

## CPP 21: Poster II

Composites and Functional Polymer Hybrids (1-7), Crystallization, Nucleation and Self-Assembly (8-17), Polymer and Molecular Dynamics, Friction and Rheology (18-22), Modeling and Simulation of Soft Matter (23-38), Glasses and Glass Transition (39-42)

Time: Tuesday 18:00–20:00

Location: Poster E

CPP 21.1 Tue 18:00 Poster E

**Tailoring Mesoporous Film Morphologies in Zinc Titanate Oxide via PS-b-PEO Guided Cooperative Self-Assembly** — •YANAN LI<sup>1</sup>, NIAN LI<sup>1</sup>, SHANSHAN YIN<sup>1</sup>, CONSTANTIN HARDER<sup>2</sup>, YUSUF BULUT<sup>2</sup>, APOSTOLOS VAGIAS<sup>3</sup>, STEPHAN V. ROTH<sup>2,4</sup>, and PETER MÜLLER-BUSCHBAUM<sup>1,3</sup> — <sup>1</sup>TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — <sup>2</sup>DESY, 22607 Hamburg, Germany — <sup>3</sup>MLZ, TUM, 85748 Garching, Germany — <sup>4</sup>Department of Fiber and Polymer Technology, KTH, SE-100 44 Stockholm, Sweden

Mesoporous ordered films have broad applications ranging from sensors to supercapacitors and biodevices due to their large surface-to-volume ratio and pore accessibility of their porous nanostructures. Here, we investigate the morphology evolutions and formation mechanisms of the morphologies of mesoporous zinc titanate oxide films obtained by changing the ratios of two inorganic precursors after calcining hybrid films consisting of organic-inorganic materials. The amphiphilic diblock copolymer self-assembles into micelles in a solvent mixture playing the role of the structure-directing template. The inorganic precursors are loaded in the micellar shell due to hydrogen bonds between poly(ethylene oxide) and precursors. We combine a sol-gel route with a spin coating to prepare hybrid films and investigate the influence of the different weight fractions of precursors and polymer concentration on the film morphologies. The inner and surface morphologies of the hybrid films are characterized using grazing incidence small-angle X-ray scattering and scanning electronic microscopy, respectively.

CPP 21.2 Tue 18:00 Poster E

**Enhancement of the Protection Performance of Eco-friendly Polymers and Nanoparticles/Polymers Coated Copper Artifact in Synthesized Marine Environments** — •MAI DIAB<sup>1</sup> and WAFAA SOLIMAN<sup>2</sup> — <sup>1</sup>National Museum of Egyptian Civilization, Cairo, Egypt — <sup>2</sup>National Institute of Laser enhancement Science, Giza, Egypt

Protective coatings based on eco-friendly polymers synthesized from renewable sources (chitosan or glycerol/chitosan polymer) have been prepared for copper artifacts protection from marine corrosion. In addition, the coating efficiency has been improved by adding a protective metal coating for copper as a corrosion inhibitor compound (ZnNi-nanoparticles) to the formulations. An accelerating corrosion test on coated copper substrates was performed to optimize the minimum amount of the inhibitor compound. Dipcoating technique was used to coat the copper specimen's surfaces. Chitosan coating was damaged when it was accelerated under marine corrosive conditions. To solve this problem, ZnNi nanoparticles were added to a chitosan-based solution. It was noticed that the significant addition of ZnNi improved the coating properties. The structural features of the coatings were evaluated by Raman spectroscopy. The surface hydrophobicity was investigated by contact angle measurements. The surface morphology changes of control and coated specimens prior to and after marine aging were evaluated by AFM and SEM. The results show that the 0.2 wt% ZnNi nanoparticles enhanced the efficiency, the mechanical hardness, and the roughness of the specimens.

CPP 21.3 Tue 18:00 Poster E

**Engineering a Dual In-Situ Strategy to Incorporate Organotitanium Nanosheets into Polyethylene Terephthalate for High-Performance Outdoor UV Fabric Shelters** — •HAILONG YU, JIA CHEN, XIANG FEI, BIN SUN, and MEIFANG ZHU — State Key Laboratory for Modification of Chemical Fibers and Polymer Materials, College of Materials Science and Engineering, Donghua University, 201620, Shanghai, China

In this study, we employed a dual in-situ approach to integrate organotitanium nanosheets into Polyethylene Terephthalate (PET), aiming to explore their applications in high-performance outdoor UV fabric shelters. Characterization techniques, including SEM, XRD, GPC, TGA, DSC, dynamic oscillatory rheology, and capillary rheometer, were utilized. Notably, the study revealed that the nanosheet struc-

ture significantly impacted PET's rheological and crystalline behavior, thereby exerting a profound influence on processing performance. We achieved uniform nanosheet dispersion within PET, enhancing structural integrity. PET/nano-Ti composites displayed outstanding UV resistance, with 80% retained strength after UV exposure, surpassing pure PET (70%). UV-A transmittance was only 2.38%, with UPF exceeding 50. These composites offer a robust choice for UV fabric shelters, including outdoor clothing and tents. This research highlights the profound impact of nanosheet composites on PET's behavior and their critical role in UV resistance, supporting the development of high-performance outdoor materials.

CPP 21.4 Tue 18:00 Poster E

**Mechanical Response of Carbon Fiber Reinforced Epoxy Composite Parts Joined with Varying Bonding Techniques for Aerospace Applications** — •FURKAN KARABOĞA<sup>1</sup>, YAHYA ÖZ<sup>1</sup>, ERDEM YUNUS<sup>2</sup>, and FATİH GÖLEÇ<sup>2</sup> — <sup>1</sup>Turkish Aerospace, Ankara, Turkey — <sup>2</sup>Bursa Technical University, Bursa, Turkey

Due to the widespread usage of composite materials in aerospace structures, the significance of composite joining methods has been increased. In this research, the impact of various joining techniques on the strength of composite joints through experimental, numerical and analytical analyses is investigated. The study compares the single lap joint shear strengths of carbon fiber reinforced epoxy composites, which are assembled using fastening with pop rivets and solid rivets, secondary bonding, co-curing and co-bonding methods. Additionally, the influence of adhesive thicknesses (from 0.2 to 0.76 mm) for secondary bonding, adhesive film existence for co-bonding and overlapping distance for co-curing on single lap shear strength is explored. Following the production of samples employing different joining methods, tests were conducted according to ASTM 5868. Furthermore, the interface damage in composites was analyzed by using a scanning electron microscope aiming to understand the damage mechanism. Evaluation of fracture mechanisms associated with bonding methods was performed by inspecting the fracture surface of composite samples. The obtained results were also analyzed numerically using software tools. The highest strength is obtained as approximately 25 MPa which deviates only 3 % from the numerical results.

