CPP 46: Poster II

Focus Session: Water - from Atmosphere to Space (with DY); French-German Session: Membranes and Porous Materials; Gels, Polymer Networks and Elastomers; Biopolymers, Biomaterials and Bioinspired Functional Materials (with BP); Complex Fluids and Colloids, Micelles and Vesicles (with DY); Charged Soft Matter, Polyelectrolytes and Ionic Liquids; Responsive and Adaptive Systems; Nanomaterials, Composites and Hybrids; Crystallization; Molecular and Polymer Dynamics, Friction and Rheology; Simulation Methods and Modeling of Soft Matter; Emerging Topics in Chemical and Polymer Physics, New Instruments and Methods

Time: Thursday 9:30–11:30 Location: P5

CPP 46.1 Thu 9:30 P5

Pressure-induced amorphization of aqueous PEG solutions — •Leah Dorothea Schwerdtfeger[1,2], Isabell Zick[1,2], and Katrin Amann-Winkel[1,2] — [1]Institut für Physik, Johannes Gutenberg Universität, Mainz — [2]Max-Planck-Institut für Polymerforschung, Mainz

Water is a fundamental substance whose behavior under supercooled temperatures shows many anomalous properties. Among the many curiosities, water can even form different amorphous states. These amorphous states are hypothesized to be directly related to two different liquid states of water, namely high- and low-density liquid. Understanding the pressure-induced amorphization of aqueous solutions can reveal how solutes alter water's phase diagram and give further insight to the predicted liquid-liquid transition.

While the impact of small molecules is known from previous studies, the role of larger polymers remains unexplored. Here, we discuss experiments on aqueous polyethylene glycol (PEG) solutions with different molar weights, studying their effect on the pressure-induced phase transitions. Our dilatometric measurements show how solutes broaden the transition from hexagonal ice to high-density amorphous ice (HDA), depending on the molar fraction. We also investigate the polyamorphic transition between low- and high-density amorphous ice (LDA-HDA), which for pure water is known to exhibit a strong temperature-dependence. The samples are further characterized by X-Ray diffraction (XRD).

CPP 46.2 Thu 9:30 P5

Phase transition in water-glycerol solutions — •Klara Holl[1,2], Louisa Kraft[1,2], and Katrin Amann-Winkel[1,2] — [1]Institut für Physik, Johannes Gutenberg-Universität, Mainz — [2]Max-Planck-Institut für Polymerforschung, Mainz

Water is omnipresent in our daily lives with many anomalous properties and a unique phase diagram. Studies of supercooled water provides insight into the hypothesis of the coexistence of two liquid states of water and a liquid-liquid transition. This proposes two different types of supercooled liquid water in a high-density and low-density liquid state, that are separated by a first order phase transition at low temperatures and elevated pressure. But how does this hypothesis impact on aqueous solutions?

Water-glycerol mixtures are often used in pharmaceuticals and act as cryoprotectants, common in biomedicine as well as automotive antifreeze. While pure water crystallizes easily, the glass-forming agent glycerol can serve as soft confinement for water. Changing the concentration of the two components alters the liquid's physical and thermodynamic properties, including depression of the crystallisation temperature.

We investigate different water-glycerol solutions at low-temperatures and high-pressure conditions using a diamond anvil cell. This allows in situ optical observation of crystallisation and glass transition. Structural changes are studied by X-ray diffraction and differential scanning calorimetry.

CPP 46.3 Thu 9:30 P5

Photooxidation of vanillic acid at the air-water interface — •Manuel Hofmann[1,2] and Ellen H.G. Backus[1,2] — [1]Institute of Physical Chemistry, Faculty of Chemistry, University of Vienna, Währinger Str. 42, 1090 Vienna, Austria — [2]University of Vienna, Vienna Doctoral School in Chemistry (DoSChem), Währinger Str. 42, 1090 Vienna, Austria

Phenolic compounds like vanillic acid, emitted from biomass burning, can form secondary organic aerosols (SOA) through aqueous phase reactions. Photooxidation of vanillic acid is a potential source of Humic-Like Substances (HULIS), that influence atmospheric chemistry through light absorption.[1]

The air-water interface provides a distinct chemical environment where structural behavior and reactions may differ from those in bulk. To specifically probe this interface, sum-frequency generation (SFG) spectroscopy and surface tension measurements are employed, offering complementary insights into molecular behavior.[2]

This study examines vanillic acid at the air-water interface across different pH values, before and after UV/H2O2-induced photooxidation. Control experiments with vanillic acid alone separate direct photolysis from radical mediated processes. Preliminary SFG spectra reveal pH-dependent vibrational signatures of adsorbed species and significant changes upon photoreaction. The goal is to identify reaction products, structural changes, and how pH affects vanillic acid photoreactivity.

[1]S. Tang et al., ACS Earth Space Chem., 4 (2020) 862-872.[2]C.-M. Saak et al., J. Phys. Chem. Lett., 15 (2024) 4546-4559.

CPP 46.4 Thu 9:30 P5

Biophysical Interaction of Steroid Hormones with Model Lipid Membranes — •Rabia Rabia[1,2,3], Prashant Hitaishi[1,2], Bridget Murphy[1,2], and Julia Herzen[3] — [1]Institute of Experimental and Applied Physics, Kiel University, Leibnizstraße 19, Kiel, 24118, Germany — [2]Ruprecht Haensel Laboratory, Deutsches Elektronen-Synchrotron DESY, Notkestraße 85, Hamburg, 22607, Germany — [3]Technische Universität München

Menopause is characterized by declining 17βestradiol (E2), increased adiposity, reduced insulin sensitivity, and higher type 2 diabetes risk. Vasomotor symptoms, such as hot flushes and night sweats, significantly impair quality of life, and transdermal E2 provides effective relief at lower doses than oral therapy, with potentially fewer systemic risks. Despite its clinical benefits, the molecular mechanisms of E2 remain incompletely understood. While steroid hormones classically act via intracellular receptors to regulate gene transcription, they also interact directly with lipid membranes, influencing packing and elasticity. We studied βestradiol, progesterone, 17αethynylestradiol, and cholesterol in DPPC and POPC monolayers at the air water interface using Langmuir isotherms and surface elasticity measurements. E2 was found to expand molecular area and reduce packing density, increasing membrane elasticity. Planned X-ray measurements will further clarify how steroid-induced reorganization of lipid interfaces modulates downstream cellular signaling.

CPP 46.5 Thu 9:30 P5

The structure and orientation of ice under confinement in Periodic Mesoporous Organosilicas (PMOs) — Niels C. Giesselmann[1], Philip Lenz[2,3], Sophia-Marie Meinert[2], Robert P.C. Bauer[1,4], Nele N. Striker[1], Michael Fröba[2,3], and •Felix Lehmkühler[1,3] — [1]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — [2]Institute for Inorganic Chemistry, University of Hamburg,Germany — [3]The Hamburg Center for Ultrafast Imaging, Hamburg, Germany — [4]Freiberg Center for Water Research, TU Bergakademie Freiberg, Germany

We studied water in periodic mesoporous organosilicas (PMOs) with pore diameters in the range of 2-5 nm. In these materials, the molecular mobility of water is influenced by the polarity of the organic moiety. We collected and analyzed X-ray scattering data of water and ice under confinement in PMOs with varying degrees of hydrophobicity and pore diameters and at varying temperature. A decrease in the density of the confined water was observed during cooling, which was strongly dependent on the organic moiety, as well as the pore diameter. We furthermore found deviations in the lattice constants of hexagonal ice in these materials compared to bulk water. In most cases, one lattice parameter was more strongly affected. This could be caused by orientational dependencies between the ice crystal and the pore. The orientation between the hexagonal crystallites in relation to the pore axis was therefore investigated using X-ray Cross Correlation Analysis (XCCA), indicating more uniformly oriented crystallites in more hydrophilic pores.

CPP 46.6 Thu 9:30 P5

Impact on snow albedo of soot aggregates inferred from their radiative properties — •Llorenc Cremonesi[1], Luca Teruzzi[1], Valentina Raspagni[2], and Marco Potenza[1] — [1]University of Milan, Milan, Italy — [2]Ca' Foscari University of Venice, Venice, Italy

Despite having a short lifespan in the atmosphere, soot aggregates are abundant and volatile enough to be found in various environments far from their sources. While suspended in the atmosphere, they influence local thermodynamic conditions and interact with water triggering cloud nucleation. These particles are also among the drivers of cryospheric degradation in climate-sensitive areas such as the Arctic and the European Alps.

The effectiveness with which soot aggregates interact with solar radiation is known to be related to their morphology as well as their composition. However, studies of their radiative properties rely on indirect or model-dependent measurements. We use a non-destructive optical technique that enables us to simultaneously measure several optical parameters on a particle-by-particle basis in situ.

Field measurements and laboratory tests show that aggregate particles exhibit exceptional scattering and absorption efficiencies relative to their mass. Directly assessing these properties obviates the need to characterise their exceptional morphological variability. By quantifying these properties, we evaluate the impact of carbon aggregates on snow, particularly in the uppermost layers.

CPP 46.7 Thu 9:30 P5

Study of nuclear magnetization transfer between water and ice phases in nanoporous solids — •Cristina Abril Gutierrez Ortigoza and Rustem Valiullin — Felix Bloch Institute for Solid State Physics, University of Leipzig, Leipzig, Germany

NMR Cryoporometry is a promising tool for the characterization of nanoporous solids. The technique relies on introducing a probe liquid into the nanopores, where a liquid and frozen phase can coexist at low temperatures. Both phases can be easily identified using NMR due to their vastly different transverse relaxation rates. The magnetization transfer mechanism between these is not well understood, especially its dependence on various parameters such as temperature and pore size. In this contribution, the magnetization transfer between water and ice in porous silica is explored, the pore structure of which is composed of well-ordered spherical nanopores connected by micropores. The measurements are performed by using the Goldman-Shen pulse sequence, which initializes the experiments in a state where all the magnetization is contained in the liquid phase. By studying how the system re-equilibrates, parameters such as the diffusion coefficient in the ice phase and the proton volume fraction in each phase are obtained. Furthermore, the non-frozen layer thickness, which refers to the liquid-like layer that forms between the ice core and the pore wall, can be obtained by exploiting the well-defined geometries of the ice and water phases. The studies were performed at different temperatures to assess the dependence of the results on this parameter. The experimental data are also compared to theoretical models.

