion that excimers are involved in the formation of 1(TT).

CPP 15.44 Mon 19:00 P4

Solution processed organic solar cells for agrivoltaic applications — •Sebastian Coen, Yunan Chen, Kerstin Märkle, and Christian Sprau — Karlsruhe Institute of Technology, Light Technology Institute

Organic solar cells (OSCs) offer a wide range of applications due to their light weight, low energy payback time, non-toxicity and mechanical flexibility. This work aims to expand these applications by fabricating semitransparent OSCs for agricultural photovoltaic applications, such as greenhouses and foil tunnels.

To facilitate future industrial production, we explore scalable processes and a fully solution-processed architecture based on non-halogenated solvents. The fabricated solar cells are studied in terms of their electrical and spectral properties and their real space morphology.

CPP 15.45 Mon 19:00 P4

Utilizing Ultrasonic Spray for the Integration of Organic Solar Cells on Cellulose Substrate — •Xinyu Jiang[1], Kang An[2], Qin Wang[2], Nadja Koelpin[1], Arik Willner[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

Cellulose nanofibrils, heralded for their eco-friendly and renewable nature, offer a significant stride toward sustainable energy solutions. Their advantageous attributes such as biocompatibility, flexibility, lightweight nature, transparency, and remarkable mechanical strength render them suitable as a base material for incorporating photovoltaic or electronic devices. We aim to explore the development of functional photovoltaics on transparent cellulose-fabricated curtains, aiming at transforming undesired sunlight into electricity. The inherent flexibility of curtains poses a fabrication challenge for solar cells, adeptly mitigated through ultrasonic spray deposition. This technique manifests as an efficacious means to engender functional layers on a large scale, ensuring a homogeneous surface with minimal roughness. Employing an advanced non-fullerene acceptor system, the resultant organic solar cell curtain showcases the promising performance, delineating a path toward substantial applications in the sustainable energy.

CPP 15.46 Mon 19:00 P4

Multiscale morphological modulation in spray-coated organic solar cells — •Shuxian Xiong[1,2], Benedikt Sochor[1], Constantin Harder[1,2], Sarathlal Koyiloth Vayalil[1], Peter Müller-Buschbaum[2], and Stephan V. Roth[1,3] — [1]Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany — [2]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [3]KTH Royal Institute of Technology, 10044 Stockholm, Sweden

The balance between phase separation and crystallization arising from the aggregations of organic semiconductor molecules defines the film morphology, resulting in multi-length scale phase transitions that enhance device performance. We investigate the morphological evolution driven by molecular self-assembly during the ultrasonic spray-coating of organic functional layers in organic solar cells. An in-depth understanding of phase transition phenomena through an analysis of both temporal (film formation kinetics) and thermal scales (annealing), with the elucidation of the intricate structure-performance nexus linked to morphological evolution and device efficiency, is achieved. We clarify the principles of effective morphological optimization to achieve high-efficiency sprayed organic solar cells, providing valuable guidance for their commercial application.

CPP 15.47 Mon 19:00 P4

Impact of amphiphilic additives on organic solar cells: Enhancing thermal stability for long term performance — •Jose Prince Madalaimuthu[1,2], Tim Matzdorff[1,2], Zhuo Xu[1,2], Md. Moidul Islam[1,2], Yisak Tsegezab Gerase[3], Hassan Ismail[1,2], Rico Meitzner[4], Aman Anand[1,2], Martin Presselt[3], Ulrich S Schubert[1,2], and Harald Hoppe[1,2] — [1]Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich-Schiller-University Jena, Jena, Germany — [2]Laboratory of Organic and Macromolecular Chemistry (IOMC Jena), Friedrich-Schiller- University Jena, Jena, Germany — [3]Leibniz Institute of Photonic Technology (IPHT), Jena, Germany — [4]Helmholtz-Zentrum Berlin GmbH, Hahn-Meitner Platz 1, 14109 Berlin, Germany

The stability of organic solar cells (OSCs) depends not only on the device architecture or effective sealing but also significantly on the morphological stability of the photoactive layer. This stability can be disrupted by alterations in the spatial arrangement of the electron donor and acceptor, which are the fundamental components of OSCs. The extent of phase separation between donor and acceptor regions within the bulk heterojunction (BHJ) plays a pivotal role in determining device performance. Consequently, various strategies have been explored to preserve the distribution of these components. One promising approach is the incorporation of amphiphilic molecules to enhance the stability of the donor-acceptor interface. This method improves thermal resilience, overall OSC performance, and mitigates morphological degradation.

CPP 15.48 Mon 19:00 P4

Interfacial encapsulation of organic solar cells — •Saib Jahan Qazi[1,2], Md Moidul Islam[1,2], Zhou Xu[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, light-weight 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 of these devices. In this study, we demonstrate solution processed interlayer encapsulation of organic solar cells using polymer-based barriers to prevent interlayer migration of impurities as well as the ingress of oxygen and moisture.

