

CPP 15: Poster I

Wetting on Adaptive Substrates (1-3), Gels, Polymer Networks and Elastomers (4-10), Biopolymers, Biomaterials and Bioinspired Functional Materials (11-16), Complex Fluids and Colloids, Micelles and Vesicles (17-19), Charged Soft Matter, Polyelectrolytes and Ionic Liquids (20-23), Energy Storage and Batteries (24-33), Responsive and Adaptive Polymers (34-38), Wetting, Fluidics and Liquids at Interfaces and Surfaces (39-41), Emerging Topics in Chemical and Polymer Physics, New Instruments and Methods (42-45)

Time: Monday 18:00–20:00

Location: Poster C

CPP 15.1 Mon 18:00 Poster C

Synthesis of diblock copolymer brush layers to control the adaptation time to water — ●BENJAMIN LEIBAUER¹, ANDRES DE LOS SANTOS PEREIRA², OGNEN POP-GEORGIEVSKI², HANS-JÜRGEN BUTT¹, and RÜDIGER BERGER¹ — ¹Max Planck Institute for Polymer Research, Mainz, Germany — ²Institute of Macromolecular Chemistry CAS, Prague, Czech Republic

The Youngs model describes the wetting behavior of an ideal surface. Recently, Butt et al. presented an adaptation model, which connects adaptation processes of the surface to dynamic contact angles [1]. In order to test the adaptation model, we used a tilted plate setup, which allows measuring velocity dependent contact angles. The applicability of the adaptation model was experimentally verified by using surfaces made of statistical copolymers. In a next step, we synthesize polymer surfaces with the aim to control the adaptation time scale upon wetting and dewetting systematically. We used the surface-initiated atom transfer radical polymerization ATRP to selectively synthesize diblock copolymer brushes. We prepared poly(2-hydroxyethyl methacrylate) (PHEMA) as a hydrophilic block from the surface and we grafted polystyrene (PS) or Poly(1-hexyl methacrylate) (PEtHexMA) as hydrophobic block on top of the PHEMA block [2]. By regulating the architecture and thickness of the polymer brush we tune the wetting properties systematically. In addition, we control the adaptation time of polymer brush surfaces by changing the drop-sample temperature.

CPP 15.2 Mon 18:00 Poster C

Effect of Low-Pressure Plasma-Treated Hydrophobic Surfaces on Sliding Water Drop Charge — ●FAHIMEH DARVISH¹, SAJJAD SHUMALY¹, XIAOMEI LI¹, YUN DONG¹, MOHAMMADREZA KHANI², GEORGE FLOUDAS¹, DORIS VOLLMER¹, and HANS-JÜRGEN BUTT¹ — ¹Max Planck Institute for Polymer Research, Ackermannweg 10, D-55128, Mainz, Germany — ²Laser and Plasma Research Institute, Shahid Beheshti University, 1983963113 Tehran, Iran

Slide electrification is the spontaneous separation of electric charges at the rear of water drops sliding over hydrophobic surfaces. This research shows how plasma-treated surfaces affect water sliding electrification. Plasma treatment reduced the contact angles and drop charging. Conversely, 64% higher drop charging was achieved using sheath treatment than to pristine sample. Based on the zeta potential, Kelvin potential, XPS measurements, we attributed the effects of plasma to two processes. First, plasma chemically changed the organic topmost layer, e.g., by oxidation and etching. Secondly, charges were deposited in the topmost layer. The surface top layer charges were less negative after sheath and more negative after bulk plasma treatment. The plasma-treated effect was neutralizable. Despite the presence of a PFOTS thin layer, we discovered that the plasma effect on the substrate governs slide electrification remotely, by using different plasma powers during glass activation prior to silanization. However, the surface roughness and contact angles remained unchanged. We demonstrated that both sheath and plasma treatment increase or decrease slide electrification to almost zero while keeping other surface properties constant.

CPP 15.3 Mon 18:00 Poster C

Partially wetted PNiPAAm brushes responses to different atmospheres — ●SIMON SCHUBOTZ^{1,2}, PETRA UHLMANN¹, ANDREAS FERY^{1,2}, JENS-UWE SOMMER^{1,2}, and GÜNTER K. AUERNHAMMER¹ — ¹Leibniz-Institut für Polymerforschung Dresden e.V., 01069 Dresden, Germany — ²Technische Universität Dresden, 01069 Dresden, Germany

In our study, we focused on the partial wetting of co-nonsolvent polymer brushes and the dynamics of a three-phase contact line moving over such brushes. We performed wetting experiments in different atmospheres and used an ellipsometer to measure the brush's thickness to understand the impact of the atmosphere on the brush. Our

findings show that PNiPAAm brushes exhibit a memory effect when depositing drops consecutively at the same position. The subsequent drops adapt the brush and change the drop's wetting behavior. In further wetting experiments, we measured water drops in an ethanol-saturated atmosphere on PNiPAAm brushes. The measurements show that an ethanol-enriched atmosphere strongly affects the memory effect reversibly. We present strategies to counter the mixing between the atmosphere and the drop.