CPP 46.8 Thu 9:30 P5

Advanced analysis of NMR cryoporometry data — •Crina Rahause, Georgiy Baroncha, and Rustem Valiullin — Felix Bloch Institute for Solid State Physics, Leipzig University, Leipzig, Germany

NMR cryoporometry is a powerful tool for structural characterisation of multi-scale nanoporous materials. It relies on probing the pore size dependent ice-liquid phase transitions of nanoconfined liquid. However, accurate interpretation of the experimental data requires a better description of phase equilibria, as well as a framework that takes into account the network topology and relaxation effects. In this contribution, we perform NMR measurement using water and octamethylcyclotetrasiloxane (OMCTS) as probe liquids inside highly ordered nanoporous alumina membranes with well-defined pore sizes ranging from 25 to 180 nanometres. OMCTS differs from water in terms of relaxation times and the thermodynamic parameters controlling phase transition suppressions; therefore, by comparing the responses of the two liquids in different porous media, we can identify key parameters which are necessary for accurately establishing an advanced cryoporometry methodology, and demonstrating the applicability of this technique to a wide range of materials.

CPP 46.9 Thu 9:30 P5

Comparison of mechanical properties and pore collapse characteristics of hyperuniform disordered anodic aluminium oxide membranes — •Rang Noh[1], Clara Twiehaus[2], Marc Thelen[1], Alexander Sprafke[3], Prerak Dhawan[3], Ralf Wehrspohn[3], Martin Steinhart[2], and Patrick Huber[1,4] — [1]Institute for Materials and X-ray Physics, Hamburg University of Technology, Hamburg, Germany — [2]Institute of Chemistry of New Materials, Osnabrück University, Osnabrück, Germany — [3]Institute of Physics, Martin Luther University of Halle-Wittenberg, Halle (Saale), Germany — [4]Center for X-ray and Nano Science CXNS, Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany

We investigate how the degree of disorder in hyperuniform Porous Anodic Aluminum Oxide (AAO) membranes influences their mechanical properties and pore-collapse behavior. Elastic moduli of AAO were measured using two different methods; Laser Ultrasonics (LUS) and nanoindentation. The indented points were captured by scanning electron microscopy to observe pore collapse characteristics. The elastic moduli from LUS and nanoindentation agree well; in general, the elastic modulus increases as both porosity and the hyperuniformity index decrease. Even at similar porosity levels, enhanced hyperuniformity results a higher elastic modulus. When the pores are ordered, the pore collapse follows directional grain paths around the indented edge and propagate further in a connected herringbone like pattern. But, in the disordered state, the irregular collapse happens, producing direction-independent crack propagation within the restricted region.

CPP 46.10 Thu 9:30 P5

Microscopic mechanisms of polymer network breakage under mechanical deformation — •Fernando Martín Salamanca[1,2] and Michael Lang[1] — [1]Institute Theory of Polymers, Leibniz-Institut für Polymerforschung Dresden e.V. Kaitzer Strasse, 4 - 01069 (Dresden) — [2]Institute of Polymer Science and Technology, Spanish National Research Council. Juan de la Cierva, 3 - 28006 (Madrid)

The failure of polymer networks arises from a subtle interplay between bond rupture, chain interactions and the underlying topology of the network. In this work, Monte Carlo simulations are used to explore how these factors shape the mechanical response of crosslinked polymers subjected to mechanical stress. The main goal is to evaluate, in a controlled manner, the key elements that modify the mechanical response by computer simulations: the criteria for bond rupture, the mathematical modelling of interactions potentials and force fields, the effect of entanglements and excluded volume. Model networks are evaluated with diverse approaches to quantify the effect of each contribution to elastic modulus. The simulations yield detailed rupture statistics and stress-strain behavior across a broad parameter space, which are compared with predictions from established theoretical descriptions of network elasticity and fracture. Overall, this work provides basic information for understanding network failure and for establishing a first-principles based model for real polymer networks.

CPP 46.11 Thu 9:30 P5

Tuning Foam Kinetics and Structure: The Role of Gas Flowrate in Microgel-Stabilized Foams — •Vera Anna Nina Alina Hesse, Joanne Zimmer, and Regine von Klitzing — Soft Matter at Interfaces, Institute for Condensed Matter Physics, TU Darmstadt, Hochschulstraße 8, D-64289 Darmstadt

The stability and microstructure of foams are critical for their performance in various applications. In this work, aqueous foams are generated by sparging gas (nitrogen) through an aqueous dispersion of PNIPAM microgels, which are used as foam-stabilizers. In specific the effect of the gas flowrate during foam production on the foam structure and kinetics is investigated. In this regard, key parameters such as the foam half lifetime, drainage (liquid content), and bubble size evolution are examined. Our findings reveal a clear dependence: In general, lower flowrates produce smaller initial bubbles, which in turn significantly improve the overall foam stability, as their structural skeleton remains intact for longer periods. On the other hand, a stability optimum is detected, with peak stability occurring at a low flowrate; further reduction however ultimately compromising stability. These findings contribute to a deeper understanding of microgel-stabilized aqueous foams and render the potential for optimizing foam generation processes.

CPP 46.12 Thu 9:30 P5

Shape and inner structure of micelles from tetrablock terpolymers in aqueous solution — •Katarina Döbler[1], Feifei

Zheng[1], Pablo A. Alvarez Herrera[1], Joachim Kohlbrecher[3], Anna P. Constantinou[2], Theoni K. Georgiou[2], and Christine M. Papadakis[1] — [1]Technical University of Munich, TUM School of Natural Sciences, Soft Matter Physics Group, Garching, Germany — [2]Imperial College London, U.K — [3]PSI, Villigen, Switzerland

Injectable hydrogels formed by LCST thermoresponsive block terpolymers consisting of thermoresponsive, hydrophilic and hydrophobic blocks are promising materials for tissue engineering by 3D bioprinting. The gel point temperature, gelation mechanism, and physical properties can be tuned by the number, sequence and length of the individual polymer blocks [1,2]. Utilizing small-angle X-ray and neutron scattering in a wide temperature range, we investigate aqueous solutions of thermoresponsive tetrablock terpolymers having different sequences of hydrophilic, hydrophobic and thermoresponsive blocks. By fitting structural models, we gain insight into the shape and size of the micelles as well as their inner structure. Moreover, the gelation mechanism is deduced from the changes of the micellar structure and correlation at the gel point.

[1] A.P. Constantinou et al., Macromolecules 2018, 51, 7019

[2] A.P. Constantinou et al., Macromolecules 2025, 58, 9122

CPP 46.13 Thu 9:30 P5

Interfacial Dilational Rheology of Microgel Layer at the air-water interface — •Jana Sänger, Atieh Razavi, Regine von Klitzing, and Amin Rahimzadeh — Soft Matter at Interfaces, Institute for condensed Matter Physics, Technical University of Darmstadt, Hochschulstraße 8, 64289 Darmstadt, Germany

Interfacial tension and dilational interfacial rheology of Poly (N-Isoprpylacrylamide) (PNIPAM) microgel layer at air-water interfaces are characterized using pendant-drop techniques. Static interfacial tension was first measured with a drop shape analyser by fitting the droplet profile to the Young-Laplace equation. To probe the interfacial elasticity of microgel dispersions, a Profile Analysis Tensiometer (PAT-1) is employed to impose controlled harmonic oscillations on pendant drops with volumes of 10 μL and microgel concentrations between 0.1 wt% and 0.015 wt%. By using a Fourier transformation, the surface dilational modulus is determined, and the elasticity modulus is then identified as the real part of the surface dilational modulus. In order to remain within the linear range of the interfacial dilational elasticity, various amplitude ratios were systematically tested, and a maximum amplitude ratio of 6% was found. Our study shows that the elastic modulus is frequency-dependent. By increasing the frequency, an increasing elastic modulus is determined. Furthermore, we observe a shift of the maximum elasticity modulus towards the lower surface pressure values by increasing the frequency.

CPP 46.14 Thu 9:30 P5

Combined TGA-MS Analysis of Actively Aged Polymers for Assessing Recycling Potential — •Judith Bünte, Inga Ennen, Karsten Rott, and Andreas Hütten — Universität Bielefeld, Universitätsstraße 25, 33615 Bielefeld, Germany

Thermogravimetric analysis (TGA) combined with mass spectrometry (MS) provides a powerful, complementary approach for characterizing the thermal stability and degradation pathways of polymers subjected to accelerated (active) aging. In this study, aged polymer samples, representing materials encountered in post-consumer recycling streams, are analyzed using simultaneous TGA-MS to monitor mass-loss events and identify evolved gaseous species. These results demonstrate that combined TGA-MS analysis can reveal chemical and structural changes that are not easily evident from bulk mechanical or spectroscopic testing alone. The findings support more accurate assessments of polymer recyclability, highlight indicators of material downcycling, and inform optimization strategies for sorting, preprocessing, and reprocessing conditions. Ultimately, this work underscores the value of TGA-MS as a diagnostic tool for improving circular-economy approaches.

CPP 46.15 Thu 9:30 P5

Synthese und Reaktivität von Betti-Basen — •Alyona Nikulina — Mikluho-Maklaya Strasse, Moskau 117198

Diese Forschung konzentriert sich auf Naphthoxazine, eine wertvolle Gruppe von Verbindungen, die für ihre biologischen Aktivitäten bekannt sind wie antimikrobielle,antidiabetische und antidepressive Wirkungen sowie für ihr Potenzial in der Entwicklung von duroplastischen Polymeren. Die Synthese dieser Verbindungen beginnt häufig mit Betti-Basen, die Zwischenprodukte für die Bildung von kondensierten 1,3-Oxazinen darstellen.Um die notwendigen Betti-Basen zu erhalten, untersuchten wir zwei Syntheserouten. Eine Strategie war eine einfache Dreikomponenten-Reaktion von β-Naphthol, sekundären cyclischen Aminen und Aldehyden. Der andere Weg umfasste zunächst die Kondensation von 2-Hydroxy-1-naphthaldehyd mit Aminen und anschließend die Reduktion der resultierenden Iminiumsalze mit Natriumborhydrid. Nachfolgende Versuche, diese Basen durch Cyclisierung mit Standardreagenzien wie Silberoxid oder Kupferacetat in die Ziel-Naphthoxazine umzuwandeln, erwiesen sich als ineffizient und ergaben geringe Ausbeuten. Da bekannt ist, dass diese Cyclisierung die Bildung eines Iminiumsalzes beinhaltet, stellten wir die Hypothese auf, dass DIAD als wirksamer Katalysator wirken würde. Das Experiment nahm jedoch eine unerwartete Wendung: DIAD allein führte nicht zu den gewünschten Naphthoxazinen. Der entscheidende Moment kam, als wir ein katalytisches System aus Kupfer(I)-iodid und Cesiumcarbonat zugaben, das eine unvorhergesehene intramolekulare Umlagerung der Betti-Basen auslöste und stattdessen zu Diketon führte.