CPP 15.49 Mon 19:00 P4

Modifying spacers for higher efficiency and stability of single-component organic solar cells — •Yakun He[1], Peter Baeuerle[2], Weiwei Li[3], Christoph Brabec[4], and Frederic Laquai[1,5] — [1]King Abdullah University of Science and Technology, Saudi Arabia — [2]University of Ulm, Germany — [3]Beijing University of Chemical Technology, China — [4]Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany — [5]Ludwig-Maximilians-Universität München, Munich, Germany.

Organic solar cells have achieved 20% efficiencies yet still lag regarding stability. Single-component materials incorporating donor and acceptor moieties in a nonconjugated method exhibit intrinsically high stability because of the restriction of morphological evolution. Nevertheless, the efficiency of single-component organic solar cells (SCOSCs) is still low compared to bulk heterojunction structures. We employ a series of dyads with similar structures but modify their spacer type and lengths to investigate the structure-morphology-performance relation. Photophysics has been studied by using steady-state and transient absorption and photoluminescence. Dyad4, with a proper long spacer, has shown the highest efficiency and surprisingly high stability under illumination. Moreover, we investigated the thermal stability of double-cable polymers by tuning the linker length between donor and acceptor moieties. Surprisingly, double-cable polymers do not show a decline of stability with the increase of space linker, and all of them display remarkably excellent stability without degradation after heating for 1000 hours at 90 degree.

CPP 15.50 Mon 19:00 P4

Photoinduced charge transfer and photophysics of functionalized Diethienopyrrole molecules from first principles — •Jannik Theile, Caterina Cocchi, and Michele Guerrini — Physics Department and Center for Nanoscale Dynamics, Carl von Ossietzky Universität Oldenburg, D-26129 Oldenburg, Germany

Donor-acceptor compounds are key components in organic electronics due to their tunable electronic and optical properties. In this work based on time-dependent density functional theory, we examine diethienopyrrole molecules, which act as electron donors, covalently combined with electron-acceptor units, focusing on their charge transfer dynamics induced by femtosecond laser excitations.

In the current symmetric molecule configuration, we find strong fluctuation patterns of the charge after laser excitation across both intensities and with and without nuclear motion, exceeding the initial changes of charge induced by laser excitation and the charge transfer (CT) remains insufficient and inconsistent throughout time evolution. Further considerations include asymmetric molecule configuration.

CPP 15.51 Mon 19:00 P4

Direct stochastic optical reconstruction microscopy (dSTORM) on cationic copolymer microgels — •Evelyn Gettinger and Thomas Hellweg — Physical & Biophysical Chemistry, University Bielefeld, Bielefeld, Germany

Microgels, three-dimensional polymer networks with colloidal dimensions, are promising candidates for catalysis, sensory and drug delivery applications due to their responsive properties. Cationic copolymer microgels, in particular, are gaining increasing attention in research, as they are suitable for conjugation with biomolecules like peptides, antibodies, and nucleic acids. Poly(NNPAM-co-DAPMA) is one such microgel that exhibits thermoresponsiveness through the monomer N-n-propylacrylamide (NNPAM) and pH responsiveness through the cationic comonomer N-3-(dimethylamino)propylmethacrylamide (DAPMA). This study investigates the network structure of Poly(NNPAM-co-DAPMA) microgels using direct stochastic optical reconstruction microscopy (dSTORM), a high-resolution fluorescence technique. Microgels with varying DAPMA concentrations were synthesized and analyzed for swelling behavior and polydispersity using photon correlation spectroscopy (PCS). Morphological properties were examined with atomic force microscopy (AFM). Post-synthetic fluorescence labeling with the anionic dye DY-654-carboxylic acid revealed a gradient of fluorophore localization from the core to the periphery and concentrated fluorophore domains, indicating a heterogeneous network with random comonomer distribution.

CPP 15.52 Mon 19:00 P4

Volume phase transition of NIPAM based copolymer microgels with non-thermoresponsive comonomers — •Jannis Krüger and Thomas Hellweg — Physical and Biophysical Chemistry, Bielefeld University

We conducted photon correlation spectroscopy (PCS) to obtain swelling curves of *N*-isopropylacrylamide (NIPAM)-based copolymer-microgels with varying content of non-thermoresponsive *N*-tert-butylacrylamide (NtBAM). Increasing NtBAM content reduces the hydrodynamic radius and broadens the volume phase transition (VPT). We analyzed the thermoresponsive contribution to the swelling curves with a cooperative Hill-like model for the Flory-Huggins interaction parameter $\chi_{\text{Hill}}(T)$ [1]. This model effectively describes the microgel swelling at various compositions. The Hill parameter ν estimates the number of water molecules leaving a polymer segment at the phase transition. A linear decrease of ν with BIS content suggests that water stays adsorbed on BIS during the VPT due to the lack of an LCST [2]. We fitted PNIPAM-*co*-NtBAM microgel swelling curves [3] with a hybrid model of χ_{Hill} for NIPAM and the original Flory-Huggins parameter χ_{FH} for NtBAM, revealing an exponential decrease in ν with x_{NtBAM}, indicating that NtBAM inhibits water adsorption of neighboring NIPAM units. Based on these results we propose a steric mechanism, which qualitatively describes the observed inhibition of microgel hydration.
[1] D. C. Leite et al., Langmuir 34 (2018), 10943. [2] S. Friesen et al., Gels 7 (2021), 42. [3] J. Krüger et al., Colloid Polym. Sci. (2024).