CPP 21.5 Tue 18:00 Poster E

**Improvement of Self Healing Functions of Composites via Microvascular Channels** — •ERAY KOSTUR<sup>1</sup>, MERVE OZKUTLU DEMIREL<sup>1</sup>, and NECDET GEREN<sup>2</sup> — <sup>1</sup>Turkish Aerospace, Ankara, Turkey — <sup>2</sup>Cukurova University, Adana, Turkey

Carbon fiber-reinforced polymer (CFRP) composites having high specific strength and modulus, are highly convenient for aerospace and automotive applications which require light-weight and high strength. However, the usage of CFRP is limited by their low crack resistance and poor off-axis strength causing material damage as a result of static and dynamic effects over its service time. Besides, prediction of the failure due to local damages are not reliable so far. This study aims to provide a composite structure with self-healing features through a novel microvascular channel mechanism while preserving its mechanical properties and as a result, to repair micro-sized cracks that occur in its structure. The effect of different channel configurations on mechanical properties is evaluated with mechanical tests. A self-healing agent was injected into microvascular channels and the reaction was triggered by a catalyst which is distributed into matrix, as the crack propagates through the channels. An enhancement of approximately 25 % is observed in the displacement values.

CPP 21.6 Tue 18:00 Poster E

**Biopolymer-Templated Deposition of Hierarchical 3D-Structured Graphene Oxide/Gold Nanoparticle Hybrids for Surface-Enhanced Raman Scattering** — •YINGJIAN GUO<sup>1,2</sup>, JUNGUI ZHOU<sup>1</sup>, CONSTANTIN HARDER<sup>1,2</sup>, GUANGJIU PAN<sup>2</sup>, SUO TU<sup>2</sup>, SARATHLAL KOYILOTH VAYALIL<sup>1</sup>, DANIEL SÖDERBERG<sup>4</sup>, PETER MÜLLER-BUSCHBAUM<sup>2,3</sup>, and STEPHAN V. ROTH<sup>1,4</sup> — <sup>1</sup>Deutsches

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Cellulose has emerged as a promising bio-based substrate capable of synergistically combining with conductive materials for diverse applications including 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 and reproducible enhancements of the Raman signal over large areas. Herein, we present a straight-forward approach utilizing the layer-by-layer spray coating method to fabricate films loaded with gold nanoparticles and graphene oxide to serve as SERS substrates. To investigate the fundamental mechanisms of enhanced SERS performance, grazing incidence small-angle X-ray scattering was employed to gain comprehensive insights into the nanostructure. Therefore, our approach provides a reference for facile and scalable production of SERS substrates.

CPP 21.7 Tue 18:00 Poster E

**Height Distribution of Microparticles in a Local-Light Driven Diffusioosmotic Flow** — ●FABIAN ROHNE — Institut für Physik und Astronomie, Karl-Liebknecht-Str.24-25, 14476 Potsdam-Golm

It has been demonstrated that separation of particles of equal size but different surface energies is possible by combination of local-light driven diffusioosmosis (local-LDDO) and microfluidic technology.[1] However, the local-LDDO causes lateral particle repulsion, which results in long-ranged particle-particle interactions observable by an increased horizontal and vertical distance. Here, we present how the height distribution influences drift motion distribution of microparticles along a pressure driven fluid flow, which depends on particle concentration, applied wavelength and fluid low.

[1] Bekir, M.; Sperling, M.; Vasquez Muñoz, D., Braksch, C.; Böker, A.; Lomadze, N.; Popescu, M. N., Santer, S. *Advanced Materials* 2023, 35, 2300358.

CPP 21.8 Tue 18:00 Poster E

**Mechanism for the formation of millimeter-long solid filaments by spin coating dilute solutions of a crystallizable polymer** — ●DA HUANG<sup>1</sup>, THORSTEN HUGEL<sup>2</sup>, and GÜNTER REITER<sup>1</sup> — <sup>1</sup>Institute of Physics, University of Freiburg, Freiburg, Germany — <sup>2</sup>Institute of Physical Chemistry, Albert-Ludwigs-Universität Freiburg, Germany

We investigated the formation of millimeter-long filaments formed by spin-coating dilute para-xylene solutions of rapidly crystallizable polyethylene chains with a contour length in the micrometer range onto mica substrates at high temperatures. These filaments were radially oriented and accumulated at the periphery of the substrate. Our observations can be explained by the stretching of polymers through the flow field induced by spinning the solution on a solid substrate. The corresponding loss in conformational entropy emphasized attractive interactions between polymers, which resulted in the formation of bundles and their assembly into long filaments. Caused by a Plateau-Rayleigh-type instability of a liquid coating on a solid filament and due to crystallization, these filaments were decorated with various small-scale structures. Still in solution, the resulting filaments experienced a Coriolis force as they were dragged towards the periphery of the sample, causing a deviation of their orientation from the radial direction. Finally, filaments adsorbed on the substrate, the solvent evaporated completely and the resulting variety of crystalline patterns and morphologies were examined by various microscopy techniques.

CPP 21.9 Tue 18:00 Poster E

**Structure formation in aqueous amine solutions** — ●LENA FRIEDRICH<sup>1</sup>, DIRK LÜTZENKIRCHEN-HECHT<sup>2</sup>, MICHAEL PAULUS<sup>1</sup>, AURÉLIEN PERERA<sup>3</sup>, MARTINA POŽAR<sup>4</sup>, and CHRISTIAN STERNEMANN<sup>1</sup> — <sup>1</sup>Fakultät Physik / DELTA, Technische Universität, 44221 Dortmund, Germany — <sup>2</sup>Fakultät für Mathematik und Naturwissenschaften, Bergische Universität Wuppertal, 42097 Wuppertal, Germany — <sup>3</sup>Sorbonne Université, Laboratoire de Physique Théorique de la Matière Condensée (UMR CNRS 7600), F75252, Paris cedex 05, France — <sup>4</sup>University of Split, Faculty of Science, 21000 Split, Croatia

Amines are associating liquids that can form transient supramolecular structures via hydrogen bonding [1]. Adding water can significantly alter the liquids' molecular structure. We studied linear, primary amines

mixed with various proportions of water, which we heated and cooled, by X-ray diffraction performed at beamline BL8 of DELTA (TU Dortmund). The structure factor pre-peak shows a peculiar concentration dependence when water is added. It significantly gains intensity with increasing water content and shifts to smaller wave-vector transfers. This effect is even more pronounced the longer the carbon chain of the amine is. With temperature increase the intensity of the pre-peak decreases. These observations are interpreted in terms of transient cluster formation using molecular dynamics simulations [2]. We thank the BMBF for funding via DAAD in the scope of the French-German collaboration PROCOPE 2024-2025 (Project-IDs 57704875 and 50951YA). [1] L. Almasy et al., *PCCP* 21, 9317 (2019); [2] M. Požar and A. Perera, *J. Mol. Liquids* 227, 210 (2017).