CPP 46.16 Thu 9:30 P5

Functional ZnPc-Polymer-Magnetic Nanocomposite Systems for Photodynamic Therapy — •Lungu Ion — Laboratory of Organic/Inorganic Materials for Optoelectronics, Institute of Applied Physics Moldova State University, 60 Al. Mateevici St., MD-2009, Chisinau, Republic of Moldova

Hybrid photosensitizing materials combining organic and magnetic components provide a promising route toward multifunctional systems for photodynamic therapy (PDT). In this work, we investigate the photophysical and magnetically induced processes in a series of functional zinc phthalocyanine (ZnPc) derivatives-ZnPc(COOH)4 and ZnPc(COOH)8 and their conjugates with dextran (Dx) and Fe3O4 nanoparticles. The systems were studied in DMSO/H2O (1:1) solutions using steady-state and time-resolved fluorescence and phosphorescence spectroscopy. All ZnPc-based compounds exhibit characteristic Q-band absorption (650-700 nm) and room-temperature phosphorescence with microsecond lifetimes, confirming efficient intersystem crossing (ISC). Dextran conjugation enhances fluorescence efficiency (ΦF = 2.37 %) and reduces aggregation, whereas Fe3O4 incorporation modifies the spin-orbit coupling, promoting magnetically assisted ISC and additional non-radiative channels. The triplet lifetimes vary between 1-9 μs, depending on molecular substitution and interfacial coupling. These results demonstrate that combining photoactive ZnPc cores with natural polymer matrices and magnetic nanoparticles enables control over excited-state dynamics and ROS generation for biomedical applications.

CPP 46.17 Thu 9:30 P5

Biopolymer-Templated Deposition of Hierarchical 3D-Structured Graphene Oxide/Gold Nanoparticle Hybrids for Surface-Enhanced Raman Scattering — •Yingjian Guo[1,2], Guangjiu Pan[2], Yusuf Bulut[1,2], Arno Jeromin[1], Thomas F. Keller[1], Andreas Stierle[1], Gergely Nemeth[3], Ferenc Borondics[3], Benedikt Sochor[1], sarathlal K. Vayali[1], Daniel Söderberg[4], Peter Müller-Buschbaum[2], and Stephan V. Roth[1,4] — [1]DESY, Hamburg — [2]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [3]Synchrotron SOLEIL, Saint-Aubin, France — [4]Department of Fibre and Polymer Technology, KTH, 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 46.18 Thu 9:30 P5

Regulation of HUVEC Adhesion by Mechanical and Biochemical Tuning of PNIPAM Microgel Coatings — •Leonie Beer, Souraj Mandal, and Regine v. Klitzing — Soft Matter at Interfaces, Department of Physics, TU Darmstadt, Darmstadt 64289, Germany

A bioactive and stable interfacial layer favouring HUVEC cell adhesion is a key factor in artificial vascular network construction. This work investigates the impact of the mechanical and biochemical properties of PNIPAM microgel (MG) coatings on HUVEC cell adhesion and proliferation on 3D printed polymeric surfaces. MG stiffness can be varied based on cross-linking, and bioactivity can be imparted by functionalizing MG with RGD-based peptide mimicking extracellular matrix (ECM) ligands. HUVEC cell culture studies showed significant effects of MG stiffness on cell adhesion and proliferation, with further improvement due to biochemical functionalization. In addition, different spacers were used to enhance cell attachment and growth.

MG adhesion on different substrates was also evaluated, revealing significantly stronger adsorption on 3D-printed polymeric surfaces compared to inorganic substrates. AFM imaging confirmed the presence of firmly adhered MGs beneath the cells, demonstrating long-term coating integrity under biological conditions.

These results demonstrate that PNIPAM MG coatings provide a robust, tunable, and bioactive platform for controlling HUVEC behaviour and represent a promising strategy for endothelialization of 3D-printed vascular structures.

CPP 46.19 Thu 9:30 P5

Crystallization behavior of electron beam modified Polylactide acid (PLA) — •Regine Boldt[1], Elisabeth Hauschild[1], Michael Müller[1], and Markus Stommel[1,2] — [1]Leibniz Institut fuer Polymerforschung Dresden, Germany — [2]Dresden University of Technology, Germany

Polylactic acid (PLA) is a polymer synthesized from renewable raw materials. The properties of PLA are essentially determined by its chemical/physical structure, such as molar mass, molar mass distribution, D-isomer content, and the resulting morphology. The morphology can be influenced by modifying the molecular structure on the one hand, and by the process parameters during processing on the other. Since PLA crystallizes very slowly, high cooling rates, which occur in processing methods such as injection molding, usually result in amorphous components. In this work, we modified PLA using high-energy electrons in order to accelerate its crystallization without adding external additives. The resulting changes in crystallization kinetics were analyzed and correlated with the morphology after irradiation. The spherulite growth rates were determined quantitatively using hot stage experiments on a light microscope. The results show that electron-modified PLA exhibits substantially increased crystal growth rates, enabling significant reductions in cooling time during processing operations such as injection molding.

CPP 46.20 Thu 9:30 P5

Diffusion and stiffness characterization of photocrosslinked hydrogels to replicate biological tissues — •Lena Hilf[1], Dimitris Missirlis[1,2], and Kai Melde[1] — [1]Institute for Molecular Systems Engineering and Advanced Materials, Universität Heidelberg — [2]MPI for Medical Research, Heidelberg

Microphysiological systems (MPS), such as organs-on-a-chip, aiming to replicate the spatial arrangement of biological tissues found in vivo are in need of a reliable and replicable way to recreate the biophysical environment including topography and mechanical properties. One possible route is via selective photocrosslinking of hydrogel scaffolds, which can be performed in situ in microfluidic platforms.

However, we still lack reliable information about key properties of potential hydrogel candidates in these systems, which influence cell adhesion and spreading, as well as the uptake of media components.

In this work, we characterize the stiffness, mesh size and diffusion constant of a range of hydrogels created using photolithpgraphy. We employ both optical and mechanical approaches, taking into account the versatility of hydrogel responses to different measurement methods.

Our results together with cell proliferation assays allow for a more targeted choice of hydrogels to serve as artifical extracellular matrices in MPS.

CPP 46.21 Thu 9:30 P5

Characterization of bimodal PMMA-PDMS suspensions using light scattering — •Katharina Gaus and Joachim Wagner — University of Rostock, Rostock, Germany

Poly-dimethylsiloxane coated PMMA particles index matched in tetraline/decaline mixtures are well defined model systems for hard spheres with tunable particle size. Binary mixtures of these core-shell particles with slightly different sizes artificially increase the polydispersity of colloidal model systems preventing crystallization at large volume fractions and thus enabling the preparation of colloidal glasses. Using a priori knowledge of both species' topology, even in the limited range of wave vectors accessible with light scattering experiments, the reliable structural characterization of mixtures is possible. Hence, such binary mixtures are promising model systems for colloidal glasses.

CPP 46.22 Thu 9:30 P5

Cycles of buckling in gel phase giant unilamellar vesicles — •Azeline Hilaire, Antonio Stocco, Jean Farago, and Fabrice Thalmann — Institut Charles Sadron, Strasbourg, France

Buckling can be observed in giant unilamellar vesicles (GUVs) in gel phase, leading to shape deformations under external stress. Such deformations may offer functional advantages, particularly for inducing motion at low Reynolds numbers.

Recently, lipid-coated microbubbles were shown to exhibit directed motion through deformation cycles, suggesting a broader potential for soft interfaces to generate propulsion. Inspired by this, we investigate whether similar mechanisms can be used in isolated GUVs under cycles of deformation, with the goal of understanding and eventually triggering symmetry-breaking dynamics. We aim to use shape hysteresis for producing directed motion.

Gel-phase GUVs were fabricated via hydration method and characterized by their ability to transition between buckled and unbuckled states. We exposed these vesicles to cyclic fields using three distinct methods: (i) oscillatory shear flows, (ii) osmotic pressure, (iii) On/Off cycles of light applied with optical tweezers. In some of these cases, the membrane exhibited buckling.

Although directed motion has not yet been observed, the buckling response establishes a first result for future efforts to induce propulsion in vesicles. These preliminary results offer a first step towards exploring whether shape hysteresis in membranes could one day be used for active functions.

CPP 46.23 Thu 9:30 P5

Dynamics of trifunctional hybrid nanoparticle assemblies — •Thomas Dartige[1], Yinan Fan[2], Clément Marque[1], Ali Abou-Hassan[2], and Antonio Stocco[1] — [1]Institut Charles Sadron, Strasbourg, France — [2]Phenix Lab, Paris, France

Active colloids are colloidal systems able to consume energy to produce work, such as directed motion. Self-propulsion in micrometric particles can be achieved through surface asymmetries, using diffusiophoresis (via asymmetric catalytic properties) or thermophoresis (via asymmetric light absorption). However, the combining of several active properties into one single colloidal system remains poorly explored. In this work, we present a hybrid system synthesized by combining distinct nanoparticles, and investigate its ability to exhibit diffusiophoresis, thermophoresis, and respond to magnetic field gradients.

CPP 46.24 Thu 9:30 P5

Physics-Informed Neural Inference with Multilayer DWBA Modeling for Quantitative GISAXS — •Özüm Emre Asirim[1,2], Yufeng Zhai[1], Marina Tropmann-Frick[2], and Stephan V. Roth[1,3] — [1]Deutsches Elektronen-Synchrotron DESY FS-SMA Notkestr. 85 22607 Hamburg Germany — [2]HAW Hamburg Berliner Tor 7 20099 Hamburg Germany — [3]KTH Royal Institute of Technology, SE-100 44 Stockholm, Sweden

Quantitative GISAXS analysis is often constrained by the complexity of multilayer scattering, film-nanoparticle coupling, and the limited availability of physically interpretable synthetic datasets for training modern inference models. We address these challenges with a physics-informed neural framework that integrates a compact multilayer DWBA formulation with a hybrid CNN-Transformer architecture. The forward model captures essential film and nanoparticle scattering through per-layer incoherent DWBA terms, normalized form factors, structure factors, and DWBA-based field enhancement, yielding a reduced and physically coherent parameter space suitable for inversion. Measurement variability is modeled through noise, detector effects, and the ability to generate time-series data for evolving structures. Leveraging this parameterization, the CNN-Transformer network jointly extracts local scattering motifs and long-range reciprocal-space correlations, enabling accurate recovery of film- and particle-level parameters. Validated through forward reconstruction using the same physics model, the workflow provides a fast, interpretable, and physically grounded solution for high-throughput GISAXS analysis.

CPP 46.25 Thu 9:30 P5

How Polymer Architecture Shapes the Phase Behavior of Polyelectrolyte Complex Coacervates — •Lena Tarrach, David Beyer, and Christian Holm — Institute for Computational Physics, University of Stuttgart, Stuttgart, Germany

Polyelectrolyte (PE) complex coacervation is an associative liquid-liquid phase separation that can occur in mixtures of oppositely charged macromolecules. Although this phenomenon is widely studied, the effects of the polymer architecture on the phase behavior of PE complex coacervates have not been considered so far. To close this gap, in this contribution, coarse-grained molecular dynamics (MD) simulations with the ESPResSo software [1] are applied to calculate the phase diagram of branched PEs with varying numbers of arms but the same overall molecular weight. The slab method is used to establish the coexistence of the coacervate phase and the supernatant solution. The number of arms of the PEs is systematically increased to assess the influence of the PE topology on the phase behavior. The obtained phase diagrams are subsequently compared to theoretical phase diagrams calculated using the random phase approximation.