CPP 15.53 Mon 19:00 P4

Amphiphilic Monomers Bridge Hydrophobic Polymers and Water — •Guido Kusters[1,2,3], Guogao Zhang[1,4], Zheqi Chen[1,5], and Zhigang Suo[1] — [1]Harvard University — [2]Eindhoven University of Technology — [3]Max Planck Institute for Dynamics and Self-Organization — [4]Xi'an Jiaotong University — [5]Zhejiang University

Water dissolves a hydrophilic polymer but not a hydrophobic polymer. However, many hydrophilic polymer monomers are amphiphilic, with a hydrophobic vinyl group for radical polymerization and a hydrophilic group, and so may form solutions with both water and hydrophobic polymers. Ternary mixtures of amphiphilic monomers, hydrophobic polymers, and water have recently been used as precursors for interpenetrating polymer networks with unusual properties. However, the phase behavior of such ternary mixtures has not been studied. Here we mix the amphiphilic monomer acrylic acid, the hydrophobic polymer poly(methyl methacrylate) and water. In the mixture, the hydrophobic polymer can form various morphologies, including solution, micelle, gel, and polymer glass. We interpret these findings by proposing that the hydrophobic and hydrophilic groups of the amphiphilic monomer enable it to function as a bridge. That is, the hydrophobic functional group binds to the hydrophobic polymer, and the hydrophilic functional group binds to water. This picture leads to a simple modification to the Flory-Huggins theory, which agrees well with our experimental data. Amphiphilic monomers offer a rich area for the development of materials of self-assembled structures with unusual properties.

CPP 15.54 Mon 19:00 P4

Mechanical Characterization of Epon 862/DETDA Epoxy Networks: Molecular Dynamics Simulations — •Djihed Rezzig[1,3], Wolfgang Verestek[2], Saad Abdeslam[1], Johannes Roth[3], and Siegfried Schmauder[2] — [1]LPMMM, Setif 1 University-Ferhat ABBAS, Algeria — [2]IMWF, Stuttgart University, Germany — [3]FMQ, Stuttgart University, Germany

Epoxy resins are widely used in advanced materials due to their exceptional mechanical properties. Among them, Epon 862/DETDA is a commonly employed thermoset system in aerospace and automotive applications. This study employs molecular dynamics simulations to investigate the mechanical behavior of the Epon 862/DETDA epoxy network. The simulations were conducted using cross-linked molecular models to represent the cured network, incorporating detailed atomic scale interactions. Mechanical behavior was evaluated by simulating stress-strain responses under tensile loading conditions and shear test for the elasticity tensor, revealing the epoxy networks high modulus and strength. Additionally, the study examines the effects of varying cross-link densities and molecular configurations on the materials performance.

CPP 15.55 Mon 19:00 P4

The effect of intracrystalline chain dynamics (ICD) in the stress relaxation of semi-crystalline polymers — •Tonghua Liu, Rose Mary Michell, Albrecht Petzold, and Thomas Thurn-Albrecht — Von-Danckelmann-Platz 3, 06120, Halle(Saale)

The intracrystalline chain dynamics (ICD) plays a significant role in semi-crystalline polymers (SC), influencing not only the polymer crystallization and morphology but also the stability of crystals and the mechanical properties, such as drawability. Here we investigate how the ICD affects the stress relaxation of SC polymers.
Plane-strain compression test is used to study the relaxation behavior after yielding point. For crystal-fixed polymers like polycaprolactone (PCL), where ICD is absent or significantly hindered, only one relaxation process is observed. In contrast, crystal-mobile polymers like high density polyethylene (HDPE) exhibit two distinct relaxation processes, which can be attributed to the additional mobility within the crystals. The two relaxation processes in HDPE demonstrate markedly distinct time scales. The faster relaxation process is observed to relax faster with increasing temperature, whereas the slower relaxation process remains unaltered within the chosen temperature range.

CPP 15.56 Mon 19:00 P4

The effect of the intracrystalline chain diffusion on the non-linear mechanical behavior of semicrystalline polymers — •Rose Mary Michell, Albrecht Petzold, and Thomas Thurn-Albrecht — Martin Luther University Halle Wittenberg, Institute of Physics, D-06099 Halle, Germany.