CPP 21.10 Tue 18:00 Poster E

**Multistep liquid-crystalline ordering of poly(3-hexylthiophene) films induced by the vacuum interface** — ●ANTON SINNER and OLEKSANDR DOLYNCHUK — Experimental Polymer Physics, Martin Luther University Halle-Wittenberg, Germany

Crystallization in liquids is often initiated at solid-liquid interfaces, which can result in enhanced nucleation kinetics and crystal orientation. However, the influence of the less specific interface to air or vacuum can be of the same importance for ordering phenomena. Elucidating these processes is especially relevant for films of functional polymers, as the structure orientation induced at interfaces can significantly affect the material properties. Here, the influence of the vacuum interface on the crystallization in films of model semiconducting polymer poly(3-hexylthiophene) (P3HT) is investigated. By using in-situ X-ray reflectivity and grazing-incidence X-ray scattering during crystallization upon cooling from the melt, we show that the ordering of P3HT films starts at the vacuum interface and undergoes multiple smectic liquid-crystalline state (SLCS) transitions. The same hierarchy of SLCS is observed during melting, largely independent of the film thickness. Furthermore, we show that the vacuum interface induces the SLCS transitions at temperatures higher than that of bulk, which still results in a significant thermal hysteresis between cooling and heating. Our results demonstrate that the SLCS formation in P3HT has both similarities and differences to surface freezing of short alkanes at the vacuum interface, providing new insights into the phenomenon.

CPP 21.11 Tue 18:00 Poster E

**Semicrystallinity in vitrimers studied by solid-state NMR** — KAY SAALWÄCHTER and ●FATEMEH FOULADI — Institut für Physik - NMR, Betty-Heimann-Str. 7, Martin-Luther Universität Halle-Wittenberg, 06120 Halle, Germany

In this study, we investigate the crystalline nature of vitrimer samples with catalyst-controlled bond dynamics by time-domain NMR. The studied vitrimer samples, synthesized by various catalysts to control bond exchange kinetics, feature covalent adaptable networks (CANs) intricately crosslinked through dynamic covalent bonds. The aim is to explore how vitrimeric exchanges influence crystallinity and identify the maximum attainable crystallinity. Specifically, crystallization kinetics was investigated via low-field <sup>1</sup>H NMR. The structural diversity in our sample raises questions about the crystallization of alkyl chains or the potential involvement of ester/thioester groups in crystal formation, which is answered by <sup>13</sup>C MAS NMR.

CPP 21.12 Tue 18:00 Poster E

**Influence of interfacial interactions on the kinetics, morphology, and crystal orientation of interface-induced polymer crystallization** — ●MARTHINUS VAN NIEKERK, OLEKSANDR DOLYNCHUK, and THOMAS THURN-ALBRECHT — Experimental Polymer Physics, Institute of Physics, Martin Luther University Halle-Wittenberg, Germany

Initiation of polymer crystallization at an interface to a solid can strongly affect crystallization kinetics that normally surpass that of homogeneous nucleation in the bulk. While heterogeneous nucleation is an activated process occurring below  $T_m$ , the process of prefreezing produces a crystalline layer above  $T_m$ , which thickens upon cooling. Both prefreezing and heterogeneous nucleation are dependent on interfacial interactions between a polymer and the underlying substrate. We present a systematic study of the crystallization of a model polymer, poly( $\epsilon$ -caprolactone) (PCL), on several substrates to elucidate the effects of interfacial interactions. We employ a system of dewetted PCL droplets on various substrates, allowing identification of individual nucleation events. AFM imaging confirms the existence of isolated droplets. Studies with polarized microscopy show large differences in

the crystallization rate of PCL droplets during cooling from the melt on different substrates. X-ray scattering shows anisotropic scattering from PCL droplets, which varies according to the substrate, proving that the substrate induces orientation of crystalline lamellae. Thus, we demonstrate the effects of interfacial interactions on interface-induced polymer crystallization.

CPP 21.13 Tue 18:00 Poster E

**Influence of Cooling Rate and Molecular Weight on Crystallization of Thin Films of Poly-(3-hexylthiophene) at the Vacuum Interface** — ●ALEXANDER J. MUCH and OLEKSANDR DOLYNCHUK — Experimental Polymer Physics, Institute of Physics, Martin-Luther-University Halle-Wittenberg, Germany

The electronic properties of organic semiconductors in general and semiconducting polymers in particular depend on the crystal orientation. It was previously shown that the interface to air or vacuum induces edge-on orientation in the model semiconducting polymer poly-(3-hexylthiophene) (P3HT) during crystallization from the melt, competing with bulk crystallization. To better understand the kinetics of this crystallization phenomenon, here we investigate the effect of cooling rate on the crystal orientation formed in P3HT films on glass substrates. Furthermore, since molecular weight  $M_w$  is known to affect the crystallinity and degree of order in bulk P3HT, we also investigate whether  $M_w$  has any effect on the crystal orientation of P3HT films. Using grazing-incidence wide angle X-ray scattering, we show that an increased cooling rate during crystallization from the melt suppresses the formation of edge-on crystals at the vacuum interface in P3HT, resulting in a more isotropic crystal orientation. Meanwhile, there is little to no difference in crystal orientation in films of P3HT with  $M_w=15\text{kg/mol}$  and  $M_w=47\text{kg/mol}$  under otherwise identical experimental conditions. Thus, our results demonstrate that the kinetics of P3HT crystallization at the vacuum interface is significantly slower than in the bulk and is weakly dependent on  $M_w$  of P3HT.

CPP 21.14 Tue 18:00 Poster E

**Integrated Simulation and Experimental Study on the UV Resistance and Crystallization of PA6/TiO<sub>2</sub> Nanocomposites** — ●HAILONG YU<sup>1,2</sup>, JENS-UWE SOMMER<sup>2</sup>, BIN SUN<sup>1</sup>, and MEIFANG ZHU<sup>1</sup> — <sup>1</sup>State Key Laboratory for Modification of Chemical Fibers and Polymer Materials, College of Materials Science and Engineering, Donghua University, 201620, Shanghai, China — <sup>2</sup>Leibniz-Institut für Polymerforschung Dresden, Hohe Strasse 6, 01069 Dresden, Germany

Addressing the heightened risk from increased UV radiation due to ozone depletion, our study developed PA6/TiO<sub>2</sub> nanocomposite fibers with enhanced UV protection. We integrated surface-modified TiO<sub>2</sub> nanoparticles into PA6 fibers using a masterbatch blending technique and performed extensive material characterizations. The study centered on the effects of TiO<sub>2</sub>, modified with agents 550 and 570, on PA6's crystallization. We observed a raised onset temperature and modified crystallinity, significantly influenced by agent 550's grafting effect on PA6's hydroxyl groups. Simulation studies provided further understanding of the structural changes impacting crystallization kinetics. A key achievement of this work is the fibers' exceptional UV resistance, demonstrated by a UPF surpassing 50, making them highly suitable for outdoor applications where robust UV protection is essential.