[1] Schubotz, S., et al., Memory effects in polymer brushes showing co-nonsolvency effects. *Advances in Colloid and Interface Science*, 2021. 294: p. 102442.

[2] Schubotz, S., et al., Influence of the Atmosphere on the Wettability of Polymer Brushes. *Langmuir* 2023, 39, 14, 4872-4880

CPP 15.4 Mon 18:00 Poster C

Simulations of Weak Polyelectrolyte Hydrogels with Divalent Counterions — ●DAVID BEYER¹, PETER KOŠOVAN², and CHRISTIAN HOLM¹ — ¹Institute for Computational Physics, University of Stuttgart, D-70569 Stuttgart, Germany — ²Department of Physical and Macromolecular Chemistry, Charles University, 128 00 Prague 2, Czechia

We use computer simulations to study a coarse-grained model of a weak (pH-responsive) polyelectrolyte hydrogel coupled to a reservoir of small ions, including a 2:1 salt. To model the ionization equilibrium of the weak groups and the exchange of small ions with the reservoir, we make use of the recently developed Grand-Reaction Monte-Carlo method (G-RxMC). We determine the free swelling equilibrium for different concentrations of the divalent salt and pH values of the reservoir. Our simulations show that even a small amount of divalent salt can significantly inhibit the swelling of the gels due to the preferential uptake of divalent ions into the gel, effectively suppressing the swelling for salt concentrations above 10mM. Interestingly, we observe that the gels exhibit a second swelling step at very high pH-values, which is in stark contrast to the behaviour in a monovalent salt solution. This behaviour arises due to an interplay of the ion partitioning and electrostatic interactions.

CPP 15.5 Mon 18:00 Poster C

On the swelling of polymer network strands — ●MICHAEL LANG and REINHARD SCHOLZ — Leibniz Institut für Polymerforschung Dresden, Hohe Straße 6, 01069 Dresden, Germany

Large scale computer simulations are employed to analyze the conformations of network strands in polymer networks at preparation conditions and at swelling equilibrium. Network strands in end-linked model networks are weakly stretched and partially swollen at preparation conditions as compared to linear polymers at the same polymer volume fraction. For increasing overlap of the chains, network swelling causes a non-ideal chain size $\propto N^\nu$ characterized by an effective scaling exponent ν approaching 7/10 on intermediate length scales. The chain size in a network consists of a fluctuating and a time average "elastic" contribution. The elastic contribution swells essentially affinely, whereas the swelling of the fluctuating part lies between the expected swelling of the entanglement constraints and the swelling of non-cross-linked chains in a comparable semi-dilute solution. The total swelling of chain size results from the changes of both fluctuating and non-fluctuating contributions.

CPP 15.6 Mon 18:00 Poster C

Impact of Curing dynamics on the Microstructure and Properties of Epoxy Thermosets — ●SAMPANNA PAHI¹, CHRISTIAN WICK¹, and ANA-SUNČANA SMITH^{1,2} — ¹PULS Group, Institute for Theoretical Physics, IZNF, FAU Erlangen-Nürnberg, 91058 Erlangen, Germany — ²Group of Computational Life Sciences, Ruder Bošković Institute, 10000 Zagreb, Croatia

Epoxy resins, essential in manufacturing, require an understanding of their curing kinetics for optimal properties. This study, using epoxy systems modeled with the recently developed Block Chemistry force-field, examines the impact of reaction kinetics on polymer chain formation. We employed a QM/MM methodology to optimize local reaction kinetics at the molecular level, enhancing curing precision. Quantum analyses and simulations showed that secondary reactions prompt early branching, while primary reactions lead to linear growth before crosslinking. Further, incorporating an isomeric mixture in the pre-polymer model resulted in denser packing, mirroring experimental densities. The study also includes loop size distribution analysis within the polymer matrix, crucial for assessing material rigidity and linking microstructural characteristics to macroscopic properties, enriching our understanding of the molecular structure-material behavior relationship in thermoset polymers.

CPP 15.7 Mon 18:00 Poster C

Probing the mechanical properties of core-shell-like PNIPAM microgels — ●MANMEET KAUR SODHI and REGINE VON KLITZING — Technische Universität Darmstadt

Stimuli-responsive liquid foams have a huge impact in terms of both fundamental research and technical applications such as catalysis, food technology, waste, since they allow a foam rupture on demand triggered by external stimuli. Temperature responsive. PNIPAM microgels (radii in the range of several 100 nm) are well-known to stabilize foams, and they have a volume phase transition temperature (VPTT) of about 32°C, i.e. below this temperature water is a good solvent and the microgels are swollen. By crossing the VPTT water becomes a poor solvent and the microgels shrink, their stiffness controlled by the degree of crosslinking, and their ability to stabilize liquid foams. This study focuses on the fundamental question of how important the softness/stiffness of the microgels is to stabilize foams. To achieve this, the mechanical properties of negatively charged individual microgel particles at solid/air interface as well as solid water interface has been studied. The data is complemented with the dynamic light scattering which not only gives us the quantitative understanding of including their hydrodynamic radius and polydispersity but also allows us to understand the behaviour of these microgels at lower critical transition temperature.