This work studies the influence of intracrystalline chain diffusion (ICD) on the mechanical properties of semicrystalline polymers by comparing PEO with fast ICD and PCL with slow ICD. Mechanical tests were performed under plane strain compression at temperatures from -10 to 55 °C and true strain rates from 0.005 to 10 min^{-1}. At large deformations, the PCL always shows a strain hardening effect, while PEO shows softening when the rate decreases, temperature increases, and molecular weight decreases. The data corresponding to the strain hardening part, which describes the network forces, was fitted using the Gaussian model. The stress-strain curve for PCL showed higher stress than the Gaussian chain model predicted. In contrast, PEO had lower stress values; this difference could be attributed to an effect linked to chain mobility. For slow ICD, the crystals act as physical crosslinking points. Otherwise, the chains can be pulled from the crystals and soften the network. In conclusion, we found systematic differences in non-linear mechanical behavior between crystal-fixed and crystal-mobile polymers. This suggests that the competition between ICD and deformation determines the non-linear mechanical behavior at large deformations of semicrystalline polymers.

CPP 15.57 Mon 19:00 P4

Exploring the role of defects in polymer networks through simulations of 4-armed polymers — •Sayam Bandyopadhyay[1,2], Sebastian Seiffert[3], 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 — [3]Department of Chemistry, Johannes Gutenberg Universität Mainz, 55128 Mainz, Germany

We simulated polymer networks formed by coarse-grained tetra-PEG (tPEG) macromolecules to investigate the effects of (connectivity) defects on network dynamics. We modeled both homoleptic and heteroleptic systems, where we modeled non-covalent bonds between functionalized end groups using an inverted Gaussian potential to control valency. The network structure was quantified through the fraction of bonded end groups and the radial distribution functions of attractive beads. Polymer mobility was characterized by examining the mean square displacement of individual tPEG molecules after gelation. To explore the impact of defects, we systematically altered the defect density by incorporating tPEG chains with inert end groups in the homoleptic systems and by varying the stoichiometry in the heteroleptic mixtures. Additionally, we examined how the bending stiffness of the polymers influenced network structure and dynamics, finding a marked slowing down with increasing stiffness. These findings provide new insights into the factors governing the role of defects in the structure and dynamics of polymer networks.

CPP 15.58 Mon 19:00 P4

Silicone implementation to car industry — •Yury Ostretsov — Moscow, Russia, Bolshaya Semenovskaya 38

Silicone is a preferred material for manufacturing automotive hoses due to its high heat resistance, resistance to aggressive chemical environments, flexibility, and durability. These properties allow silicone hoses to maintain shape and performance under extreme temperatures and pressure fluctuations, reducing the risk of leaks or failures. Additionally, silicone is lightweight compared to rubber alternatives, contributing to overall vehicle efficiency. Its ability to withstand ozone and UV exposure also enhances longevity, making it a reliable choice for various automotive applications.

CPP 15.59 Mon 19:00 P4

Water flow decrease of track-etched polyethylene terephthalate membranes in filtration applications — •Ana Ambroz[1,2], Zhen Yao[2], Christopher Rojas[3], Polina Angelova[2], Irena Petrinic[1], and Armin Gölzhäuser[2] — [1]Univeristy of Maribor, Maribor, Slovenia — [2]University of Bielefeld, Bielefeld, Germany — [3]CNM Technologies GmbH, Bielefeld, Germany

Track-etched (TE) membranes, with their precise pore size, controlled porosity, and defined pore geometry, are industrially applied as highly sensitive and fast filters for bacteria in the food, cosmetic and pharmaceutical industries, as control barriers in glucose sensors, and as biomolecule selective barrier in implants. Additionally, they are being investigated for their potential in reverse and forward osmosis for water purification and cold concentration. However, their tendency to lose performance over time presents a significant challenge, particularly in high-throughput and durable applications. In this work, we evaluate the performance of track-etched polyethylene terephthalate (TE-PET) membranes as nano- and microfilters in low-pressure reverse osmosis (LPRO) and dead-end filtration systems. Monitoring water flux through the TE-PET membranes at different low pressures (0.02-10 bar) revealed a gradual decrease over time, varying with porosity and pore size. Specifically, membranes with low porosity ($<$1.5%) and small pore sizes ($<$1.5 um) exhibited a significant reduction in water flux. The decline is attributed to membrane swelling and the formation of a sol-gel film within the pores, with additional contributing factors discussed.