[1] Florian Weik, Rudolf Weeber, Kai Szuttor, Konrad Breitsprecher, Joost de Graaf, Michael Kuron, Jonas Landsgesell, Henri Menke, David Sean, and Christian Holm. ESPResSo 4.0 - an extensible software package for simulating soft matter systems. The European Physical Journal Special Topics, 227(14):1789-1816, 2019. doi:10.1140/epjst/e2019-800186-9.

CPP 46.26 Thu 9:30 P5

Self-assembled Micelles from Charged Block Copolymers: Insights from Small-Angle X-ray Scattering (SAXS) — •Yijun Zhao[1], Varvara Chrysostomou[2], Athanasios Skandalis[2], Stefano Da Vela[3], Stergios Pispas[2], and Christine M. Papadakis[1] — [1]TUM School of Natural Sciences, Soft Matter Physics Group, Garching, Germany — [2]Theoretical and Physical Chemistry Institute, NHRF, Athens, Greece — [3]EMBL at DESY, Hamburg, Germany

Block copolymer micelles have been widely studied due to their ability to load drugs. Positively charged micelles have been proposed to complex DNA, enabling efficient gene therapy. To achieve highly tunable morphology, self-assembled micelles from the diblock copolymers PDMAEMA-b-PLMA and the triblock terpolymers PDMAEMA-b-PLMA-b-POEGMA are investigated in aqueous solution [1]. Here, PDMAEMA stands for the weak polycation poly(2-(dimethylamino)ethyl methacrylate), PLMA for the hydrophobic, but soft poly(lauryl methacrylate), and POEGMA for the hydrophilic poly(oligo(ethylene glycol) methacrylate). Small-angle X-ray scattering (SAXS) on dilute aqueous solutions revealed that PDMAEMA-b-PLMA forms ellipsoidal core-shell micelles, with their size and inner structure depending on temperature and the pH value. For the triblock terpolymers, the micellar structures depend strongly on the block lengths.

[1] V. Chrysostomou et al., J. Polym. Sci. 63 1684-1694 (2025).

CPP 46.27 Thu 9:30 P5

Pump-probe spectroscopy on the polyelectrolyte donor polymer PTHS for solar cell applications — •Mick Gindorf[1], Anna Köhler[1], Christopher Vogt[2], and Johannes C. Brendel[2] — [1]Chair of Soft Matter Optoelectronics, University of Bayreuth — [2]Chair of Macromolecular Chemistry I, University of Bayreuth

Poly(3-hexylthiophene) (P3HT) is a well-researched donor polymer for application in organic solar cells (OSCs). Side chain modification of P3HT with sulfonate groups yields PTHS, a polyelectrolytic donor polymer with high hole transport mobility [1]. This polyelectrolyte possesses two key advantages: Firstly, exchange of the cationic counter ions enables insolubilization of the donor layer, allowing simple fabrication of donor-acceptor bilayer systems by sequential spin coating with a wide variety of acceptors, including both fullerene and non-fullerene acceptors (NFAs). Secondly, adjusting the counter ion composition enables tuning of the donor energy level and thereby the donor-acceptor energy level offset (E_{off}), which is critical for achieving high open circuit voltages (V_{oc}). These properties make PTHS an ideal model system for the investigation of exciton dissociation in OSCs with spectroscopic techniques, including time-resolved transient absorption spectroscopy. Probing the exciton dissociation dynamics as a function of E_{off} on a picosecond timescale in different donor-acceptor systems yields valuable insights into the energetic and entropic contributions that help overcome the exciton binding energy in OSCs.

1) Brendel, J. et al. Chem. Mater. 2014, 26, 6, 1992-1998

CPP 46.28 Thu 9:30 P5

PEDOT Molecular Imprinting in PEDOT:PSS/PDADMA Layer-by-Layer Films — •Martin Hunger, Muhammad Khurram, and Christiane A. Helm — martin.hunger@uni-greifswald.de

PPEDOT:PSS films are widely used because they offer high conductivity & tunable electro-optical properties. We prepare PEDOT:PSS films with a thickness of up to 150 nm using Layer-by-Layer assembly. We vary the preparation conditions: flow cell, dip coating, PEDOT:PSS concentration in solution, and rinsing steps. Whenever PDADMA is the top layer, UV-vis-IR absorption spectroscopy shows that there is significantly less PEDOT in the films than when PEDOT:PSS is the top layer. Films prepared using the flow cell have the highest electrical conductivity (approx. 200 kS/m) with PEDOT:PSS. When PEDOT is the top layer, conductivity is reduced by a factor of 100. The conductivity of films prepared with dip coating with PEDOT:PSS as the top layer is one order of magnitude lower or more. When PDADMA is the top layer, conductivity drops by an additional 4 to 5 orders of magnitude. Thus, during assembly, PEDOT can be selectively removed and subsequently rebound to the film, leaving behind well-defined molecular cavities that preserve their shape and enable reconstruction of percolative pathways.

CPP 46.29 Thu 9:30 P5

PDADMA/PSS Multilayer Buildup in NaBr Solution: Vertical PSS Diffusion and Unusual Growth — •Per-Ole Hilken, Issam Assi, and Christiane A. Helm — Institute of Physics, University of Greifswald, Germany

Polyelectrolyte multilayers form by sequential adsorption of oppositely charged polyelectrolytes. The interfaces between the adsorption layers are fuzzy; in the exponential growth regime of PDADMA/PSS (poly(diallyldimethylammonium)/polystyrene sulfonate) multilayers PSS diffuses vertically through the film. We determine its vertical diffusion coefficient D_{PSS} using a quartz crystal microbalance with dissipation (QCM-D). The scaling laws for D_{PSS} in dependence of the NaBr concentration are similar to those found with NaCl in the deposition solution (Sill et al., Macromolecules 2025), however, the diffusion coefficient is one to two orders of magnitude larger. The dependence on PSS molecular weight M_{PSS} is qualitatively the same as with NaCl in the deposition solution: Polymer diffusion dominates multilayer buildup when $M_{PSS} < 76$ kDa.; at larger M_{PSS}, site diffusion dominates; i.e. diffusion of charged repeat units with their counterions. For polyelectrolyte multilayers in the non-exponential growth regimes it is well known and also found with that an increase in the salt concentration leads to thicker multilayers. This is not the case if the NaBr concentration exceeds ≈ 0.6 M; additionally, film stability becomes an issue. To understand the unusual behavior, the dissipation during film build-up is quantified. The surface topography is investigated with AFM.

CPP 46.30 Thu 9:30 P5

Structural influences on nonlinear optical activity in the heterocubane family — •Alexander Kapp and Simone Sanna — alexander.kapp@pysik.uni-giessen.de

Recent progress in the study of molecular clusters with extreme nonlinear optical response has highlighted their potential for coherent broadband light generation. To extend the library of suitable candidate materials, we investigate the linear and nonlinear optical properties of a family of heterocubanes with the general formula $[(RM)_4Pn_4]$, where M = C, Si, Ge, Sn, Pn = N, P, As, Sb, Bi, and R = H, Me, Ph. Using *ab initio* density functional theory, we analyze their structural and electronic characteristics, including optimized geometries, symmetry features, band gaps on different theoretical levels and shape of the HOMO–LUMO orbitals. Both the linear and the nonlinear (SHG) optical responses of all systems are computed using the Yambo code. Clear trends emerge that link the optical activity to the choice of pnictogen, tetrel, and substituent. These findings help identify promising candidates for nonlinear optical applications and contribute to a deeper understanding of structure–property relations in heterocubane materials.

CPP 46.31 Thu 9:30 P5

A micellar solution from thermoresponsive block copolymers during pressure jumps — •Yandong Wang[1], Geethu P. Meledam[1], Leonardo Chiappisi[2], Cristiane Henschel[3], André Laschewsky[3,4], Alfons Schulte[5], and Christine M. Papadakis[1] — [1]TUM School of Natural Sciences, Soft Matter Physics Group, Garching, Germany — [2]ILL, Grenoble, France — [3]Universität Potsdam, Germany — [4]Fraunhofer IAP, Potsdam-Golm, Germany —

[5]University of Central Florida, Orlando, U.S.A.

The diblock copolymer PMMA-b-PNIPAM, consisting of a hydrophobic poly(methyl methacrylate) and a thermoresponsive poly(N-isopropylacrylamide) block, forms core-shell micelles in dilute aqueous solution at atmospheric temperature. These micelles aggregate upon heating or applying pressure. Previous studies have shown that the micellar shell remains hydrated in the two-phase region under high pressure, in contrast to the strongly dehydrated micelles observed in the two-phase region at atmospheric pressure [1]. In this work, we analyzed the micellar transition kinetics during rapid pressure jumps using time-resolved small-angle neutron scattering (SANS). The system was driven from the one-phase region into the two-phase region at target pressures in both low- and high-pressure regimes.
[1] P. A. Alvarez Herrera et al., Macromolecules 2024, 57, 10263.

CPP 46.32 Thu 9:30 P5

Photoresponsive Interfacial Behavior of Hybrid Photosensitizer-Surfactant Mixtures — •Phat Tan Pham[1], Julius Gemen[2], Frank Glorius[2], and Björn Braunschweig[1] — [1]Universität Münster, Institut für Physikalische Chemie, Corrensstr. 28/30, 48149 Münster — [2]University of Münster, Organisch-Chemisches Institut, Correnssstraße 40, 48149 Münster

Fluid interfaces that adapt to external triggers such as light or temperature are of great interest for driving changes in soft matter systems like foams and emulsions. Arylazopyrazoles (AAPs), as photo-responsive surfactants, can control surface tension and molecular organization at air-water interfaces through E/Z photoisomerization. However, light-induced switching of AAP derivatives is typically limited to UV and green light. To overcome this, we combined AAP with the water-soluble photosensitizer resazurin (Rez) and achieved pronounced interfacial changes under 625 nm red-light irradiation. By tuning the AAP/Rez molar ratio, we further introduced history-dependent, quasi-adaptive changes in surface tension and molecular structure. The latter was examined in situ with surface tensiometry and vibrational sum-frequency generation (SFG) when the samples where irradiated at 365, 520, or 625 nm. We propose that red-light activation occurs at the interface, through photoexcited Rez moieties at 625 nm and subsequent intersystem crossing to adjacent interfacial AAP molecules. These results demonstrate a new strategy to extend the optical control of photo-responsive surfactants into the red-light region.