CPP 21.15 Tue 18:00 Poster E

**Engineering Anisotropic Photoluminescence in Quantum Dot Metasurfaces** — ●LAVANYA BERI<sup>1,2</sup>, OLHA AFTENIEVA<sup>2</sup>, SWAGATO SARKAR<sup>2</sup>, and TOBIAS A.F. KÖNIG<sup>2,3</sup> — <sup>1</sup>Indian Institute of Technology Delhi — <sup>2</sup>Leibniz-Institut für Polymerforschung Dresden e.V. (IPF), Hohe Straße 6, 01069 Dresden, Germany — <sup>3</sup>Center for Advancing Electronics Dresden (cfaed), Technische Universität Dresden, Helmholtzstraße 18, 01069 Dresden, Germany

Quantum dots are high-performance, solution-processed materials with high photoluminescence quantum yield. Due to these exceptional properties, quantum dots can serve as building blocks for metasurfaces and are of broad interest for photonic applications. Here, we propose a metasurface with anisotropic photoluminescence due to its structuring. With the help of the template-assisted self-assembly methods [Advanced Functional Materials, 31(36), 2105054], we arrange highly luminescent quantum dots into the so-called blazed grating with intrinsic geometrical asymmetry. The latter modifies quantum dots' otherwise omnidirectional emission profile [ACS nano, 17(3), 2399-2410], enhancing it along the particular resonant directions. We demonstrate the asymmetry of the periodic structure using angle-resolved

Fourier spectroscopy. This approach may pave the way toward unidirectional light propagation and lasing [Advanced Optical Materials, 11(6), 2202226].

CPP 21.16 Tue 18:00 Poster E

**Probing pre-crystallization dynamics** — ●ATMIKA BHARDWAJ<sup>1,2</sup>, JENS-UWE SOMMER<sup>1,2</sup>, and MARCO WERNER<sup>1</sup> — <sup>1</sup>Institut Theorie der Polymere, Leibniz-Institut für Polymerforschung Dresden e.V., Hohe Strasse 6, 01069 Dresden, Germany — <sup>2</sup>Institute für Theoretische Physik, Technische Universität Dresden, Zellescher Weg 17, 01062 Dresden, Germany

Polymer crystallization is a fundamental process influencing material properties, yet understanding the molecular intricacies preceding crystallization remains a challenge. This research builds on our prior work in generating unsupervised machine-learning labels for amorphous and crystalline phases in polymer crystallization [A. Bhardwaj, J.-U. Sommer and M. Werner, arXiv:2311.00454 (2023)]. Our focus extends to the exploration of the polymer melt, to quantify the latent information contained within its molecular conformations prior to crystallization. Through the analysis of the spatial distribution of molecular fingerprints, we characterize the subtle changes in molecular arrangements that precede the crystalline transition. Our study strives to advance the understanding of polymer crystallization, offering a new perspective for informed material design.

CPP 21.17 Tue 18:00 Poster E

**Polymer crystallization in bulk and on substrates: flat histogram Monte Carlo simulation** — ●EVGENIYA FILIMONOVA, TIMUR SHAKIROV, and VIKTOR IVANOV — Martin-Luther-University Halle-Wittenberg, Halle (Saale), Germany

We use the stochastic approximation Monte Carlo (SAMC) simulation to study crystallization in melts of short polymers chains in the bulk and under confinement (between two hard walls). SAMC allows to sample configurations uniformly over the whole interval of energies in microcanonical ensemble and analyse the transition between amorphous melt at high energies and homogenous crystal at low energies, with a variety of inhomogeneous partially crystalline configurations inbetween. We have proposed new methods for analysis of local crystal ordering based on bond order parameters calculated for properly averaged particle coordinates, which has allowed us to observe the coexistence of domains with different local crystalline symmetries. In melts confined between two walls, we observe a coexistence of an isotropic structure in the center of the film with ordered structures at the walls at intermediate values of energies. Our aim is to identify physical factors which are responsible for one of two possible scenarios of surface-induced polymer crystallization: heterogeneous nucleation or prefreezing.

CPP 21.18 Tue 18:00 Poster E

**Molecular dynamics study on the impact of water distribution on nanoscopic friction in case of monolayer MoS<sub>2</sub>** — ●MILJAN DAŠIĆ<sup>1,2</sup> and IGOR STANKOVIĆ<sup>2</sup> — <sup>1</sup>Institute of Organic Chemistry and Biochemistry of the Czech Academy of Sciences, Flemingovo náměstí 2, 166 10, Prague, Czech Republic — <sup>2</sup>Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia

We have designed and applied a molecular dynamics (MD) simulation setup for the study of nanoscopic frictional phenomena in case of monolayer MoS<sub>2</sub>. Our design represents a typical AFM experiment, comprising an amorphous SiO<sub>2</sub> probe in tribo-contact with a monolayer crystalline MoS<sub>2</sub> plate. Based on experimental conditions, we implemented two clearly distinguishable setups, regarding the water distribution: (1) large quantity of water - SiO<sub>2</sub> probe is fully immersed in water and surrounded by water molecules, and (2) ambient water - water coating is attached to the probe, which is surrounded by lateral vacuum gaps. We determined the force-distance characteristics of a fully-immersed probe at several temperatures, revealing that some water molecules get trapped in the probe-plate gap, with their number decreasing as temperature increases. We obtained well-defined stick-slip friction loops via sliding simulations. Considering the slip regime: fully-immersed probe mainly moves in single-slip regime, while ambient water distribution promotes multiple-slips. Amount of water, and especially its distribution, strongly influence the stick-slip frictional behaviour of the studied tribosystem.

CPP 21.19 Tue 18:00 Poster E

**Particles Formation in the Drying of Polymer Solution**

**Droplets** — ●MENGMEG WU, HSIAO-PING HSU, and KURT KREMER — Max-Planck-Institut für Polymerforschung, Ackermannweg 10, Mainz 55128, Germany

Due to the unique properties such as large specific surface area, high permeability and low density, porous polymer nano- or micro-spheres are promising for various applications including biomedical, pharmaceutical, tissue engineering and degradable electronic applications. We develop a coarse-grained polymer solution droplet model to study the particle structure's formation of drying polymer solution droplets. By inducing a high degree of polymer entanglement and maintaining below the glass transition temperature, highly porous particles are generated followed by a rapid evaporation of the solvent in a vacuum. For a drying droplet in a vacuum, the temperature experiences a decrease owing to solvent vaporization. Such temperature reduction results in a decrease in polymer solubility during evaporation, consequently impacting the drying dynamics of polymer droplets. Our investigation explores how the cooling of droplets during solvent evaporation influences the final morphology of polymer particles.

CPP 21.20 Tue 18:00 Poster E

**Diffusion Dynamics in Glassy Polymer Films through MD Simulations** — ●SHARON VOLPE, HSIAO-PING HSU, and KURT KREMER — Max-Planck-Institut für Polymerforschung, Ackermannweg 10, Mainz 55128, Germany

Case II diffusion presents a unique challenge in materials science and polymer engineering. The slow rearrangement of the polymer chains in the glassy state leads to an anomalous sorption behavior: a sharp front is observed as an interface that moves at a constant velocity between the swollen plasticized region and the unswollen glassy region. Unraveling the microscopic mechanisms of Case II diffusion is fundamental for tailoring materials with precise diffusion properties, with applications ranging from drug delivery to food packaging. This study employs Molecular Dynamics (MD) simulations to investigate Case II diffusion in glassy polymer films. A dedicated explicit solvent model is developed to control and vary the solvent-polymer interactions. Our focus is on exploring diffusion for different solvent qualities, their impact on diffusion profiles and the chain characteristics in the swollen region. In certain conditions, the observed diffusion patterns align with the characteristic behavior of Case II diffusion. The simulations provide insights into the interplay between solvent and glassy polymer films and contribute to the knowledge of molecular diffusion in these materials.