CPP 15.60 Mon 19:00 P4

Intermolecular bonds - connecting structure and dynamics — •Martin Tress[1], Friedrich Kremer[1], and Jan Philipp Gabriel[2] — [1]Peter-Debye-Institute for Soft Matter Research, Leipzig University, Leipzig, Germany — [2]Institute of Materials Physics in Space, German Aerospace Center, Köln, Germany

Descriptions of the glass transition often consider temperature dependent changes in the specific volume to explain the tremendous increase in relaxation time, and empricial data confirm the general role of thermal expansion [Nat Phys 19 (2023) 694]. However, since glassy dynamics happens on molecular scale, macroscopic thermal expansion might be too coarse. Here we use infrared spectroscopy data to extract intermolecular hydrogen (H)-bond lengths in wide temperature ranges. For water, the H-bond expansion coefficient differs strongly from the macroscopic one, which is easily assigned to considerable structural reorganization in the water network [JCP 160 (2024) 234502]. Their comparison reveals that the most compact molecular arrangement is formed in the range ~316-331 K (i.e. well above the density maximum). This coincides with several pressure-related anomalies which confirms this characteristic point in the supra-molecular arrangement. These results confirm our earlier approach to deduce inter-molecular H-bond lengths in polyalcohols [JCP 154 (2021) 024503] and open a new alley to investigate the role of inter-molecular expansion as a precursor to structural relaxation on a bond-specific level.

CPP 15.61 Mon 19:00 P4

Single-molecule spectroscopy of organic laser gain media — •Janne Becker, Robert Schmidt, Steffen Michaelis de Vasconcellos, and Rudolf Bratschitsch — Institute of Physics, University of Münster, Germany

Since the first experiments on pentacene [1], single-molecule spectroscopy has been performed for applications ranging from cell biology and medicine to organic laser media and single-photon emission [2]. To design and use these specialized molecules, their photophysical properties have to be investigated. Here, we perform single-molecule spectroscopy to study organic laser gain media. To isolate single molecules, we dilute the organic material down to concentrations of the order of nmol/L with ultra-pure solvents and measure characteristic fluorescence lifetimes and spectra.

References:

[1] W. E. Moerner and L. Kador, Physical Review Letters, 62, 2535. (1989)

[2] H. Miller et al, Rep. Prog. Phys. 81 024601 (2018)

CPP 15.62 Mon 19:00 P4

XPS study of redox mechanism in $Na_{2.5-x}Fe_{1.75}(SO_4)_3$ cathode material for high-voltage sodium-ion batteries — •Neama Imam[1], Karsten Henkel[1], Anna Milewska[2], Janina Molenda[2], Ehrenfried Zschech[1], and Jan Ingo Flege[1] — [1]Applied Physics and Semiconductor Spectroscopy, Brandenburg University of Technology Cottbus-Senftenberg, Germany — [2]AGH University of Krakow, Faculty of Energy and Fuels, Krakow, Poland

A multiplet splitting model based on the original work by Gupta and Sen has been used to track the redox mechanism and electronic structure of $Na_{2.5-x}Fe_{1.75}(SO_4)_3$, a high-performance cathode material for sodium-ion batteries (SIBs). This high-purity, off-stoichiometric open-channel cathode material with a tailored sodium-ion distribution, synthesized using an optimized solid-state route, demonstrates a high operating voltage of ∼3.8 V, surpassing the values reported for other cathode materials in the literature. X-ray photoelectron spectroscopy (XPS) was employed to analyze the evolution of the material's electronic structure at various charging potentials. $Fe2p_{3/2}$ spectra decomposition using the multiplet splitting model revealed the gradual oxidation of Fe^{2+} to Fe^{3+} during battery charging while transitioning from its pristine state ($x = 0$) with the presence of only Fe^{2+} at the cathode surface to the highest sodium de-intercalation level ($x = 1.61$). This result is consistent with the electrochemical analysis.

CPP 15.63 Mon 19:00 P4

Multiscale dynamics simulations of amorphous polyethylene terephthalate — •Andoni Ugartemendia[1], Alessandro Mossa[2], and Giorgia Brancolini[3] — [1]Institute of Nanoscience, CNR-NANO S3, via G. Campi 213/A, 41125 Modena, Italy — [2]Institute of Nanoscience, CNR-NANO S3, via G. Campi 213/A, 41125 Modena, Italy — [3]Institute of Nanoscience, CNR-NANO S3, via G. Campi 213/A, 41125 Modena, Italy

In the last decades, multiwall polymers have become widely used in food packaging due to their excellent mechanical and barrier properties. Unfortunately, the recycling of these materials is difficult and costly, leading to environmental problems. An understanding of the polymers properties is crucial towards the development of new recycling technologies. However, their computational modeling poses a great challenge since the dynamics span over several time scales. As a result, a multiscale approach becomes mandatory to gain access to the slower degrees of freedom. In this regard, coarse grained (CG) models have drawn considerable attention recently. CG models neglect the fastest degrees of freedom, flattening the rugged potential and thus, allowing higher time steps. In this work, we adopt a multiscale protocol to characterize several properties of polyethylene terephthalate (PET). First, atomistic molecular dynamics (MD) simulations are performed for amorphous PET systems with varying chain lengths. Then, the atomistic data is employed to derive a CG force field based on the iterative Boltzmann inversion (IBI). Finally, the structural data obtained with atomistic and CG simulaions are compared.