CPP 46.33 Thu 9:30 P5

Thermoresponsive Microgel Membrane for applications in an Electrochemical Device — •Aditi Gujare[1], Stefanie Uredat[2], Jonas Runge[2], Domenico Truzzolillo[1], Julian Oberdisse[1], and Thomas Hellweg[2] — [1]Soft Matter Physics Team, Laboratoire Charles Coulomb, University of Montpellier, Montpellier, France — [2]Physical and Biophysical Chemistry, Bielefeld University, Bielefeld, Germany

Microgels based on NIPAM are thermoresponsive with a volume phase transition temperature (VPTT) of 33°C. The VPTT has been observed to shift by copolymerizing these microgels with comonomers such as N-hydroxymethyl acrylamide (HMAM).[1] Different sets of copolymers have been tested, NIPAM-co-HMAM and NIPMAM-co-HMAM. These microgels have been observed to have a VPTT up to 60°C. The copolymer microgels based on the comonomer HMAM has an alcohol group, making it prone to condensation at high temperatures (above 90°C) resulting in formation of a membrane. These thermoresponsive, chemically crosslinked membranes have been prepared by dropcasting and crosslinking at 100°C. Such membranes can be prepared in a range of thickness, of 30-800 μm. The resistance of these membranes of different thickness, comonomer content, and at different temperatures are being tested. Resistance measurements at room temperatures show that thicker membranes are more resistive in a certain concentration of an electrolyte. [1]Gujare,Uredat,Runge,Morgenstern,Truzzolillo,Hellweg,Oberdisse, Langmuir 2025, 41, 45, 30442

CPP 46.34 Thu 9:30 P5

Correlating molecular properties of tetraphenylethylene substituted tetraphenyl heteoadamantanes to nonlinear optical activity — •Eva Westenfelder Gil and Simone Sanna — Institut für Theoretische Physik, Justus-Liebig-Universität Gießen, Germany

Recent studies have demonstrated white light generation from molecular clusters with adamantane-like cores and various substituents [1,2]. Subsequent investigations on isolated molecules revealed correlations of the structural, electronic and optical properties [3]. Building on this foundation, we focus here on further investigating structural, electronic, and (nonlinear) optical properties from first principles for isolated molecules with modified cores. In this contribution, we report on $[(PhSn)_3(TPESi)S_6]$ and $[(PhSn)_3(TPESi)Se_6]$ clusters, which are modeled within density functional theory. Distinct changes in the spectral signatures can be observed. The presented results expand on theoretical foundations for the design of tailored nonlinear optical sources.

[1] N. W. Rosemann *et al*, Science 2016, 352, 1301

[2] N. W. Rosemann *et al*, J. Am. Chem. Soc. 2016, 138, 50, 16224-16227

[3] F. Ziese *et al*, 2024. J. Phys. Chem. A 128, 8360-8372

CPP 46.35 Thu 9:30 P5

Modeling Structural and Electronic Properties of Functional Organic Molecules — •Linda Düren and Simone Sanna — Institut für Theoretische Physik, Justus-Liebig-Universität Gießen, Germany

In this work, various organic molecules with the general composition $[(RT)_4E_6]$ are investigated using density functional theory (DFT) to model their structural, electronic, and optical properties. Ground-state geometries and energies, as well as the frequency-dependent optical parameters, are calculated for the isolated clusters. The study includes *tetraphenyladamantane* and its halogenated derivatives, as well as other heteroadamantanes with a heterogeneous ligand field of the type $(MeC)(CH_2)_3(PhSn)E_3$ with E = S, Se, Te, CH_2.

The theoretical results provide insights into the relationship between molecular structure and optical behavior, building on previous studies of nonlinear optical responses in organotetrel and (hetero)adamantane-type clusters [1] and amorphous molecular materials for directed supercontinuum generation [2]. The results are compared with experimental data where available and demonstrate the potential of these classes of molecules for applications in optics.
[1] Ziese et al., *J. Phys. Chem. A* **128**, 8360 (2024)
[2] Dehnen et al., *ChemPhotoChem* **5**, 1032 (2021)

CPP 46.36 Thu 9:30 P5

Tuning PNIPAM Phase Transition and Interfacial Structures — •Zugeng Cong, Michael Hardt, and Björn Braunschweig — University of Münster, Institute of Physical Chemistry, Münster, Germany

In this work, we aim to introduce the concept of a self-regulating negative-feedback system in which an exothermic photochemical process would be coupled to the thermo-responsive polymer PNIPAM. In such a scheme, reaction-generated heat would raise the solution temperature, trigger PNIPAM collapse, increase turbidity, and thereby limit light penetration—providing an intrinsic mechanism to suppress further heat generation. For that, we characterize the PNIPAM phase transition through temperature-dependent turbidity measurements while varying SDS and NaCl concentrations as well as the water-ethanol co-solvent composition. To elucidate interfacial contributions, surface-specific sum-frequency generation (SFG) spectroscopy is used to probe adsorption layers at the air-water interface, taken as a model for micellar environments. These measurements reveal how surfactant loading, solvent composition, and electrolyte concentration reorganize interfacial structures below and above the PNIPAM phase-transition temperature. This provides the physicochemical basis required for designing a feedback-controlled photochemical soft matter system.

CPP 46.37 Thu 9:30 P5

Quasi-elastic neutron scattering of perdeuterated poly(N-isopropylacrylamide) and hydration changes across the demixing transition — •Alfons Schulte[1], Eric Rende[1], Marcell Wolf[2], Thomas Müller[3], Dirk Schanzenbach[4], Andre Laschewsky[4,5], and Christine M. Papadakis[6] — [1]Department of Physics and College of Optics and Photonics, University of Central Florida, Orlando, U.S.A. — [2]Heinz Maier-Leibnitz Zentrum (MLZ), TUM, Garching, Germany — [3]FZ Jülich, JCNS at MLZ, Garching, Germany — [4]Institut für Chemie, Universität Potsdam, Potsdam-Golm, Germany — [5]Fraunhofer-Institut für Angewandte Polymerforschung, Potsdam-Golm, Germany — [6]TUM School of Natural Sciences, Soft Matter Physics Group, Garching, Germany

We investigate the hydration dynamics of perdeuterated poly(N- isopropylacrylamide) (PNIPAM-d10) to elucidate the molecular mechanism of its demixing transition. Quasi-elastic neutron scattering (QENS) and Raman spectroscopy were measured in a 25 wt% PNIPAM-d10 aqueous solution over the temperature range from 298 to 325 K. There is a significant upward shift in the cloud point by about 4 degrees. Deuteration suppresses incoherent scattering from the polymer, allowing a clear view of hydration water dynamics. The dynamic susceptibilities reveal the relaxation processes for bulk and bound water, with the bound fraction decreasing sharply near the transition. The relaxation times of hydration water are consistently lower than in the protiated polymer, indicating faster local dynamics. Raman spectra show abrupt C-D band frequency shifts at the transition, reflecting side-group dehydration.

CPP 46.38 Thu 9:30 P5

Thermoresponsive Microgels with hydrophilic Monomers — •Stefanie Uredat[1], Aditi Gujare[2], Jonas Runge[1], Domenico Truzzolillo[2], Julian Oberdisse[2], and Thomas Hellweg[1] — [1]Physical and Biophysical Chemistry, University Bielefeld, Bielefeld, Germany — [2]Laboratoire Charles Coulomb (L2C), University of Montpellier, CNRS, Montpellier, France.

To develop fully smart membranes for use in low-temperature fuel cells operating at around 80-90 °C it is essential to achieve a high volume phase transition temperature (VPTT) within this range. To reach these high VPTTs, new monomers are required for microgel synthesis. The most common and researched monomers have a VPTT around the human body temperature [1]. To rise the VPTT we increased the hydrophilicity of the monomers by adding a hydroxy group to the well-known NIPAM and got HIPAM (N-(2-hydroxyisopropyl)acrylamide).

To tune the VPTT to higher Temperatures a series of microgels with two different main monomers (NIPAM and NIPMAM) with different contents of HIPAM as comonomer were synthesised. The microgels were observed by Dynamic Light Scattering and AFM. With higher HIPAM content the VPTT of the microgels increases and widens. We also observe a jump in size with increasing hydrophilic monomer content. We also investigated a second hydrophilic monomer N-(hydroxymethyl)acrylamide (HMAM). [2]

[1] Uredat, Runge, Gujare, PCCP, 2024, 2732. [2] Gujare, Uredat, LANGMUIR 2025, 41, 45, 30442 [3] The authors acknowledge funding from the DFG (505656154) and ANR (ANR-22-CE92-0052-01)

CPP 46.39 Thu 9:30 P5

The phase transition of perdeuterated thermoresponsive polymers — •Chenrui Ding[1], Kuno Schwärzer[2], Alfons Schulte[3], and Christine M. Papadakis[1] — [1]TUM School of Natural Sciences, Soft Matter Physics Group, Garching, Germany — [2]JCNS-1, FZ Jülich GmbH, Germany — [3]University of Central Florida, Department of Physics and College of Optics and Photonics, Orlando, U.S.A.

The interaction of thermoresponsive polymers with water has been amply studied with respect to the cloud point temperature and the latent heat at the transition, using, among others, turbidimetry and differential scanning calorimetry (DSC) [1]. New information on the polymer-water interaction can be gained using perdeuterated polymers. We present results on poly(N-isopropyl acrylamide) (PNIPAM) and poly(N-isopropyl methacrylamide) (PNIPMAM) and their perdeuterated versions in aqueous solution as a function of polymer concentration and establish the transition behavior.

1. C.-H. Ko, C. M. Papadakis et al., Macromolecules 53, 6816 (2020)

CPP 46.40 Thu 9:30 P5

Steel Mesh-Supported SNW-1/CsPbBr3 Nanocomposite: Photocatalyst for Sustainable Ammonia Production — •Negin Khosroshahi and Vahid Safarifard — Iran University of Science and Technology, Tehran 16846-13114, Iran

The conversion of solar energy into chemical energy through photocatalysis is an important field of interest in green energy generation and environmental improvement [1]. Nevertheless, its effectiveness currently falls short of expectations, primarily due to the issue of charge recombination. To address this challenge, the photocatalytic effect has become an optimistic approach for enhancing processes [2]. In this research, we have developed a Steel Mesh-Supported SNW-1/CsPbBr3 nanocomposite by combining covalent-organic frameworks with metal halide perovskite. To gauge their effectiveness, the heterostructure was assessed by employing multiple characterization methods including XRD, IR, FESEM, DRS, EDX, VSM, PL, EIS, Zeta, and BET. After the composite's preparation and characterization, we examined its photocatalytic activity in nitrogen reduction. The SNW-1/MHP/Steel mesh nanocomposite exhibited exceptional performance in ammonia generation. These findings suggest that the SNW-1/MHP/Steel mesh nanocomposite holds promise as an environmentally friendly and cost-effective photocatalyst, capable of addressing the challenges of sustainable ammonia production. This study presents a promising method for identifying effective photocatalytic materials using mesh substrates to address environmental concerns.