CPP 15.8 Mon 18:00 Poster C

Study of core-shell nanogels via molecular computer simulations — ●ALLA DOBROSERDOVA¹ and SOFIA KANTOROVICH² — ¹Ekaterinburg, Russia — ²University of Vienna, Vienna, Austria

Nanogels represent a new class of smart materials. They consist of a permanently cross-linked network of dilute polymers. We consider core-shell nanogels, where the polymers in the shell can have different lengths. Considering some magnetic core particles, we make nanogels with a magnetic core. We can also consider the magnetic particles of the shell along with the magnetic particles of the core. We study how the intensity of the magnetic dipole-dipole interaction affects the magnetic and structural properties of the nanogel.

CPP 15.9 Mon 18:00 Poster C

Influence of single particle softness on the elasticity of microgel covered interfaces — ●CARINA SCHNEIDER, SEBASTIAN STOCK, JOANNE ZIMMER, and REGINE VON KLITZING — Department of Physics, TU Darmstadt, Hochschulstraße 8, 64289 Darmstadt

Softness strongly influences the behavior of microgels (MG) adsorbed at liquid interfaces. Therefore, it is fundamental to understand and quantify its effect via the microscopic scale on the macroscopic layer. For this purpose, we spread homogeneous and heterogeneous poly-NIPAM MGs at the air-water interface of a Langmuir trough, and determine the compression isotherms. This enables the calculation of the compression dependent elasticity. We control the stiffness of the MG particles by varying the cross-linker density. To artificially increase the stiffness of the single particles we add latex particles to the system. Simultaneously, we observe the lateral structure formation, by transferring and subsequently scanning the particle layer on a Silicon wafer using atomic force microscopy. The elasticity of the particle layer at the interface exhibits a maximum as a function of the surface pressure. Counterintuitively, the maximum value increases with decreasing stiffness of the particles.

CPP 15.10 Mon 18:00 Poster C

How Ultrasound Accelerates Microgel Adsorption Kinetics at Liquid Interfaces — ●LUCA MIRAU¹, SEBASTIAN STOCK¹,

AMIN RAHIMZADEH¹, SONJA WISMATH², MATTHIAS RUTSCH², MARIO KUPNIK², and REGINE VON KLITZING¹ — ¹Soft Matter at Interfaces, Institute for Condensed Matter Physics, TU Darmstadt, Hochschulstraße 8, 64289 Darmstadt — ²Measurement and Sensor Technology, TU Darmstadt, Merckstraße 25, 64283 Darmstadt

Poly-N-isopropylacrylamide (PNIPAM) based microgels (MGs) are surface-active and offer great opportunities as stabilizers of emulsions and foams. Due to their thermosensitive response the MGs enable also destabilization on demand. However, emulsion formation implies energy input by stirring or ultrasonication. To understand this formation process, it is important to understand the interfacial adsorption of the MGs. A fast trigger to affect the adsorption process is given by ultrasonication. The present study shows the effect of ultrasound on the adsorption kinetics of PNIPAM MGs at the water-oil interface monitored by drop shape tensiometry. The adsorption kinetics of MGs accelerates with increasing ultrasonication intensity. The variation of different parameters, such as ultrasonic frequency, MG crosslinker density, concentration, phase composition and temperature, indicates that both acoustic streaming as well as ultrasound induced deswelling of MGs due to breakage of hydrogen bonding cause this acceleration.

CPP 15.11 Mon 18:00 Poster C

Water-based lignin colloidal particle and cellulose nanofibrils hybrid films with UV-block ability by spray deposition — ●SHOUZHENG CHEN^{1,2}, CONSTANTIN HARDER^{1,3}, IULIANA RIBCA⁴, YUSUF BULUT^{1,3}, PETER MÜLLER-BUSCHBAUM^{3,5}, MATS JOHANSSON⁴, JULIEN NAVARRO², and STEPHAN ROTH^{1,4} — ¹Deutsches Elektronen-Synchrotron DESY, Notkestraße 85, 22607 Hamburg, Germany — ²Institute of Wood Science, Universität Hamburg, 20146 Hamburg, Germany — ³Physik-Department, Lehrstuhl für Funktionelle Materialien, Technische Universität München, James-Frank-Strasse 1, 85748 Garching, Germany — ⁴KTH Royal Institute of Technology, Department of Fibre and Polymer Technology, 10044 Stockholm, Sweden — ⁵Technische Universität München, Heinz Maier-Leibnitz Zentrum (MLZ), Lichtenbergstr. 1, 85748 Garching, Germany

Cellulose nanofibrils (CNFs) have hydrophilic interfaces and establish self-entangled networks, making them natural biopolymer substrate materials. Lignin is a natural UV-shielding material due to its high content of phenolic groups. We prepared hybrid films from CNFs and water-based colloidal lignin particles (CLP) by spray deposition using layer-by-layer stacking as well as premixing. The resulting nanostructures were correlated with water imbibition, UV shielding ability and visible light transparency of the films. We found that CNF acts as a directing agent in the premixed system to dominate the uniform distribution of CLP in the thin film, which allows to optimizing the visible light transparency while maintaining the UV-shielding ability.