CPP 21.21 Tue 18:00 Poster E

**Modeling fracture formation and propagation in cured epoxy resins under mechanical stress** — ●BARISCAN ARICAN<sup>1</sup>, CHRISTIAN WICK<sup>1</sup>, and ANA-SUNČANA SMITH<sup>1,2</sup> — <sup>1</sup>PULS Group, Institute for Theoretical Physics, IZNF, FAU Erlangen-Nürnberg, 91058 Erlangen — <sup>2</sup>Group of Computational Life Sciences, Division of Physical Chemistry, Ruder Bošković Institute, 10000 Zagreb, Croatia

Epoxy resins, integral in manufacturing, play a crucial role due to their versatility. Understanding fracture mechanisms in these materials is paramount for determining mechanical properties. This study focuses on developing a multiscale simulation framework, integrating molecular dynamics (MD) with quantum mechanics/molecular mechanics (QM/MM), to consecutively assess and break bonds, simulating fracture propagation. MD simulations of straining crosslinked epoxy resin extend until the potential occurrence of fracture-inducing bond breakage, determined by bond elongation and referred to as the classical criteria. Subsequently, QM/MM calculations are performed on a small subsystem excised from the main system, precisely identifying actual fracture events through spin contamination assessment. Reaction site topology is then updated with broken bond information to create or propagate the fracture. Classical criteria triggering QM/MM calculations are optimized, ensuring computational resources focus on relevant fracture events. This work provides valuable insights into epoxy resin fracture behavior, advancing our understanding of these materials at the molecular level.

CPP 21.22 Tue 18:00 Poster E

**Effects of plasma treatments and temperature on the triboelectric charging behavior of polymers in stirring and shaking charging processes** — ●ALINA BACHMANN — Frankfurt am Main, Hessen, Germany

This study evaluates the triboelectric charging behavior of polymers. Examining the effect of different plasma pretreatments and temper-

atures, the saturation charging of various multi-component polymer blends was conducted.

Within the experimental procedure, the saturation charge through stirring and shaking charging processes was compared. The charge-to-mass ratio and surface charge density serve as crucial parameters for characterising the treated surfaces.

The results of the study find application in the electro-sorting of plastics based on triboelectricity. Since this phenomenon is not scientifically understood to a full extent, the generated data contributes to a more optimised implementation in the technical field.

CPP 21.23 Tue 18:00 Poster E

**Balancing short- and long-range interactions in Machine Learning Force Fields** — ●TOBIAS HENKES, IGOR POLTAVSKY, and ALEXANDRE TKATCHENKO — Université du Luxembourg

Nowadays, highly accurate and data-efficient Machine Learning (ML) Force Fields (FFs) are an established method in computational chemistry and physics. MLFFs can enable simulations of large, complex systems with quantum chemical accuracy by using predefined molecular descriptors or learned representations. However, even state-of-the-art ML models can struggle with handling long- and short-range interactions equally. They often employ a locality assumption, naturally emphasizing short ranges. To overcome this constraint, we embed a coarse-grained description of the global environment into an accurate local atomic representation. Effectively, the ML model now has a balanced picture of local and global features and uses this to simultaneously reproduce long- and short-range effects. We showcase the proposed methodology in the Gradient Domain Machine Learning (GDML) framework. Herein, we utilize a hierarchical descriptor that includes local and global features with adjustable attention weights. The modified GDML approach shows an improved accuracy compared to the default architecture for extended systems such as solvated molecules and liquid water. Ultimately, the developed embedding approach can aid any MLFF model in striking a balance between short- and long-range interactions.

CPP 21.24 Tue 18:00 Poster E

**Spiropyran/Merocyanine Amphiphile in Organic and Aqueous Media** — ●OLGA GUSKOVA — IPF Dresden, Dresden, Germany

This theoretical study delves into the molecular and photophysical characteristics of an amphiphilic compound containing spiropyran in both organic and aqueous environments. In organic solvents, the system exhibits positive photochromism: under UV radiation, the colorless spiropyran transitions to a vibrant merocyanine isomer. Conversely, in aqueous solutions, a negative photochromism is observed: the orange-red merocyanine form becomes more thermodynamically stable in water, and exposure to UV and visible light results in partial or complete photobleaching. The underlying rationale for this phenomenon is elucidated through density functional theory calculations and classical modeling, including thermodynamic integration. The explanation lies in the molecular properties of merocyanine. Following the ring-opening reaction, this molecule transforms into a zwitterionic form. The presence of three charged groups on the periphery of a flat conjugated backbone promotes the self-assembly of merocyanine molecules in water, leading to the formation of elongated associates with stack-like building blocks. Molecular dynamics simulations of the aqueous solution, with a concentration above the critical micelle concentration, confirm this self-assembly phenomenon. This work is supported by DFG. For more information see: V. Savchenko, N. Lomadze, S. Santer, O. Guskova, *Int. J. Mol. Sci.* 23 (2022) 11535.

CPP 21.25 Tue 18:00 Poster E

**Equilibrium self-dissociation free energy of nanoconfined water from classical simulations** — ●KIRA FISCHER, HENRIK STOOS, and ALEXANDER SCHLAICH — SC SimTech, University of Stuttgart

Understanding the electrodynamic properties of water in confinement is essential for the development of efficient, cost-effective and environmentally friendly energy storage solutions, in particular water-only batteries. Experiments have shown that the construction of such batteries is possible, but a comprehensive understanding of all the phenomena involved is still lacking. Ab-initio studies have inconclusively reported that the self-dissociation barrier of water might be affected by nano-confinement, but sampling the right ensemble poses an unsolved challenge in such simulations.

In this study, molecular dynamics simulations, including lambda dynamics, are used to investigate the equilibrium self-dissociation of confined water at the nanoscale. We focus on the ion pairs  $\text{H}_3\text{O}^+$  and

$\text{OH}^-$ , which are important contributors to the electrodynamic behavior of water, and try to understand the effects of nano-confinement and interfaces on the electrodynamic properties of water.

CPP 21.26 Tue 18:00 Poster E

**Atomistic Simulations of Conjugated Polymers - A Bottom-up approach** — ●RICHARD SCHÖMIG and ALEXANDER SCHLAICH — SC Simtech, University of Stuttgart, Germany

Conjugated polymers show remarkable properties due to their semi-conducting nature and their swelling behaviour in contact with an electrolyte, making them promising materials for next-generation sensors, artificial muscles, artificial synapses or for neuromorphic computing. Their complex band-structure combined with the fine details of doping requires a careful treatment of the electronic structure problem, making computational access to the mechanic response and the swelling dynamics infeasible. On the other hand, established coarse-graining approaches and classical polymer theory will miss important details that characterize the system's response and dynamics. Here, we develop atomistic simulation approaches for the adsorption, swelling, and transport behaviour by means of molecular dynamics simulations. We benchmark our approach against the experimental mechanic behaviour.