CPP 46.41 Thu 9:30 P5

Engineering MOF@MOF Heterojunction for Photocatalytic N2 Reduction to NH3 — •Maedeh Atoufi Kashani, Negin Khosroshahi, and Vahid Safarifard — Iran university of science and technology, Tehran, Iran

Photocatalytic nitrogen fixation is a promising green alternative to the Haber-Bosch process, but cobalt-based MOFs typically suffer from poor stability in water. Here, two Co-terephthalate frameworks were synthesized via solvothermal routes: MOF-71 from Co(NO3)3.6H2O and ultrathin Co-BDC nanosheets from CoCl2.6H2O in the presence of triethylamine, water, and ethanol. Both materials showed high phase purity and strong visible-light absorption. To improve the limited stability of Co-BDC, a Ce-based MOF overlayer was constructed on Co-BDC and MOF-71, forming a Ce-Co MOF-on-MOF composite. The Ce shell enhanced water stability, facilitated charge separation, and promoted N2 activation at the heterointerface. As a result, the Ce-Co-BDC composite delivered markedly higher ammonia production and durability than pristine Co-BDC. This work highlights the critical roles of precursor chemistry and Ce-Co interfacial engineering in developing robust MOF photocatalysts for solar-driven nitrogen fixation. [1] S. Nabi, M.M. Bhat, A. Hamid, A.Y. Bhat, A.U. Bashir, Q. Jan, P.P. Ingole, M. Bayati, M.A.J.A.S.S. Bhat, (2025) e00112. [2] G. Song, Y. Shi, B. Yang, Y. Yang, H.J.I.C. Pang, 64 (2025) 6265-6274.

CPP 46.42 Thu 9:30 P5

Structural Insights into Supported Ionic Liquid Phases — •Yufei Wu[1], Julius Schlüter[2], Chandan K. Das[3], Zhuo Chen[1], Alexis Bordet[1], Maria Fyta[3], and Thomas Wiegand[1,2] — [1]Max Planck Institute for Chemical Energy Conversion, Mulheim an der Ruhr, Germany — [2]Institute of Technical and Macromolecular Chemistry, RWTH Aachen University, Aachen, Germany — [3]Computational Biotechnology, RWTH Aachen University, Aachen, Germany

Metal nanoparticles supported on molecularly modified surfaces (MMSs) offer significant potential for the development of advanced materials chemistry, particularly in catalysis. In this work, we focus on supported ionic liquid phases (SILPs) as a representative class of MMS materials. The SILP material was synthesized by functionalizing an amorphous silica surface with a layer of phosphonium-based ionic liquid (IL) covalently bound to the silica. The structural features of the SILP, specifically the conformation of the phosphonium IL cations, were characterized using magic-angle spinning (MAS) solid-state NMR spectroscopy. To complement the experimental findings, all-atom molecular dynamics (MD) simulations were performed on IL-modified silica surfaces. These simulations provided atomic-level insights into the structural organization and conformational dynamics of the IL molecules in the SILP materials. This combined approach paves the groundwork for future studies aimed at realizing SILP materials as efficient catalytic templates.

CPP 46.43 Thu 9:30 P5

Towards stable passivation layers on III-V-semiconductor nanowires for photoelectrochemical water splitting applications — •Chris Yannic Bohlemann, Pavithira Manoharan, Sahar Shekarabi, Peter Kleinschmidt, Thomas Hannappel, and Juliane Koch — Technische Universität Ilmenau, Fundermentals of Energy Materials, Ilmenau, Germany

The production of green hydrogen is expected to play a crucial role in achieving a sustainable, climate-neutral economy. Although III-V semiconductors offer record solar-to-hydrogen conversion efficiencies, the large-scale deployment is limited by the scarcity of the required materials. III-V nanowires (NWs) are a promising approach, as they require less material than planar films, and exhibit an enhanced optical absorption, as well as benefit from a high surface-to-volume ratio [1].

However, the instability of III-V materials in aqueous electrolytes leads to rapid corrosion and short lifetimes of photoelectrodes. To address this limitation, we investigated the growth behavior, electrical properties, and corrosion stability of GaAsP NWs and subsequently passivated with GaP(N) shells grown via metal-organic vapor-phase epitaxy. Scanning electron microscopy was used to examine the growth quality, crystal orientation, defect structures, and degradation before and after extended operation under water splitting conditions. Our results demonstrate that the application of a GaP(N) passivation layer significantly enhances the structural integrity and durability of the NWs during continuous photoelectrochemical water splitting.

[1] J. Koch et al., Adv. Energ. Sust. Res. e202500156, 2025.

CPP 46.44 Thu 9:30 P5

A Bottom-Up Coarse-Grained Model of Nanoparticles Decorated with Oppositely Solvent-Responsive Diblock Copolymers for Reversible Self-Assembly — •Daniel Otschkowski and Arash Nikoubashman — Leibniz-Institut für Polymerforschung Dresden e.V., Dresden, Germany

Polymer-grafted nanoparticles (PGNPs) combine the optical, magnetic, or electronic functionality of inorganic cores with the elasticity and responsiveness of polymer chains. This hybrid character offers multiple, orthogonal design parameters for controlling the structure and properties of PGNP-based materials. In this work, we study spherical NPs grafted with amphiphilic diblock copolymers composed of two blocks with opposing solvent affinities, enabling reversible transitions between assembly and disassembly states. In the assembly state, the inner polymer block is solvophilic while the outer block is solvophobic, thus collapsing into attractive patches; in the disassembly state, the inner block forms a dense polymer shell which is surrounded by a stabilizing hydrophilic polymer corona. To access device-relevant time and length scales, we develop a bottom-up coarse-grained (CG) model, where we describe the PGNPs in the assembly state as particles with flexible, spring-tethered patches. Smoothly varying the effective interactions allow the CG model to reproduce the continuous transition between both states. This approach enables efficient simulation of large PGNP systems and provides insight into their reversible, stimuli-responsive behavior.

CPP 46.45 Thu 9:30 P5

Organic cathodes based on polyaniline and cellulose for aqueous Zn-ion batteries — •Ramsha Wasi Khan[1], Meriem Boudjenane[1], Gilles Wittmann[1], Xaver Brehms[2], Simon Schraad[3], Xinyu Jiang[3], Stephan V. Roth[3], and Lucas P. Kreuzer[1] — [1]Heinz Maier Leibnitz Zentrum (MLZ), TUM, Garching, Germany — [2]CEA, Grenoble, France — [3]DESY, Hamburg, Germany

Aqueous zinc-ion batteries are promising candidates for a non-toxic and safer alternative to lithium-ion batteries, where organic cathodes provide distinct advantages of sustainability, tunability and mechanical flexibility. In this work, we investigate the role of polyaniline (PANI) as an organic cathode material, motivated by its high theoretical capacity, reversible redox chemistry, and intrinsic electrical conductivity. To enhance stability against humidity-induced degradation, cellulose derivatives are employed as green binders, enabling regulation of water uptake and improved mechanical stability. Comprehensive multiscale characterization is conducted to optimize the electrochemical performance and structural integrity of PANI-based cathodes, as well as understand the morphological changes and nanoscale water dynamics under humidity. Advanced techniques such as cyclic voltammetry, scanning electron microscopy (SEM), and quasi-elastic neutron scattering (QENS) are used to support this analysis. It was observed that the use of composite cellulose films as a binder with an optimized composition effectively triples the current density and improves peak reproducibility as well as the water uptake behaviour of the film.

CPP 46.46 Thu 9:30 P5

Integration of Ag_2S nanocrystals into flexible polymer matrices — •Dolores García de Viedma Guerra, Peijiang Wang, and Beatriz Hernández Juárez — Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC), Madrid E-28049, Spain

A broad range of modern optical technologies, for instance flexible photonics, require luminophores to be embedded within mechanically versatile host materials [1]. Usually, transferring nanocrystals from colloidal dispersions into polymer networks alters their physicochemical environment, which promotes surface traps and can thus signify a loss in photoluminescence [2].

In this work we investigate Ag_2S nanocrystals integrated into flexible polymer matrices with the goal of preserving their NIR response. We assess nanocrystal dispersion and spatial homogeneity, and probe their optical performance under 808 nm laser excitation via photoluminescence measurements and infrared spectroscopy, while NIR imaging maps emission uniformity. The results yield bright, uniform nanocrystal-polymer composites suitable for optoelectronic integration.

[1] Gordillo, H. et al. "Polymer/QDs Nanocomposites for Waveguiding Applications".*Journal of Nanomaterials* 2012, 960201, 2012.

[2] Marcus Jones et al. "Signatures of Exciton Dynamics and Carrier Trapping in the Time-Resolved Photoluminescence of Colloidal CdSe Nanocrystals". *The Journal of Physical Chemistry* C 2009, 113 (43), 18632-18642.

CPP 46.47 Thu 9:30 P5

Exploring the length limit for freestanding electrodeposited Ni nanowires — •Anneliese Wirth and Karin Leistner — Chemnitz University of Technology, Chemnitz 09107, Germany

Magnetic nanowire arrays are of interest from a fundamental and application point of view due to the shape anisotropy and high surface-to-volume ratio. This can be advantageous for 3D memory devices, micro-hard magnets and catalysis. The goal of this project is to obtain freestanding Ni nanowire arrays in order to functionalize their surface and possibly apply electrolytic gating strategies for 3D magneto-ionic materials in the future.[1] The Ni nanowire synthesis is performed by electrodepositing Ni into aluminum oxide membranes that serve as templates. Afterwards, the template is removed via dissolution of the aluminum oxide to achieve freestanding nanowires. For nanowires with high aspect ratio, this step usually leads to the collapse of the wires into agglomerated bundles.[2] This causes the loss of the nanowires' perpendicular alignment to the substrate. We show an optimized synthesis that avoids the collapse of nanowires with high aspect ratio in a large-scale array with a total size of around 0.5 cm^2. The deposition time during the electrodeposition is varied to obtain nanowires reaching up to more than 10 μm length while the diameter is fixed to 200 nm. Scanning electron microscopy indicates that the freestanding nature is related to irregularities of the nanowires which are introduced by the specific template geometry and lead to the stabilization of the array. [1] M. Nichterwitz et. al, ACS Mater. Au 2024, 4, 55. [2] N. Winkler et. al, J. Mater. Chem. 2012, 22, 16627.

CPP 46.48 Thu 9:30 P5

Structure and Morphology Investigations of Perovskite Nanocrystal Film — •Azam Davoodabadifarahani[1,2], Thomas Baier[1], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]University of Applied Sciences, Munich, Germany

In recent years, perovskite quantum dot solar cells with the ABX3 structure have shown great promise due to their high power conversion efficiency (PCE), high photoluminescence quantum yield (PLQY) and narrow photoluminescence (PL) peak. Within the presented work, the active layer consists of PQD thin films based on CsPbI3 and FAPbI3, which exhibit high photoelectric performance. However, CsPbI3 has a challenge with phase instability and FAPbI3 suffers from weak structural stability. To balance the performance and stability of the active layer, FAxCs1-xPbI3 PQDs are employed as the light-absorbing layer. The samples are evaluated using various optical and structural characterization techniques, such as PL spectroscopy, scanning electron microscopy (SEM), X-ray diffraction (XRD) and grazing incidence x-ray scattering (GIXS) to observe the influence of the synthesis process, temperature, and deposition techniques on the crystal size, orientation, phase, and stability, all of which determine the external quantum efficiency and optical performance.