CPP 15.64 Mon 19:00 P4

Fourth-Generation High-Dimensional Neural Network Potentials for Molecular Chemistry in Solution — •Djamil Abdelkader Adel Maouene[1,2], Moritz Richard Schäffer[1,2], Moritz Gubler[3], Stefan Goedecker[3], and Jörg Behler[1,2] — [1]Theoretische Chemie II, Ruhr-Universität Bochum, Germany — [2]Research Center Chemical Sciences and Sustainability, Research Alliance Ruhr, Germany — [3]Department Physik, Universität Basel, Switzerland

Machine learning has become a powerful tool in chemistry and materials science, as high-dimensional neural network potentials (HDNNPs) provide accurate representations of multidimensional potential energy surfaces for atomistic simulations. In this study, we compare the performance of two types of HDNNPs; 2G-HDNNPs and 4G-HDNNPs, in modeling organic molecules in aqueous solution. While 2G-HDNNPs have proven effective in many systems in capturing local interactions based on atomic environments, they fail in scenarios where long-range charge transfer plays a critical role. These cases are better addressed by 4G-HDNNPs, which take into account atomic charge variations caused by structural or electronic changes even at distant regions in the system. Both methods are demonstrated using a model organic molecule.

CPP 15.65 Mon 19:00 P4

Insights into Machine Learning Interatomic Potentials for simple analytical model systems — •Mirko Fischer and Andreas Heuer — Institute for Physical Chemistry, University of Münster, Corrensstraße 28/30, 48149 Münster

During the past 10 years Machine Learning interatomic potentials

(MLIP) have gained popularity for Molecular Dynamics simulations with quantum chemical accuracy. Although it is a rapidly evolving field, many questions remain open. These include issues of interpretability, modeling different interaction types and how to select training data properly. MLIPs are rarely applied to simple model systems, for which the interactions of particles can be described analytically, to investigate these questions. Instead, MLIPs are mostly applied directly to realistic molecular systems for which the ground truth interactions must be approximated by methods like Density Functional Theory. By training an Atomic Cluster Expansion as a systematic and generally interpretable model for a Lennard-Jones model system, we aim to study how interaction types, system size and temperature affect the learned model in a systematic manner. The obtained interactions can be directly compared to the known true analytical interactions. Moreover, we fit a MLIP for an amorphous silica system to study structure and dynamics in a glass-forming system, where low-energy states are important. The question emerges, how to select the training data best and if such low-energy (low temperature) states must be explicitly included in it or if the MLIP is able to extrapolate from high-energy (high temperature) states to low energy states.

CPP 15.66 Mon 19:00 P4

Efficient Millisecond Timescale Modeling of Hydroxide Ion Dynamics in Aqueous Systems: A Multiscale Simulation Approach — •Jonas Hänseroth[1,2], Daniel Sebastiani[2], and Christian Dressler[1] — [1]Theoretical Solid State Physics, Institute of Physics, Ilmenau Universitiy of Technology, Ilmenau, Germany — [2]Theoretical Chemistry, Institute of Chemistry, Martin-Luther-University of Halle-Wittenberg, Halle (Saale), Germany

An adapted combined Molecular Dynamics/Lattice Monte Carlo (cMD/LMC) approach models hydroxide ion transport across extended systems and millisecond timescales.[1] The method surpasses classical Molecular Dynamics in efficiency while maintaining the accuracy of ab initio Molecular Dynamics, allowing the study of aqueous potassium hydroxide systems over a wide concentration range (3-61 wt.-%). The cMD/LMC algorithm allows simulations involving thousands of atoms at low computational cost, yielding diffusion coefficients consistent with ab initio benchmarks. This framework can provide insights into the dynamics of hydroxide ion in systems such as anion exchange membranes, which are essential for fuel cell technology. [1] J. Chem. Theory Comput. 2014, 10, 10, 4221-4228

CPP 15.67 Mon 19:00 P4

Confinement-induced dynamics in binary liquid mixtures: insights from molecular simulations — •Anam Sara, Pascal Merle, Siegfried Stapf, and Christian Dressler — Technische Universität Ilmenau, Germany

In this work, we investigate the behavior of binary liquid mixtures confined within silica nanopores, examining how confinement impacts the diffusion and relaxation properties of mixtures such as cyclohexane/acetone, cyclohexane/tetrahydrofuran (THF), water/acetone, and water/THF [1]. Experimental NMR measurements revealed deviations in diffusion coefficients and relaxation times of these mixture under confinement [2,3]. To interpret these observations, we perform molecular dynamics (MD) simulations to get atomistic insights into the structure and dynamics of these mixtures within the pores. Our primary objective is to characterize how confinement alters the microphase separation, component density distribution along the pore axis, and preferential interactions with pore walls.

[1] G. Guevara-Carrion, T. Janzen, Y. Muñoz-Muñoz, J.Vrabec, The Journal of Chemical Physics, 144, (2016).