CPP 15.12 Mon 18:00 Poster C

Coarse-grained modeling of nucleic acid coacervates — ●SOUMEN DE KARMAKAR and THOMAS SPECK — Institute for Theoretical Physics IV, University of Stuttgart, Heisenbergstr. 3, Stuttgart 70569, Germany

Membraneless biomolecular condensates, consisting of several components such as multivalent proteins, RNA, and DNA, are ubiquitous in cellular environments. Recent in vitro studies demonstrate the condensation of single-stranded DNA (ssDNA) [1] or RNA [2] with increasing temperature reminiscent of lower critical solution temperatures (LCST) in thermoresponsive polymers. The observed LCST suggests that entropic interaction play a significant role in addition to the conventional enthalpy dominated interactions in other biomolecular condensates. To shed more light on the possible mechanism of LCST in the single component biomolecular condensates, we employ a minimal coarse-grained model and implicitly incorporating background ions that are essential for the formation of condensates. Our numerical study exhibits phase separation in line with the experiments of ssDNA and RNA. Our results provide insight into the design of hierarchical structures composed of several components of biomolecular assemblies.

[1] Merindol et al., Nat. Nanotech. 13, 730-738 (2018). [2] Wadsworth et al., Nat. Chem. (2023), 1755-4349.

CPP 15.13 Mon 18:00 Poster C

Are alginate - pullulan sponge-like composites suitable to help heal a skin wound? — ●EMMA BOBU¹, KLARA MAGYARI², ALEXANDRA DREANCA³, and MONICA BAI⁴ — ¹Doctoral School in Physics, BBU, Cluj, Romania — ²Interdisciplinary Research Institute on Bio-Nano-Sciences, BBU, Cluj, Romania — ³Faculty of Veterinary Medicine, UASVM, Cluj, Romania — ⁴Faculty of Physics, BBU, Cluj,

Romania

A major health issue that needs to be addressed is external bleeding, which occurs every day in people around the world, due to accidents or surgery. Normally, the body reacts immediately to stop the bleeding and heal the wound, but there are deep and uncontrolled bleedings, and the body needs external help for hemostasis. First, we need to absorb the blood and keep the wound moist. The natural polymers chosen for this purpose are calcium alginate and pullulan, because of their good swelling properties and biocompatibility. Therefore, the final material CAlg-Pll has a sponge-like structure that absorbs the fluid to increase the viscosity and concentration of the blood in the wound while keeping the environment moist. That stops the bleeding and prevents big losses. The samples were synthesized and characterized by XRD, FT-IR, and Raman spectroscopy. For the in vitro tests, the samples were immersed in simulated body fluid to see the bioactivity, swelling ratios, and degradability and were again investigated by XRD, FT-IR, Raman spectroscopy, and SEM. The next assay was the evaluation of coagulation rate and time. The materials are stable in biological fluid, absorb the excess fluid in the wound, and are nontoxic.

CPP 15.14 Mon 18:00 Poster C

In situ X-ray studies of temperature-controlled structures in polylactic acid — ●REGINE BOLDT¹, LAURA MEINIG¹, ERIC EUCHLER¹, ANNA KATHARINA SAMBALE¹, KAI UHLIG¹, MATTHIAS SCHWARTZKOPF², and MARKUS STOMMEL^{1,3} — ¹Leibniz-Institut für Polymerforschung, Dresden, Germany — ²Deutsches Elektronen Synchrotron DESY, Hamburg Germany — ³TUD Dresden University of Technology, Dresden, Germany

Poly(lactic acid) (PLA) is a frequently used biopolymer. It is used, for example, as films for food packaging and in agriculture in the form of mulch films. PLA is also used in medicine as implant or suture material. To precisely control application-specific material properties, a better understanding of the formation of relevant structures and identifying influential process parameters is essential. In this work, we focused on investigating the formation of crystalline structures at different temperatures. It is known that PLA crystallizes in two different modifications depending on the temperature: (i) the metastable α' -phase and (ii) the thermodynamically stable α -phase. We investigated the formation of the different phases using in situ synchrotron X-ray scattering experiments. Using a newly developed experimental setup, PLA was heated to melt and then cooled to different temperatures and monitored the crystallite formation as a function of time. As a result, new insights into the process-controlled formation of α' - and α -phases were achieved.

CPP 15.15 Mon 18:00 Poster C

Computing thermodynamic and kinetic properties for the primary reactions during sucrose pyrolysis — ●OLIVER HEYMER, JAKOB KRAUS, and JENS KORTUS — Institute of Theoretical Physics, TU Bergakademie Freiberg, Leipziger Str. 23, D-09599 Freiberg, Germany

The thermodynamic properties of the hydrolysis of sucrose as well as the formation of anhydrofructose were investigated at the gold-standard CCSD(T)-level. This level of accuracy enables the comparison of results obtained from perturbation theory and density functional theory. By combining climbing image nudged elastic band calculations with subsequent transition state optimizations, it was possible to report minimum energy paths and highest-energy transition states for both reactions.