CPP 46.49 Thu 9:30 P5

Surface-induced morphology and in-plane order in thin films of polydiketopyrrolopyrroles — •Anton Sinner and Oleksandr Dolynchuk — Martin Luther University Halle-Wittenberg, Germany

Board-like conjugated polymers are of particular interest in the context of surface-induced ordering because they often exhibit a preferred out-of-plane molecular orientation in thin films. Recent studies of ordering in conjugated polymer films have found that the free surface induces the formation of sanidic liquid crystalline (LC) mesophases with out-of-plane, smectic-like positional order between polymer chains. However, the question of whether the surface influences the in-plane order between polymer chains during ordering remained open. Here, we use atomic force microscopy to investigate the surface morphology and nanoscale structure formed on the surface of polydiketopyrrolopyrrole (PDPP) films after slow cooling and ordering from the melt. We find that the surface morphology consists of disc-like crystallites with diameters roughly equivalent to the polymer contour length and heights equivalent to several out-of-plane polymer layers. Thus, the observed LC morphology is consistent with the earlier study of out-of-plane molecular order. On a larger scale, multiple LC discs arrange into string-like morphologies, suggesting the existence of orientational order among them. Quantitative analysis of the surface morphology allows for calculating a distance-dependent orientation correlation function for six-fold symmetry, which indicates the presence of quasi-long-range order on the surface of PDPP films.

CPP 46.50 Thu 9:30 P5

Investigation of structure and transport properties in redox-active polymers — •Laura Hölzer[1] and Diddo Diddens[2] — [1]Institut für Physikalische Chemie, Universität Münster, 48149 Münster, Germany — [2]Helmholtz Institute Münster, Forschungszentrum Jülich GmbH, 48149 Münster, Germany

Organic radical batteries are seen as an alternative to traditional lithium-ion batteries. Their advantages include fast charge and discharge processes, and mechanical flexibility. However, high power densities are required for their application in the Internet of Things. To achieve this, good charge transport is essential. This transport mechanism is guided by two factors: the movement of electrons along the polymer, which is dictated by its structure, and the compensation of charge by counterions, which affects their mobility. The focus here is on a cathode material consisting of a redox-active polymer such as poly(2,2,6,6-tetramethylpiperidinyloxy-4-ylmethacrylate) (PTMA), which is in contact with a solvent. Classical molecular dynamics simulations of a PTMA cathode model are carried out. These provide insights into the structural properties and dynamics of charge transport. An outlook on the behaviour at interfaces around the cathode is given.

CPP 46.51 Thu 9:30 P5

Ex-Situ Investigation of Latex Deformation — •Simon Schraad[1,2], Shuxian Xiong[1,2], Helder Marques Salvador[3], Benedikt Sochor[1], Sarathlal Koyiloth Vayalil[1,4], Peter Müller-Buschbaum[2], and Stephan V. Roth[1,5] — [1]DESY, Hamburg, Germany — [2]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [3]CPP, Venlo/Poing, Netherlands/Germany — [4]UPES, India — [5]KTH, Department of Fibre and Polymer Technology, Stockholm, Sweden

Colloidal polymer latexes are used in ink-jet printing to form a pigment stabilizing layer on top of the cellulose layer. The latex film formation (LFF) is influenced by humidity, temperature, minimum film formation temperature (MFFT), and glass transition temperature (T_g). Exceeding MFFT polymer colloids begin to deform and further heating above the T_g polymers interdiffuse and coalesce into a homogeneous coating layer. Here we investigate cellulose nanofibrils (CNF) thin films coated with polystyrene colloids (diameters ranging from 100 to 500 nm) and commercially available polymeric colloids with different MFFT (Neocryl A639 and A1127). The samples were prepared by spray coating at temperatures below and above their T_g. Scanning electron microscopy revealed the size and shape of the colloids. Grazing incidence small angle scattering data shows contributions of spherical form factors from the colloids with respective diameters, which changes upon heating. 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 46.52 Thu 9:30 P5

A DFTB Pseudoatom-Based Fragmentation Strategy — •Kevin Mächtel — Karlsruher Institut für Technologie, Institut für Physikalische Chemie, Karlsruhe, Germany

Theoretical investigations of charge transport mechanisms in large molecular systems often rely on efficient fragmentation strategies, to reduce computational costs. In conventional approaches, link atom fragmentation has been used for this purpose, but pseudoatom approaches offer a more versatile alternative. They enable more efficient molecular fragmentation, simplifying the overall fragmentation process. In this study, we develop a novel density functional tight-binding pseudoatom fragmentation scheme for complex molecular systems. We tested our approach on 9,10-di(quinolin-6-yl)phenanthrene and demonstrated strong agreement with the established link atom method.

CPP 46.53 Thu 9:30 P5

Benchmarking the Transferability of Machine Learning Interatomic Potentials for Polymers — •Mirko Fischer and Andreas Heuer — Institute for Physical Chemistry, University of Münster, Corrensstraße 28/30, 48149 Münster

Machine Learning Interatomic Potentials (MLIPs) enable molecular dynamics (MD) simulations with nearly quantum-chemical (QM) accuracy and have been successfully applied to various molecular systems. However, their systematic application to polymer systems has not yet been explored. A key challenge arises from the large molecular size, which makes QM reference calculations for the training data computationally demanding. Moreover, relaxation processes and diffusive behavior in polymers require long simulation times, making a direct comparison between MLIP-based and *ab initio* MD simulations infeasible.

In this study, we first train Atomic Cluster Expansion (ACE) potentials for small oligomers on MD reference data, thereby circumventing the need for expensive QM reference simulations and enabling long, cost-efficient MD trajectories. We then benchmark the transferability of the trained ACE potentials to longer polymer chains with respect to density, structural, and dynamic properties. The insights gained allow us to identify an optimal oligomer chain length that balances training cost and transferability. Based on this, we can efficiently train a QM-accurate potential for polymers on QM reference data in a second step.

CPP 46.54 Thu 9:30 P5

Fourth-Generation High-Dimensional Neural Network Potentials for Molecular Chemistry in Solution — •Djamil A. A. Maouene[1,2], Moritz R. 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 potentials have become essential tools in chemistry and materials science, offering accurate, efficient representations of high-dimensional potential energy surfaces for atomistic simulations. Here we compare two generations of high-dimensional neural network potentials (HDNNPs) 2G-HDNNPs and 4G-HDNNPs in their ability to model organic molecules in aqueous solution. 2G-HDNNPs perform well for systems dominated by local interactions because they rely on descriptors of the immediate atomic environment. However, in cases of long-range charge transfer 4G-HDNNPs provide a more reliable description by explicitly accounting for charge redistribution in the system as a function of its global structure. We illustrate these differences for organic molecules in water.

CPP 46.55 Thu 9:30 P5

Controlling porosity in supraparticles: A simulation study using spherical and rod-shaped particles — •Kritika Kritika[1,2], Mayukh Kundu[3], Michael Howard[3], and Arash Nikoubashman[1,2] — [1]Leibniz Institute of Polymer Research Dresden, Germany — [2]Institute of Theoretical Physics, TU Dresden, Germany — [3]Department of Chemical Engineering, Auburn University, Auburn, USA

Supraparticles (SPs) are large assemblies of smaller colloidal particles, whose properties can be tuned by modifying, e.g., the chemistry, shape, and size of the individual constituent particles and their arrangement within the SP. SPs can be formed through droplet drying, a process commonly observed in both everyday life and industrial applications, such as spray drying and printing. Porous SPs are of particular interest, since their high surface area and tunable pore size distribution make them ideal materials for catalysis, photonics, and adsorption applications. In this computational study, we explore the drying-induced formation of SPs made from spherical and rod-shaped particles. After drying, we selectively remove one of the particle components, leaving behind a highly porous SP. The initial volume fraction between spherical and rod-shaped particles plays a key role in shaping the porosity within the SP, while increasing the aspect ratio of the rods further amplifies the porosity of the SPs. Additionally, we observed that slower drying leads to a distinct increase in average pore size.

CPP 46.56 Thu 9:30 P5

Demystifying the decoupling of conformation and phase behavior in PNIPAM cononsolvency — •Ved Mahajan and Nico F. A. van der Vegt — Department of Chemistry, Technical University of Darmstadt

Cononsolvency describes the situation in which a polymer becomes insoluble in a mixture of two individually good solvents. PNIPAM, a widely studied thermoresponsive polymer, exhibits a strong coupling between its temperature-driven coil-globule transition and its phase behavior at low methanol concentrations; however, these two responses decouple as the methanol content increases. In this work, we use a minimal physical model, a hydrophobic polymer in water-methanol mixtures, that reproduces these key experimental observations. Despite its simplicity, the model captures both the emergence of cononsolvency and the crossover from coupled to decoupled thermal responses. At low methanol concentration, the polymer conformation remains temperature dependent, whereas at high methanol concentration, it becomes insensitive to temperature. In contrast, hydrophobic aggregation consistently strengthens with increasing temperature. Together, these results reveal a simple mechanism for the observed decoupling: the differing temperature sensitivities of polymer collapse and hydrophobic aggregation, both rooted in the hydrophobic effect.

CPP 46.57 Thu 9:30 P5

Molecular insights into the anion-dependence of the double-layer capacitance — •Richard Schömig[1], Xuqiang Xu[2], Jana Zaumseil[2], and Alexander Schlaich[1] — [1]Institute for Physics of Functional Materials, Hamburg Technical University, Hamburg — [2]Institute for Physical Chemistry, Heidelberg Universiy, Heidelberg

Mixed ionic-electronic conductors are promising candidates for organic electrochemical transistors (OECTs). Single-walled carbon nanotubes (SWCNTs), a key example, show transconductance and capacitance responses that are strongly influenced by the properties of the surrounding electrolyte [1]. To uncover the mechanisms governing this behavior, we perform molecular dynamics simulations of aqueous electrolytes containing ions of different sizes and concentrations under varying applied potentials. As a simplified model for the more complex SWCNT electronic structure, we here use graphene as the electrode material. Employing atomistic constant-potential simulations, we investigate how these electrolyte characteristics shape the interfacial structure and differential capacitance. Analysis of the hydrogen-bond network and associated free-energy changes highlights the central role of ion size in determining interfacial behavior.