[2] D. Bellaire, H. Kiepfer, K. Münnemann, H. Hasse, J. Chem. Eng.Data, 65, 793-803 (2020).

[3] Stapf, S., Siebert, N., Spalek, T., Hartmann, V., Gizatullin, B., and Mattea, C. (2023).

CPP 15.68 Mon 19:00 P4

Density of states in hard disks: Concentration dependency via SAMC simulation — Timur Shakirov[1,2], Malte Kautzsch[1], and •Viktor Ivanov[1] — [1]Martin-Luther-University Halle-Wittenberg, Halle (Saale), Germany — [2]Indivumed GmbH, Hamburg, Germany

We propose a new variant of SAMC sampling for determining the density of states as a function of the concentration of particles. The system is modelled as a set of dimensionless points, i.e., points with zero diameter. The minimal points separation, d_{min}, is chosen as the sampling parameter determining the macrostate. Thus, the density of states and the visiting histogram depend on the minimal distance d_{min} and are accumulated at each step of the algorithm according to the standard SAMC procedure. In a microstate (particular configuration of points' positions) with a given value of the minimal distance between points, d_{min}, one can replace the points with the hard disks of the diameter d_{min} (or less). This creates a system with a specific value of the concentration φ. We apply this algorithm for the two-dimensional system of hard disks to study its phase behaviour at different concentrations and compare the results with KTHNY theory and the previous simulations.

CPP 15.69 Mon 19:00 P4

Multiscale Simulation Framework for Functional Polymer Systems — •Steffen Kampmann[1], Alexander Croy[2], Arezoo Dianat[1], and Gianaurelio Cuniberti[1,3] — [1]Institute for Materials Science and Max Bergmann Center for Biomaterials, TU Dresden — [2]Chair of Theoretical Chemistry, Institute of Physical Chemistry, Friedrich Schiller University Jena — [3]Dresden Center for Computational Materials Science (DCMS)

Functional, mechanically resilient polymer and polymer-based nanocomposite films play an important role for strain gauges or organic light-emitting diode (OLED) displays [1-3]. The modelling and simulation workflow presented here enables the generation of disordered polymer systems and the linking of the mechanical and electronic properties from the atomistic to the microscopic size scale. Here, the focus is on the relationship between deformation and conductivity behavior. To calculate the multi-scale material behavior, we use density functional tight binding (DFTB) calculations, molecular dynamics simulations, and the finite element method. The in-situ processing, evaluation as well as the exchange of the generated data across simulation methods is performed using our Python framework. The multi-scale computational workflow indicated here represents a computationally efficient assessment of the properties of the polymer systems at different scales. [1] K. Grabowski, et al., Computational Materials Science, 135, 169*180, (2017) [2] R. Luo, et al., Progress in Organic Coatings, 162, 106593 (2022) [3] L. Liu, et al., Organic Electronics, 89, 106047 (2021)

CPP 15.70 Mon 19:00 P4

Investigation of electrolyte dynamics with interfaces: Insights from simple MD-models — •Katharina Kintrup[1,2], Youssef Mabrouk[1,2], Diddo Diddens[1,2], and Andreas Heuer[1] — [1]Institut für Physikalische Chemie, Corrensstraße 28/30, 48149 Münster, Deutschland — [2]Helmholtz-Institut Münster, Corrensstraße 48, 48149 Münster, Deutschland

Molecular Dynamics (MD) simulations are a common tool to investigate transport properties of electrolytes. Typically, periodic boundary conditions (pbc) are applied to simulate energetically closed systems, which are contrary to experimental systems with interfaces. Electrophoretic NMR (eNMR) experiments show that the incompressibility is dominating the transport properties of electrolytes, leading to an application of local conservation of volume. [1] Inspired by this, we set up simplified models to simulate binary liquids, imitating ionic liquids (IL), within interfaces, resulting in energetically open systems. After applying external (electric) fields, various properties of the model systems such as average velocities, number densities, volume densities, etc. were evaluated. A transition from local conservation of momentum towards local conservation of volume was observed. The velocities of all systems portrayed oscillations due to sound waves. A general analysis of dynamic processes on different time scales for systems without explicit charges was achieved. A comparison between systems with and without explicit charges was conducted, proving the superiority of the advanced charged model due to higher incompressibility. [1] J. Phys. Chem. Lett, 2022, 13, 8761-8767

CPP 15.71 Mon 19:00 P4

Evidence for unusual solvation shell of aqueous Fe^{3+} at high dilution — •Amrita Goswami, Elvar Örn Jónsson, and Hannes Jónsson — Science Institute and Faculty of Physical Sciences, University of Iceland, VR-III, 107 Reykjavík, Iceland