CPP 21.27 Tue 18:00 Poster E

**Energy conversion during microphase separation in polyoxyethylene-polyoxybutylene diblock copolymers modeled by self-consistent field theory** — ●THORE POHL, HUICHEN SHU, and MICHAEL FISCHLSCHWEIGER — Clausthal University of Technology, Clausthal-Zellerfeld, Germany

The microscale phase behavior of polyoxyethylene-polyoxybutylene diblock copolymers is particularly intriguing and has already undergone thorough experimental investigation in the literature. Specifically, in-situ small-angle X-ray scattering (SAXS) has been employed to characterize phase transition temperatures and polymorphisms. Through these experiments, four distinct microstructures have been identified: cubic, hexagonal, lamellar, and bicontinuous-cubic. Modeling phase transitions, especially the spatial evolution of phases at a microscopic level, remains incomplete for this particular material system. One approach to modeling the polymorphic phase behavior of block copolymers involves utilizing self-consistent field theory (SCFT). Chemical information of the monads is encoded into a set of continuous sequence descriptor functions defined in the contour space domain. In this study, the three-dimensional microstructure and phase behavior of polyoxyethylene-polyoxybutylene diblock copolymers are computed. The interaction functional to be integrated incorporates one interaction energy parameter that is, herein determined inversely through experimental SAXS measurements. Phase change enthalpies for specific compositions and corresponding microstructures could be modeled using SCFT.

CPP 21.28 Tue 18:00 Poster E

**Understanding Cellulose-Hemicellulose interactions by molecular dynamics simulation** — ●HANIEH MIANEHROW<sup>1</sup>, YU OGAWA<sup>2</sup>, JAKOB WOHLERT<sup>3</sup>, and SILVIA VIGNOLINI<sup>1</sup> — <sup>1</sup>Max Planck Institute of Colloids and Interfaces, Potsdam Science Park, Am Mühlberg 1, 14476 Potsdam — <sup>2</sup>University Grenoble Alpes, CNRS, CERMAV, 38000 Grenoble, France — <sup>3</sup>Department of Fibre and Polymer Technology, Wallenberg Wood Science Center, KTH Royal Institute of Technology, Teknikringen 56, 100 44 Stockholm, Sweden

Structural coloration in plants, achieved through the arrangement of cellulose microfibrils into helicoidal architectures within the cell wall, is a widespread strategy observed in various plant species. However, the mechanism of such organization is not well-understood. This work focuses on studying interactions between cellulose and hemicelluloses, specifically xylan, using molecular dynamics (MD) simulations. Three model xylan chains with different substitution patterns are created, and the extent of their interactions with the cellulose surface is studied by MD simulation. In addition, the conformation of each xylan chain in the presence of cellulose is also investigated. This helps to understand the effect of the substitution pattern on xylan-cellulose interaction. Results show that the substitution pattern of xylan affects the extent of adhesion between xylan and cellulose and the conformation of xylan on cellulose. This could help explain the origin of structural coloration in some plants.

CPP 21.29 Tue 18:00 Poster E

**Many-body potentials and optimized mapping schemes**

**for systematic coarse-graining** — ●SAYAN DUTTA<sup>1,2,3</sup>, DENIS ANDRIENKO<sup>4</sup>, and ARASH NIKOUBASHMAN<sup>1,2,3</sup> — <sup>1</sup>Johannes Gutenberg-Universität Mainz — <sup>2</sup>Leibniz-Institut für Polymerforschung — <sup>3</sup>Technische Universität Dresden — <sup>4</sup>Max-Planck Institut für Polymerforschung Mainz

The field of organic semiconductors is largely influenced by diverse molecular compounds which need efficient computational protocols for pre-screening. To reveal the structure-property relationship between the small molecule chemistry and the materials properties that the condensed systems exhibit (like the glass transition temperature), brute-force atomistic molecular simulations are often intractable due to the large gap in relevant length- and time-scales. To tackle these challenges, multi-scale coarse-grained models are promising approaches, which systematically reduce the number of degrees of freedom and smooth the rugged energetic landscapes. Often, the effective coarse-grained potential is approximated by a pairwise interaction which neglects explicit many-body correlations. However, such many-body contributions can play an important role in inhomogeneous systems, such as thin films or droplets, where the local particle density fluctuates strongly. To address this short-coming, we introduce local density dependent potentials (LDP), which include many body interactions in a mean field way. Our computational framework consists of an accurate coarse-grained model, endowed with LDPs, which is expected to improve the coarse-grained model for inhomogeneous systems.

CPP 21.30 Tue 18:00 Poster E

**Cononsolvency consequences at finite polymer concentration** — ●MARTIN MELČÁK and JAN HEYDA — University of Chemistry and Technology, Prague Technicka 5, 16628, Prague 6 - Dejvice, Czech Republic

Cononsolvency, a rare situation in polymer physics, when a mixture of two good solvents creates a poor solvent, is experimentally known and at the macroscopic level is well-described process. However, despite intensive theoretical and simulation research, the microscopic origin and driving forces behind this phenomenon remain unclear. In this contribution, we employ coarse-grained molecular dynamics simulations to model the chain-chain interaction and aggregation of many polymer chains in explicit solvent-cosolvent mixtures. We have systematically varied the strength of monomer-cosolvent interactions, which resulted in cosolvent exclusion, enrichment, or even bridging. We have calculated effective interactions between two polymer chains, providing a link from the cosolvent effect on a single polymer chain to finite polymer concentrations, utilizing the statistical-thermodynamic framework of Kirkwood-Buff theory. Finally, the cosolvent effect on the polymer state is summarized in the form of a phase diagram.

CPP 21.31 Tue 18:00 Poster E

**oxDNA Molecular Dynamics ecosystem applied to the analysis of "Hairygami"**. — ●MICHAEL MATTHIES<sup>1</sup>, MATTHEW SAMPLE<sup>2</sup>, HAO LIU<sup>2</sup>, and PETR ŠULC<sup>1,2</sup> — <sup>1</sup>Technische Universität München, Garching bei München, Germany — <sup>2</sup>Arizona State University, Tempe, USA

In the rapidly evolving field of nucleic acid and nucleic acid-protein hybrid nanostructure design, computational methods play a crucial role. oxDNA is a popular coarse-grained Molecular dynamics model which recently got extended by an extensive ecosystem. We showcase these improvements on the practical case of analyzing the conformational space of several archetypical rectangular DNA origami structures influenced by oligonucleotide extensions (nicknamed "Hairygami")<sup>[1]</sup>. These extensions, usually used to attach functional elements to the origami structures induce a curvature of the structures in the bulk. We characterize the phenomenon using the oxDNA ecosystem and provide experimental verification.