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CPP 46.58 Thu 9:30 P5

Computing static and dynamic structure in colloidal models for solutions of globular proteins — •Sven Köbler — Institute of Applied Physics, University of Tübingen, Tübingen, Germany

Crowded solutions of globular proteins are commonly probed using neutron and X-ray scattering to obtain static and dynamic structure factors across a broad range of concentrations. Complementary insight can be gained from Brownian dynamics simulations based on coarse-grained colloidal models; however, extracting meaningful scattering observables particularly dynamic structure factors which requires fast and scalable trajectory analysis tools. We present an efficient computational framework for calculating both static structure factors $S(q)$ and intermediate scattering functions $F(q,t)$ directly from simulation trajectories. Our tools are highly optimized and build with CUDA compatibility to exploit computing speeds of GPUs. Its performance is demonstrated using binary colloidal models designed to mimic mixtures of bovine serum albumin (BSA) and ferritin. The resulting simulated scattering functions are compared with experimental X-ray photon correlation spectroscopy data.

CPP 46.59 Thu 9:30 P5

Dynamic properties of telechelic polyisobutylene with sticker ends: atomistic vs. coarse-grained molecular dynamics simulation — •Anastasiia Pivovarova and Viktor Ivanov — Martin-Luther-University Halle-Wittenberg, Halle (Saale), Germany

Modeling associating polymer networks, such as telechelic polyisobutylene (PIB) with barbiturate stickers, requires not only constructing accurate coarse-grained (CG) interaction potentials but also resolving the inherent problem of accelerated dynamics. This challenge becomes evident when comparing Green-Kubo viscosity calculations across different levels of resolution. Atomistic simulations of PIB with barbiturate end groups reproduce the expected rheological behavior of associating systems, yielding a viscosity of about 3.32 Pa*s. In contrast, CG simulations performed for pure PIB used as an initial step toward a full CG description of the telechelic system show a pronounced reduction in viscosity, reflecting substantially faster dynamics intrinsic to coarse-graining. These observations illustrate how dynamical acceleration can dominate the predicted viscoelastic properties even when structural features are reproduced, underscoring the need for systematic strategies to recover realistic dynamical behavior in CG models of associating polymer networks.

CPP 46.60 Thu 9:30 P5

Density of states in monodisperse and polydisperse hard disks: Concentration dependent SAMC estimation — •Viktor Ivanov, Joram Heimbold, Malte Kautzsch, and Timur Shakirov — Martin-Luther-University Halle-Wittenberg, Halle (Saale), Germany

We propose a new variant of flat-histogram Monte Carlo, where the density of particles is the control parameter for the density of states and the visiting histogram. We simulate a system of point particles with zero diameter. The square of the minimal interparticle distance, r_{min}^2, is used as the control parameter for a macrostate. The density of states and the visiting histogram depend on r_{min}^2 and are updated at each step of the algorithm according to the usual SAMC rules. For a microstate (particilar configuration of particles) with a given value of the minimal distance between particles r_{min} one can replace the points with the hard disks of the diameter r_{min} or smaller, which corresponds to a system with a specific particle density. We apply this algorithm to 2d systems of monodisperse and polydisperse hard disks (with diameter distributions $1/d^2$) and study the density driven crystallization transition. For monodisperse hard disks the transition from the liquid to the hexatic phase proceeds via a first-order like pseudo-phase transition, whereas the transition from the hexatic to the crystalline phase is continuous. With increasing polydispersity, crystallization is significantly suppressed, such that no transition to the crystalline phase is observed for a 10% variation in particle radii.

CPP 46.61 Thu 9:30 P5

Benchmarking bond dissociation energies with plane-wave pseudopotential and Gaussian all-electron methods — •Yue Pan[1], Jochen Heil[2], Ali Karimi[2], and Arash Mostofi[1] — [1]Imperial College London, South Kensington Campus, London, SW7 2AZ, UK — [2]Continental Reifen Deutschland GmbH, Hanover, Germany

Accurate homolytic bond dissociation energies (BDE) are important for understanding bond breaking processes in molecules. They are also frequently used to benchmark the accuracy of different method for electronic-structure calculations. Most calculations of BDE focus on datasets of small gas-phase molecules and, accordingly, are carried out with localised-orbital methods, while systematic comparisons to periodic plane-wave DFT remain scarce. This is relevant for modelling interfacial failure processes in hybrid systems such as polymer nanocomposites, in which molecules are attached to inorganic surfaces, and it becomes less clear which method is more suitable from the perspective of accuracy and efficiency.

In this work, we benchmark the performance of two widely used approaches for DFT calculations, namely the plane-wave basis pseudopotential methods and Gaussian all-electron methods. We use C*C bond dissociation in gas phase hydrocarbons and surface-anchored molecules. We then compare our calculated BDEs with theoretical results obtained from highly accurate quantum chemistry methods and experimental values. Our work represents a step towards a better understanding of bond breaking and interfacial failure in materials.

CPP 46.62 Thu 9:30 P5

Continuum Modeling of Light-Matter Interaction in Polymer-Based Hollow-Core Optical Fibers with Different Geometrical Configurations — •Zehra Gizem Mutlay and Mustafa Ordu — UNAM - National Nanotechnology Research Center and Institute of Materials Science and Nanotechnology, Bilkent University, Ankara 06800, Türkiye

Recent studies have demonstrated that nested hollow-core optical fibers (HCFs) can achieve attenuation below 0.1 dB/km while maintaining broad transmission bandwidths. This performance demonstrates the promise of air-guided waveguides as alternatives to conventional solid-core optical fibers. In this work, we perform continuum modeling based on the finite-element method to investigate light interaction with polymer in HCFs by implementing three- and four-tube cladding structures. The analysis involves designs with and without nested elements and supporting bars. Our comparative investigation includes silica- and polymer-based structures to identify how intrinsic material properties and geometrical parameters influence mode confinement, optical loss, and transmission behavior. The findings show that even minor changes in geometry or material composition significantly influence light propagation, which underlines the sensitivity of optical guidance to light-material interaction. This study establishes a continuum-based framework for analyzing electromagnetic behavior in polymer systems and lays the groundwork for developing 3D-printed polymer-based hollow-core fibers with reduced attenuation for future applications in optical and materials physics.

CPP 46.63 Thu 9:30 P5

General Polarization Dependent Dynamic Light Scattering Using the Dynamic Mueller Matrix — •Reinhard Sigel — Independent Scientist, Markdorf, Germany

The Mueller Matrix for a general description of the polarization transfer of an optical system is combined with Dynamic Light Scattering (DLS) [1]. Azzam's procedure [2] based on two rotated quarter wave plates is combined with photo correlation measurements to detect the Dynamic Mueller Matrix, which contains all possible polarization dependent correlation functions. The related Siegert relation is derived. Applications are dynamic ellipsometric light scattering [3] experiments on soft colloidal particles and 3D correlation ellipsometry [4] experiments on soft interfaces [5].

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CPP 46.64 Thu 9:30 P5

Versatile X-Ray Reflector Extension Setup for Grazing-Incidence Experiments for Liquid Surface Study at the Beamline P03/PETRA III — •Jan Rubeck, Andrei Chumakov, and Matthias Schwartzkopf — DESY, Notkestr. 85, 22607 Hamburg, Germany

Existing beamlines for in situ GISAXS on liquids are either limited in angular range or incompatible with the large sample-detector distance required for submicron resolution. We present a low-cost, easily assembled beam-tilting extension for synchrotron-based ultra-small-angle X-ray scattering (USAXS) facilities, enabling grazing-incidence (GI-) and transmitted scattering (GIUSAXS, GTUSAXS) studies on liquid surfaces. The setup is compatible with standard USAXS beamlines and requires only 0.5 m of space at the sample stage. It allows X-ray beam incidence angles of up to 0.6° at the liquid surface, equal to twice the angle of incidence on a reflector and below its critical angle of reflector materials, and provides access to a q-range of approximately 0.003-0.5 nm^{-1}. The system was tested at P03 beamline (DESY) using polystyrene nanoparticles, self-assembled at the air/water interface. The proposed scheme enables selective depth profiling and expands the research capabilities of existing SAXS synchrotron facilities for in situ studying submicron nanostructured objects at liquid surfaces under GI-geometry, combined also with GIWAXS and TXRF techniques. https://doi.org/10.1107/S1600577525003431

CPP 46.65 Thu 9:30 P5

Hybrid field coupling in nanoscale infrared spectroscopic imaging of nano-structured soft matter — •Sharon Xavi[1], Mashiat Huq[1], Matthias Zeissberger[2], Daniela Täuber[1,2], and Christin David[1,3] — [1]Friedrich Schiller University Jena, 07743 Jena — [2]Leibniz Institute of Photonic Technology, 07745 Jena — [3]University of Applied Sciences, 84036 Landshut, Germany

Anisotropic intensity distributions are frequently observed on nanostructured surfaces in the emerging field of nanoscale infrared (IR) spectroscopic imaging methods, including mid-IR scattering scanning optical nearfield microscopy (IR-sSNOM) and methods combining mid-IR illumination with mechanical detection using atomic force microscopy (AFM-IR). Such methods bridge the gap between high-resolution structural imaging in electron and atomic force microscopy and chemical imaging in conventional far-field IR spectroscopy by overcoming the limitations of optical diffraction in far-field IR spectroscopic imaging. In the mid-IR spectral region, the hybrid field coupling of the incident field with a polymer nanosphere and a metallic AFM probe is nearly as strong as the plasmonic coupling in case of a gold nanosphere [Anindo et al., J. Phys. Chem. C, 2025, 129, 4517]. We modeled this hybrid field coupling on varied nanostructured surfaces to enhance the understanding of the observed anisotropies and contribute to the development of advanced applications of these methods [Ali et al. Anal. Chem., 2025, 97, 23914].

CPP 46.66 Thu 9:30 P5

Learn how to switch off: In-silico Modelling of Thermal Ring-closing Process in Spiropyran Derivatives — •Bowen Cheng, Robert Strothmann, Hendrik Heenen, and Karsten Reuter — Fritz-Haber-Institut der MPG, Berlin, Germany

Spiropyran (SP) and its derivatives undergo a ring-opening reaction via UV radiation and a ring-closing reaction in thermal conditions, making them excellent candidates for photoswitches. One key aspect that governs the sensitivity of such photoswitches is the rate of the thermal ring-closing process. A main challenge in modelling this process is the existence of various thermally accessible conformers, leading to a complex reaction network.

In this study, we highlight a combined workflow using machine-learned interatomic potential (MLIP) and a microkinetics model (MKM) to address this. With a fine-tuned MACE-OFF24 foundation model, we predict different transition state energies within the reaction network using the nudge elastic band method, and correlate these energies to experimental observations using the MKM.

Our workflow can be migrated between different SP derivatives to reveal the effect of functional group decorations. Our findings demonstrate the potential of using MLIPs to predict transition states and enable larger-scale studies of complex reaction networks. We also aim to condense our workflow as a new descriptor for *in-silico* screening in future spiropyran photoswitch design.