At temperatures ranging from 0 to 1500 K, it was found that the hydrolysis reaction is both exothermic and exergonic. For the formation of anhydrofructose, endothermic behavior in the same temperature range was reported. Additionally, this reaction is endergonic from 0 to 450 K and becomes exergonic reaching a temperature of 500 K.

The identification of transition states allowed for an estimate of activation energies and therefore standard reaction rate constants. Lastly, it was possible to study interesting mechanistic aspects that occur during the reactions.

CPP 15.16 Mon 18:00 Poster C

Conformation of star-like molecular brushes with amphiphilic diblock copolymer side arms — ●WENQI XU¹, LAURA FIETZKE², FEIFEI ZHENG¹, MONTSERRAT ROMAN-QUINTERO¹, PEIRAN ZHANG¹, DMYTRO SOLOVIOV³, RAINER JORDAN², and CHRISTINE M. PAPADAKIS¹ — ¹TUM School of Natural Sciences, Technical University of Munich, Garching, Germany — ²Faculty of Chemistry and Food Chemistry, Technical University of Dresden, Germany — ³EMBL at

DESY, Hamburg, Germany

Poly(2-oxazoline)s are considered versatile platforms for biomedicine thanks to their biocompatibility and rich architectural possibilities. While linear brushes with amphiphilic copolymer sidearms from poly(2-oxazoline)s have been amply investigated, studies on star-like brushes are still scarce. In the present work, we investigate molecular brushes, in which diblock copolymers from hydrophilic methyl(2-oxazoline) and hydrophobic *n*-butyl(2-oxazoline) are grafted onto star-shaped poly(methyl methacrylate) backbones having functionalities ranging from 2 to 5. The size and shape of the star brushes were investigated in dilute aqueous solutions using dynamic light scattering and synchrotron small-angle X-ray scattering. Our results show that the star brushes are ellipsoids whose degree of elongation depends on the functionality and the relative length of the backbone.

CPP 15.17 Mon 18:00 Poster C

Dynamics of Colloidal Hard-Sphere Systems: A Rescaled Mode Coupling Theory Study — ●JOEL DIAZ MAIER and JOACHIM WAGNER — Institut für Chemie, Universität Rostock, 18051 Rostock, Germany

Intermediate scattering functions of liquid-like structured suspensions containing model hard-sphere particles are determined by means of static and dynamic light scattering experiments. The structure and short-time dynamics can be quantitatively described by employing multi-component Percus-Yevick integral-equation theory for the structure factors and the $\delta\gamma$ -expansion for hydrodynamic functions. Rescaled multi-component mode coupling theory (RMCT) can quantitatively describe the full, experimentally determined collective dynamics across the entire range of volume fractions investigated within the fluid range when the structure factors used for the calculation of the MCT vertices are rescaled to a lower effective volume fraction. Apart from the scaling factor, RMCT provides a parameter-free, correct description for long-time self-diffusion coefficients and the shear viscosity in the limit of small shear gradients.

CPP 15.18 Mon 18:00 Poster C

Binary mixtures of magnetic shape-anisotropic particles: the role of depletant — MARGARET ROSENBERG¹, ●EKATERINA NOVAK², ELENA PYANZINA², and SOFIA KANTOROVICH¹ — ¹University of Vienna, Vienna, Austria — ²Ekaterinburg, Russia

The introduction of non-magnetic particles into a dispersion of magnetic soft (or hard) spheres is recognized to promote the phase separation of the system. Our goal is to explore whether a comparable effect exists in binary mixtures of magnetic shape-anisotropic particles. In this paper, specifically, we undertake a theoretical and computational study of systems comprising either ellipsoids or platelets. We scrutinize the microstructure to assess if the introduction of depletants leads to quantitative or qualitative changes in the radial distribution functions, structure factors, orientational correlations, bond order parameters and static magnetic susceptibility. This research has been partially supported by the RSF Grant No. 19-72-10033. Computer simulations were performed at the Vienna Scientific Cluster (VSC-4).

CPP 15.19 Mon 18:00 Poster C

Electrostatic Screening in Highly Concentrated Salt Solutions — ●ESTHER OHNESORGE, THOMAS TILGER, and REGINE VON KLITZING — Department of Physics, Technische Universität Darmstadt, Darmstadt, 64289, Germany

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

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

To elucidate the underlying mechanism, we performed colloidal probe AFM (CP-AFM) measurements in different types of salt solutions, close to their solubility limit. As confining surfaces, silica and mica were compared to study the influence of the surface charge den-

sity and to bridge the gap between CP-AFM and SFA.