[1] M. Sample, H. Liu, M. Matthies, P. Šulc, arXiv:2302.09109, (2023)

CPP 21.32 Tue 18:00 Poster E

**Understanding electrolyte transport properties with interfaces under applied forces: Insight from MD-simulations** — ●KATHARINA KINTRUP<sup>1</sup>, YOUSSEF MABROUK<sup>1,2</sup>, DIDDO DIDDENS<sup>1,2</sup>, and ANDREAS HEUER<sup>1</sup> — <sup>1</sup>Institut für Physikalische Chemie, Corrensstraße 28/30, 48149 Münster, Deutschland — <sup>2</sup>Helmholtz-Institut Münster, Corrensstraße 48, 48149 Münster, Deutschland

Transport properties of electrolytes can be conveniently studied via Molecular dynamics (MD) simulations. However, whereas typically MD simulations are performed with periodic boundary conditions

(pbc), experimental systems involve fixed electrodes. As a consequence, the conservation of momentum, observed in MD simulations, is violated. Indeed, previous electrophoretic NMR (eNMR) experiments suggest that the conservation of local volume [1] rather than momentum conservation is the mobility determining constraint.

We performed molecular dynamics (MD) simulations for a simplified binary model, imitating ionic liquids. Starting with an equilibrium configuration, we record the respective center-of-mass velocities after application of an electric field for both boundary conditions and for various box sizes. Whereas in the presence of pbc momentum is naturally conserved, we observe a complex oscillatory time dependence of the two velocities with fixed walls. Their ratio approaches a value nearly compatible with local volume conservation, in qualitative agreement with experiment. A physical picture is formulated, based on the emergence of the generation of standing sound waves. [1] *J. Phys. Chem. Lett.* 2022, 13, 37, 8761-8767

CPP 21.33 Tue 18:00 Poster E

**Orientation of dynamically asymmetric diblock copolymers in shear flow** — ●NIKLAS BLAGOJEVIC and MARCUS MÜLLER — Institut für Theoretische Physik, Universität Göttingen

The ability of diblock copolymers to assemble into periodic structures with length scales in the nanometer range offers many applications. For practical applications, it is often desirable that the microstructures have a high degree of order even on large length scales and are oriented in a desired direction. It is possible to order and orient the microstructures by shearing the copolymer melt. However, the details of the orientation mechanism under shear are not fully understood. In experiments, different orientations are found depending on copolymer type and shear amplitude. Lamellae-forming copolymers were in some cases oriented parallel to the shear gradient and in other cases perpendicular. In our simulations, we analyse the effect of a dynamical asymmetry, where one block has slower time scales than the other. We can show that the parallel orientation is preferred for high dynamic asymmetries while the perpendicular is preferred for small asymmetries. To investigate this, we conducted molecular dynamics simulations of a highly coarse-grained polymer melt using dissipative-particle dynamics under shear flow. We controlled the dynamic asymmetry via a friction parameter as well as via so-called slip-springs, which represent entanglements of the polymers. Different settings were used to determine the stable orientation, for example the simulation of a system with differently oriented lamellae under shear or the simulation of a quench from a disordered state under shear.

CPP 21.34 Tue 18:00 Poster E

**Modeling Electronic Coupling in Polymeric Radical Batteries** — ●SOUVIK MITRA, DIDDO DIDDENS, and ANDREAS HEUER — Institut für physikalische Chemie, Universität Münster, Corrensstraße 28/30, 48149 Münster

We examine the electronic coupling in PTMA, a redox-active polymer often used in organic radical batteries (ORBs). Our study reveals the significant influence of both distance and relative orientation of the redox pairs on the electronic coupling, which suggests that the electronic communication between the redox centres heavily depends on both intramolecular properties as well as the complex intermolecular environment in the electrode material. Additionally, our study highlights the limitations of the frontier molecular orbital (FMO) method in this context. Our findings underline the significance of integrating molecular dynamics and advanced electronic structure methods, like complete active space self-consistent field (CASSCF), to provide a holistic understanding of electronic coupling for charge transfer reactions in organic electrodes. In this framework, we will also introduce a regression analysis designed to predict electronic coupling across various conformations of the redox pairs.

[1] 10.26434/chemrxiv-2023-rn9bj

CPP 21.35 Tue 18:00 Poster E

**Aggregation of copolymer chains consisting of flexible and semi-flexible segments: A stochastic approximation Monte Carlo simulation** — ●JULIA MARTEMYANOVA, TIMUR SHAKIROV, VIKTOR IVANOV, and WOLFGANG PAUL — Martin-Luther-University Halle-Wittenberg, Halle (Saale), Germany

We use flat histogram Monte Carlo simulations based on the stochastic approximation Monte Carlo (SAMC) algorithm to study aggregation behavior of several multi-block copolymer chains consisting of flexible and semi-flexible segments with equal composition. We compare algorithms with the one-dimensional density of states, which depends on

the total energy, and with the two-dimensional density of states, which depends on the energy of intramolecular stiffness and on the energy of non-valence interactions. We present data on different non-trivial morphologies of aggregates, including several structures with high orientational ordering of bonds and with microseparation of segments of different types. Our aim is to identify single chain morphologies which are able to aggregate in a shape-persistent fashion. We also want to learn to which degree such aggregation is stable without the presence of specific interactions like, e.g., hydrogen bonding. We acknowledge the financial support from DFG (project PA 473/18-1).

CPP 21.36 Tue 18:00 Poster E

**Stabilizing alpha-Helicity of a Polypeptide in Aqueous Urea** — ●LUIS ANDRE BAPTISTA DOS SANTOS<sup>1</sup>, YANI ZHAO<sup>1</sup>, KURT KREMER<sup>1</sup>, DEBASHISH MUKHERJI<sup>2</sup>, and ROBINSON CORTES-HUERTO<sup>1</sup> — <sup>1</sup>Max Planck Institute for Polymer Research, Mainz, Germany — <sup>2</sup>Quantum Matter Institute, University of British Columbia, Canada

We propose a mechanism for alpha-helix folding of polyaniline in aqueous urea that reconciles experimental and simulation studies. Over 15 $\mu$ s long, all-atom simulations reveal that, upon dehydrating the protein's first solvation shell, a delicate balance between localized urea residue dipole interactions and hydrogen bonds dictates polypeptide solvation properties and structure. Our work clarifies the experimentally observed tendency of these alanine-rich systems to form secondary structures at low and intermediate urea concentrations. Moreover, it is consistent with the commonly accepted hydrogen-bond-induced helix unfolding, dominant at high urea concentrations. These results establish a structure-property relationship highlighting the importance of microscopic dipole-dipole orientations/interactions for the operational understanding of macroscopic protein solvation.

CPP 21.37 Tue 18:00 Poster E

**Heat transport across nanometre-sized gaps** — ●OSCAR MATEOS, PABLO M. MARTINEZ, OSCAR GUTIERREZ, GUILHERME VILHENA, and JUAN CARLOS CUEVAS — Universidad Autonoma de Madrid, Spain

Calorimetry has recently achieved a significant milestone by measuring heat transport through a single-atom junction, positioning us to investigate heat transfer across various distances, from atom-sized contacts to more extensive separations. When metals come into contact, heat is primarily carried by electrons at close proximity, while at greater distances, it is transported by photons in a Planckian or super-Planckian manner. However, when the separation reaches the nanometer scale, a transition from thermal radiation to conduction is expected. Recent experiments have shown that heat flux between gold contacts at sub-10nm distances exceeded conventional theories by several orders of magnitude, challenging our understanding of heat transfer across vacuum gaps.