Solvated Fe^{3+} in water is a particularly important system, relevant, for instance, for the widely studied charge transfer Fe3+/Fe2+. However, the solvation shell of such highly charged cations is still poorly understood, particularly at for concentrations less than 1 M. In this regime of high dilution, experimental data and high-level calculations are sparse. For instance, most density-functional theory calculations are performed at a concentration of 0.8 M or higher, with uniform background charge. Simulations for such dilute solutions can provide insight inaccessible to other techniques. Using extensive molecular dynamics simulations with empirical potentials and DFT geometry optimizations of selected configurations, we study the effect of solution concentration on the solvation structure of aqueous Fe^{3+}. The solvation shell is found to undergo abrupt transitions between two states: an octahedral (OH) state with 6-fold coordination, and a metastable capped trigonal prism (CTP) state with 7-fold coordination. Further, we have developed a QM/MM (quantum-mechanical/molecular mechanical) method to study dilute solutions of aqueous Fe^{3+} with DFT-level accuracy, with a polarizable water model. References: Goswami et al., J. Phys. Chem. Lett., 2024

CPP 15.72 Mon 19:00 P4

Exploring Pathways of Supramolecular Self-Assembly at Liquid-Liquid Interfaces — •Mephin Philip Alamcheril[1], Friederike Schmid[1], and Shikha Dhiman[2] — [1]Institute for Physics, Johannes Gutenberg University Mainz — [2]Department of Chemistry, Johannes Gutenberg University Mainz

A self-assembly process usually occurs through thermodynamic pathways but the co-existence of different intermediates and diverse pathways of self-assembly have been observed. Liquid droplets are one such intermediate in many self-assembly processes, particularly in biological systems, which form through liquid-liquid phase separations (LLPS). Even though LLPS is a very well-known phenomena in polymer chemistry, only little is known about the possible role of LLPS in synthetic small molecule-based self-assembly.

In this project, we aim to study the possible mechanism of self-assembly at the surface of phase separated liquid droplets to explore the structure and dynamics at various stages of self-assembly and provide insights into how it can be controlled and manipulated for various applications. To that end, we develop a simple coarse-grained model for monomers in explicit solvent that self-assemble into fibers. The model is designed to represent BTA-like molecules in water. It is able to capture key characteristics of the experimental system such as the competition of fibril formation and liquid-liquid phase separation. We use it to examine the pathways of fibril formation from phase separated droplets.

CPP 15.73 Mon 19:00 P4

Isoconversional effect in epoxy polymerization process — •Sampanna Pahi[1], Christian Wick[1,2], and Ana Sunčana Smith[1,2,3] — [1]PULS Group, Institute for Theoretical Physics , FAU Erlangen-Nürnberg, Germany — [2]Group of Computational Life Sciences, Division of Physical Chemistry, Ruder Bošković Institute, Zagreb, Croatia — [3]Competence Unit for Scientific Computing (CSC), FAU, 91058 Erlangen, Germany

Isoconversional methods are essential for understanding the kinetics and predicting thermodynamic data in epoxy polymerization. While these methods have been experimentally validated, their computational modeling remains underexplored. In this study, we use molecular dynamics (MD) simulations and Quantum Mechanics/Molecular Mechanics (QM/MM) transition state (TS) analyses to investigate mechanisms and energetic barriers in epoxy thermoset curing, focusing on isoconversional effects. We generated post-a-priori QMMM reactive sites with hydrogen-bonded systems to examine the influence of hydrogen bonding on the curing process. Initial results without hydrogen bonds showed higher activation energies than experimental values, with some outliers showing lower energies. Adding hydrogen bonds, especially hydroxyl (OH) bonds, reduced activation energies and explained these discrepancies. Radial distribution function (RDF) analyses showed OH bond formation is more likely than amine (NH) bonds, highlighting hydrogen bonding*s critical role in isoconversional effects during epoxy curing.

CPP 15.74 Mon 19:00 P4

A Multiscale MD-QM/MM Approach for Modeling Fracture Behavior in Epoxy Resins — •Barişcan Arican[1], Christian Wick[1], and Ana-Sunčana Smith[1,2] — [1]PULS Group, Institute for Theoretical Physics, IZNF, FAU Erlangen-Nürnberg, 91058 Erlangen — [2]Group of Computational Life Sciences, Division of Physical Chemistry, Ruder Bošković Institute 10000 Zagreb, Croatia

Epoxy resins, with their exceptional mechanical properties, are indispensable in advanced engineering applications. However, understanding their fracture behavior at the molecular level remains a challenge. This study presents a multiscale framework that couples molecular dynamics (MD) simulations with quantum mechanics/molecular mechanics (QM/MM) calculations to analyze bond rupture and crack propagation in epoxy networks. The MD component monitors strain accumulation and identifies critical bond elongation thresholds indicative of imminent fracture. When these thresholds are met, the simulation transitions to QM/MM calculations, where bond breakage is determined dynamically by considering the surrounding chemical environment. This on-the-fly approach enables efficient and accurate modeling of fracture events and their impact on larger-scale material behavior, providing a foundation for future studies of epoxy resin failure mechanisms.