CPP 15.20 Mon 18:00 Poster C

The simulations of structural, thermodynamical, and mechanical characteristics of the mixture of ionic liquid and water using molecular dynamics: example of [bmim]⁺[PF₆]⁻ ionic liquid — ●MATEJA JOVANOVIĆ^{1,2}, MILJAN DAŠIĆ^{1,3}, and IGOR STANKOVIĆ¹ — ¹Scientific Computing Laboratory, Center for the Study of Complex Systems, Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Zemun, Serbia — ²Institute of Technical Sciences of SASA, K. Mihailova 35/IV, 11000 Belgrade, Serbia — ³Institute of Organic Chemistry and Biochemistry of the Czech Academy of Sciences, Flemingovo nam. 2, CZ-16610 Prague 6, Czech Republic

We present a study of the structural, thermodynamical, and mechanical properties of an ionic liquid 1-Butyl-3-methylimidazolium hexafluorophosphate [bmim]⁺[PF₆]⁻ water mixtures. Our simulation setup allows varying parameters of the system: temperature, concentration of ionic liquid, and shear rate of the system. We report significant changes compared to neat water or ionic liquids in the boiling temperature, diffusion coefficient, and viscosity. Even modest molar fractions of [bmim]⁺[PF₆]⁻ significantly affect the boiling point. The self-diffusion coefficient of water for the system with a lower concentration of ionic liquid is similar to the self-diffusion coefficient of neat water, and it decreases with increasing concentration of ionic liquid. Viscosity is investigated using equilibrium Green-Kubo relation and non-equilibrium molecular dynamics. In both cases, the viscosity coefficient increases with the increasing weight fraction of ionic liquid.

CPP 15.21 Mon 18:00 Poster C

Effect of different network topologies on swelling and mechanical properties of hydrogels — ●SOMESH KURAHATTI, MARIANO BRITO, DAVID BEYER, and CHRISTIAN HOLM — Institute for Computational Physics, Stuttgart, Germany

Polyelectrolyte gels exhibit larger swelling ratios than their uncharged counterpart because of the interplay between osmotic pressure induced by the dissociated counterions and the larger stretching induced by the self-repulsion of the backbone charges. Changing the charge density or varying the network constraints affects the swelling capacity as well as the mechanical moduli, which can be shown to also exhibit a strong influence on the desalination efficiency. In the current project, we explore the coupling between bulk modulus and equilibrium swelling of the polyelectrolyte hydrogels and their relation with different network architectures, by analysing various hydrogel conformations including different topologies and network defects. We investigate the bulk modulus and equilibrium swelling as a function of strand length under different salt concentrations and ionization degrees, and compare our results to existing scaling theories. As a result we find a universal coupling between these two quantities in different salinity regimes. The universal coupling can be broken by replacing linear polyelectrolyte strands by bottlebrush polyelectrolytes. Our results are helpful to develop a rational design of functional hydrogels.

CPP 15.22 Mon 18:00 Poster C

Concentration dependent pKa-values in mixtures of trimethylamine N-oxide (TMAO) and amino acids — ●JULIA KEIL, VARUN MANDALAPARTHY, and NICO VAN DER VEGT — Department of Chemistry, Technical University, Darmstadt

The stabilizing effect of trimethylamine N-oxide (TMAO) on proteins is known to be pH-dependent. In our investigation of this pH-dependent action, we studied protonation-deprotonation equilibria in mixed systems containing amino acids and TMAO by performing constant pH molecular dynamics simulations at different pH values. We found that the presence of TMAO causes a decrease in the pKa of acidic and basic groups, while the presence of acidic groups increases the pKa of TMAO. The observed changes in acidity and basicity of the titratable groups correlate with the TMAO concentration. Our results thus indicate a coupling between the equilibria of different titratable groups.

We propose a Wyman-Tanford binding model to explain the underlying mechanism of the observed behavior. Based on this, the accumulation of molecules around a titratable group favors the protonation state which is better stabilized by the presence of these molecules. That leads to a shift in the protonation-deprotonation equilibrium of titratable groups and results in a change of the pKa. More concisely, we find a favorable interaction between deprotonated acidic groups and protonated basic groups and an unfavorable interaction between different protonated basic groups to explain the observed changes of

pKa values in mixed solutions of titratable groups.

CPP 15.23 Mon 18:00 Poster C

Using the Light Polarization to Control the Properties of Photoresponsive Metal-Organic Frameworks — ●TAHER AL NAJJAR, ANEMAR BRUNO KANJ, CHUN LI, and LARS HEINKE — Karlsruhe Institute of Technology, Karlsruhe, Germany.

Controlling the properties of materials by applying external stimuli such as light is highly desirable for many applications. One promising realization is the incorporating photochromic molecules in the crystalline, nanoporous structure of metal-organic frameworks (MOFs). MOFs are a class of crystalline nanoporous materials with several unique properties because of their tailorable ordered structures and high surface area. Azobenzene molecules, which respond to light stimulations by isomerisation between its thermodynamically stable trans state and the excited cis state, are among the most popular photochromic molecules and can be used to functionalize MOFs. Using MOFs with fluorinated azobenzene moieties have demonstrated applications such as photoswitchable adsorption, membrane separation and ionic conduction. In this poster, a photoresponsive pillared-layer MOF thin film with incorporated fluorinated azobenzene molecules is presented. In addition to the photoisomerization upon unpolarized light of different wavelengths, the effect of the light polarization is explored. It is found that the polarization can be used to selectively isomerize the functional moieties in the MOF and, thus, to modify the material properties. We show that the polarization can be another useful parameter to control the material properties.