In this presentation, we propose to provide an atomic-level description of heat transport across sub-10nm gap between two metallic surfaces with conductivity values ranging nW/K on gaps as large as 5nm. The all-atom molecular dynamics simulations not only provide results in quantitative agreement with the aforementioned experiments but also settle a nearly decade long paradox.

CPP 21.38 Tue 18:00 Poster E

**Structure Formation of Nanoparticles on a Polymer Brush: Effect of Polymer-Nanoparticle Interaction** — ●BHUVAN POUDEL, HSIAO-PING HSU, and KURT KREMER — Max Planck Institute for Polymer Research, Mainz, Germany

The prospect of composite materials based on a polymer brush and nanoparticles (NPs) depends on the precise spatial arrangement of NPs within the brush. Therefore, understanding the insertion mechanism and controlling the distribution of NPs in the brush is crucial for optimal applications of nanocomposite materials. We here approach this problem by performing extensive molecular dynamics simulations of the brush-NP system. The brush is described by a weakly semiflexible bead-spring model and NPs are considered as hard spheres of diameter seven times larger than a bead size. As the attraction between polymers and NPs is weak, NPs tend to spread and form a monolayer on the brush surface. The thickness of such a layer is about the size of an NP. As the interaction strength is increased beyond a threshold value, NPs start to penetrate into the brush. Our findings indicate that the assembly of NPs in/on a brush can be precisely controlled by tuning the strength of attraction between polymers and NPs.

CPP 21.39 Tue 18:00 Poster E

**Microrheology under pressure using XPCS** — ●FIONA BERNER<sup>1,2</sup>, TOBIAS ECKLUND<sup>1,2</sup>, LOUISA KRAFT<sup>1,2</sup>, NELE STRIKER<sup>3</sup>, FABIAN WESTERMEIER<sup>3</sup>, FLORIAN SCHULZ<sup>4</sup>, FELIX LEHMKUELER<sup>3</sup>, WERNER STEFFEN<sup>1</sup>, and KATRIN AMANN-WINKEL<sup>1,2</sup> — <sup>1</sup>Max Planck Institute for Polymer Research, Germany — <sup>2</sup>Johannes Gutenberg University, Department of Physics, Germany — <sup>3</sup>Deutsches Elektronen-Synchrotron (DESY), Germany — <sup>4</sup>University Hamburg, Germany

Glycerol is a glass-forming liquid with a glass transition temperature around  $T_g \approx 180$  K at ambient pressure. The transition strongly depends on parameters such as the heating and cooling rate. We aimed to investigate the pressure dependence of glycerol's glass transition and viscosity via a microrheological approach, a mixture of 80 % glycerol in water. Our group implemented a diamond anvil cell and a cryostat to the P10 Coherence Applications Beamline of Petra III at DESY.

Coherent X-rays from modern storage-ring-based radiation facilities provide unique capabilities to investigate both the structure and molecular-level dynamics of disordered soft matter systems. X-ray photon correlation spectroscopy (XPCS) can determine the dynamics on the timescale of  $\mu$ s to hundreds of s.

We calculated the intensity auto-correlation function  $g_2$  for small scattering vectors  $|\vec{q}|$  and determined the relaxation rate for different pressures and temperatures. We observe that the applied pressure slows down the system, leading to a shift toward a higher glass transition temperature.

CPP 21.40 Tue 18:00 Poster E

**Microrheology under pressure using XPCS** — ●FIONA BERNER<sup>1,2</sup>, LOUISA KRAFT<sup>1,2</sup>, TOBIAS ECKLUND<sup>1,2</sup>, KLARA HOLL<sup>1,2</sup>, NELE STRIKER<sup>3</sup>, FABIAN WESTERMEIER<sup>3</sup>, FLORIAN SCHULZ<sup>4</sup>, FELIX LEHMKUELER<sup>3</sup>, WERNER STEFFEN<sup>1</sup>, and KATRIN AMANN-WINKEL<sup>1,2</sup> — <sup>1</sup>Max Planck Institute for Polymer Research, Germany — <sup>2</sup>Johannes Gutenberg University, Department of Physics, Germany — <sup>3</sup>Deutsches Elektronen-Synchrotron (DESY), Germany — <sup>4</sup>University Hamburg, Germany

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sition temperature.

CPP 21.41 Tue 18:00 Poster E

**Temperature-dependent Raman spectroscopic characterization of poly(furfuryl alcohol)** — DURVAL BERTOLDO MENEZES<sup>1</sup>, FRANCESCO D'AMICO<sup>2</sup>, THOMAS SEPPERER<sup>3</sup>, ARTUR BENISEK<sup>4</sup>, and ●MAURIZIO MUSSO<sup>4</sup> — <sup>1</sup>Instituto Federal do Triângulo Mineiro, Campus Uberlândia, 38.400-970 Uberlandia, Minas Gerais, Brazil — <sup>2</sup>Universität Salzburg / Fachbereich Chemie und Physik der Materialien — <sup>3</sup>Jakob-Haringer-Strasse 2a — <sup>4</sup>University of Salzburg, Department of Chemistry and Physics of Materials, Jakob-Haringer-Strasse 2a, 5020 Salzburg, Austria

Recently we employed FTIR and Resonant Raman spectroscopy to investigate the chemical constitution of the polymer polyfurfuryl alcohol (PFA) synthesized in different ways, and appearing macroscopically different: the first one being a liquid and viscous commercial sample, the second one, produced following a thermosetting procedure, being a self-prepared solid and rigid sample.

As a continuation, we have performed a set of temperature dependent Raman spectroscopic measurements in order to study the evolution of these Raman spectra during the glass transition in thermosetted PFA, adopting the same spectral analysis previously performed by us to infer about the glass transition of the polymer poly(methyl methacrylate).

Compatible with Differential Scanning Calorimetry (DSC) data, the Raman spectral features of the thermosetted PFA changed with temperature, this spectral evolution being a clear indication of the PFA glass transition.

CPP 21.42 Tue 18:00 Poster E

**Properties of stable ensembles of Euclidean random matrices modeling the vibrations in low-temperature glass** — ●PHILIPP BAUMGÄRTEL, FLORIAN VOGEL, and MATTHIAS FUCHS — Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany

Using coupled disordered harmonic oscillators we investigate the vibrational properties of amorphous solids. Earlier findings suggest that this Euclidean random matrix ensemble features low temperature vibrational anomalies of glasses. By exact numerical diagonalization and a finite size study we analyze the spectra of the harmonic oscillators [1]. We observe a low-frequency regime of extended modes leading to a Debye like vibrational density of states. At larger frequencies the density of states shows an excess over the Debye behavior resembling Wigner's semicircle law. We discuss that the corresponding modes follow the statistics known from the Gaussian orthogonal ensemble. We reveal that the sound waves are damped by Rayleigh scattering even though the ERM system is purely harmonic. Additional calculations performed in two spatial dimension suggest that the two dimensional systems behave very similar to the three dimensional ones.

In conclusion, the Euclidean random matrix model captures salient features of the vibrational phenomena in glass at low temperatures.

[1] P. Baumgärtel, F. Vogel and M. Fuchs. arXiv:2309.08028, 2023