CPP 15.24 Mon 18:00 Poster C

Operando study on structure-activity relationship between electrolyte components and electrochemical performance for all-solid-state lithium-ion batteries — ●YINGYING YAN¹, LIANGZHEN LIU³, YUXIN LIANG¹, FABIAN A.C. APFELBECK¹, GUANGJIU PAN¹, and PETER MÜLLER-BUSCHBAUM^{1,2} — ¹TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — ²TUM, MLZ, 85748 Garching, Germany — ³TUM School of Natural Sciences, Chair of Inorganic and Metal-Organic Chemistry, 85748 Garching, Germany

All-solid-state lithium-ion batteries (ASSLIBs) have received extensive attention as one of the most promising power sources for flexible and wearable electronics. However, the practical application of ASSLIBs has been hindered by poor interfacial stability and inferior ionic conductivity. Solid polymer electrolytes (SPEs), as an important component in ASSLIBs, play a crucial role in determining the overall electrochemical properties, specifically for PEO and PEO-based derivatives, because of their superior interfacial compatibility, wide electrochemical windows and high ionic conductivity. Several strategies have been adopted to address the above issues, nevertheless, the SPEs degradation mechanism is still not clear and needs to be further studied. Therefore, we combined electrochemical characterization and morphological structure characterization to elucidate the structure-activity relationship between the component structure of the electrolyte and the electrochemical performance.

CPP 15.25 Mon 18:00 Poster C

Temperature dependent crystal structure of Ethylene Carbonate — ●LEA WESTPHAL^{1,2,3}, VOLODYMYR BARAN⁴, PETER MÜLLER-BUSCHBAUM^{1,2}, FLORENCE PORCHER^{3,5}, and ANATOLIY SENYSHYN² — ¹TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — ²MLZ, TUM, Garching, Germany — ³Laboratoire Leon Brillouin, UMR12 CEA-CNRS, Gif-sur-Yvette Cedex, France — ⁴DESY, Hamburg, Germany — ⁵ESS, Lund, Sweden

Performance and safety/stability of Li-ion batteries can be improved by joint optimisation of the charge-storing electrode materials and charge transfer-mediating liquid electrolytes. Most of the research on this has been focused on the electrodes, whilst electrolytes are less studied. An important class of solvents used in liquid electrolytes are linear and cyclic carbonates, because of the combination of physical/chemical properties, electrochemical performance and stability in a mixture with two or more solvents together with a lithium salt. Ethylene carbonate (EC), being the only solvent able to provide the protective SEI layer, is present in almost all commercial batteries, mixed with other solvents. [1] After the determination of the crystal structure of EC [2], this contribution presents room temperature data obtained by Neutron Powder Diffraction at SPODI (FRM II), Total Scattering and temperature dependent Powder X-Ray Diffraction data from beamline P02.1

(DESY), showing the structural evolution at different temperatures.

- [1] J.-M. Tarascon & M. Armand, *Nature* 414, 359-367 (2001).
 [2] C.J. Brown, *Acta Cryst.* 7, 92-96, (1954).

CPP 15.26 Mon 18:00 Poster C

Construction of cobalt oxyhydroxide nanosheets with rich oxygen vacancies as high-performance lithium-ion battery anodes — •YONGHUAN FU^{1,2}, HUAPING ZHAO¹, JIANHONG LIU², and YONG LEI¹ — ¹Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany — ²Graphene Composite Research Center, College of Chemistry and Environmental Engineering, Shenzhen University, Shenzhen, P. R. China

Cobalt oxyhydroxide (CoOOH) is a promising anode material for lithium-ion batteries (LIBs) due to its high electronic conductivity and theoretical specific capacity. Herein, CoOOH nanosheets are successfully obtained using a facile one-pot method, and a hierarchical nanoporous structure is formed by oxidizing cobalt hydroxide (Co(OH)₂) in NaOH and (NH₄)₂S₂O₈ solution. The CoOOH anode shows better electrochemical performance compared to Co(OH)₂ and Co₃O₄ electrodes when applied to LIBs. The hierarchical nanoporous structure and high electronic conductivity of the CoOOH anode contribute to its outstanding initial discharge capacity, high initial coulombic efficiency, and excellent cyclability. Experiments and density functional theory (DFT) calculations confirmed that the high ICE and prominent rate capability of the nanosheets could be ascribed to the rapid and complete conversion reaction of CoOOH upon lithiation/delithiation facilitated by hydroxyl groups and oxygen vacancies. This study provides new insights into the structure-property relationship of transition-metal oxyhydroxide anode materials for LIBs.

CPP 15.27 Mon 18:00 Poster C

In-situ interface film forming on the high-voltage LiCoO₂ cathode by a tiny amount of nanoporous polymer additives — •RUOXUAN QI¹, MING YANG³, TIANLE ZHENG¹, YA-JUN CHENG^{3,4}, and PETER MÜLLER-BUSCHBAUM^{1,2} — ¹TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — ²MLZ, TUM, Garching, Germany — ³NIMTE, CAS, Zhejiang Province, P. R. China — ⁴College of Renewable Energy, Hohai University, Jiangsu Province, P. R. China

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

CPP 15.28 Mon 18:00 Poster C

3D Electrodeposition Porous Cu for Long-cycling Lithium-Metal Batteries — •LYUANG CHENG¹, ZHUIJUN XU¹, TIANLE ZHENG¹, YINGYING YAN¹, RUOXUAN QI¹, YUXIN LIANG¹, FABIAN A. C. APFELBECK¹, YAJUN CHENG², and PETER MÜLLER-BUSCHBAUM^{1,3} — ¹TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — ²Hohai University, 213022 Changzhou, China — ³TUM, MLZ, 85748 Garching, Germany

Lithium (Li) metal is the ultimate anode for rechargeable batteries. Its high specific capacity (3860 mAh g⁻¹) and low voltage (*3.04 V vs standard hydrogen electrode) warrant optimal cell energy density. However, these anodes rely on repeated plating and stripping of Li, which leads to consumption of Li inventory and the growth of dendrites that can lead to self-discharge and safety issues. To address these issues and problems related to the volume change of these anodes, a number of different porous conductive scaffolds have been reported to create high surface area electrodes on which Li can be plated reliably. While impressive results have been reported in literature, current processes typically rely on either expensive or poorly scalable techniques. Herein, we report a scalable fabrication method to create porous Cu anodes using a one-step electrodeposition process. The areal loading,

pore structure, and electrode thickness can be tuned by changing the electrodeposition parameters, and we show the in-situ WAXS images with lithium growth which can help explain the mechanism of dendrites. We also provide a feasible method to fabricate the porous Cu cathodes with different electrodeposition solution concentrations.

CPP 15.29 Mon 18:00 Poster C

Operando study of structure evolution with PEO-LLZTO composite electrolyte in all-solid-state lithium batteries — •TANNU GARG¹, YUXIN LIANG¹, and PETER MÜLLER-BUSCHBAUM^{1,2} — ¹TUM School of Natural Sciences, Chair for Functional Materials Garching, Germany — ²MLZ, TUM, Garching, Germany

Solid-state lithium batteries are promising for next-generation energy storage due to their potential for high energy density and safety. This proposal focuses on the operando study of the poly(ethylene oxide) (PEO)-LLZTO composite electrolyte in all-solid-state lithium batteries, with a specific emphasis on observing the structure evolution in bias conditions. The composite electrolyte consists of PEO + LiTFSI matrix and inorganic filler Li_{6.4}La₃Zr_{1.4}Ta_{0.6}O₁₂ (LLZTO) in varying weight percentages. The study aims to investigate the phase segregation and polymer region shrinkage with increasing LLZTO content. Additionally, it will explore the diffusion behavior of Li⁺ ions and the generation of interfaces in different composite electrolytes. The proposal also outlines plans for X-ray scattering analysis and charge/discharge cycling of LLZTO to further enhance the understanding of the system. The study will contribute to the ongoing efforts to develop high-performance all-solid-state lithium batteries by providing insights into the behavior and evolution of PEO-LLZTO composite electrolytes under bias conditions.

CPP 15.30 Mon 18:00 Poster C

Use of High-concentration Lithium-ion Electrolyte to Overcome Challenges of High-temperature Lithium Batteries — •TIANLE ZHENG¹ and PETER MÜLLER-BUSCHBAUM^{1,2} — ¹TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — ²TUM, MLZ, 85748 Garching, Germany

Lithium secondary batteries (LSBs) have witnessed explosive growth in the last decade. Traditional Li-ion batteries, on the other hand, are severely constrained in high-temperature applications due to the low thermal stability of the electrolyte/electrode interface and electrolyte decompositions in the cell. Herein, we demonstrate a new electrolyte that achieves excellent stable long-term cycling at 100°C, well beyond the typical 60°C limits of normal conventional Li-ion batteries. The highly concentrated lithium oxalate difluoroborate (LiODFB) is selected as the only lithium salt with a carefully designed high thermal stability solvent group. As a result, this unique high-concentration electrolyte promotes the formation of a stable and inorganic solid electrolyte interface (SEI) layer on the electrode at elevated temperature, leading to improved performance in MCMB/Li and lithium iron phosphate (LFP)/Li half-cells. Moreover, it achieves reversible capacities of 160 and 350 mA h/g, respectively, with Coulombic efficiencies (CEs) > 99.3%. Subsequently, we further investigate the mechanism of high-concentration electrolytes by molecular dynamics (MD) simulations and XPS characterization techniques, exploring a new way for future high-temperature electrolytes for Li-ion batteries.

CPP 15.31 Mon 18:00 Poster C

Development of a novel type of solid polymer electrolyte for solid-state lithium battery applications based on lithium-enriched PEO/PVP blend polymer — •MAYANK GARG¹, YUXIN LIANG¹, and PETER MÜLLER-BUSCHBAUM^{1,2} — ¹TUM School of Natural Sciences, Chair of Functional Materials, 85748 Garching, Germany — ²MLZ, TUM, 85748 Garching, Germany

The growing demand for thin, flexible energy storage devices for applications like flexible electronics and wearable technologies has intensified interest in Solid Polymer Electrolyte (SPE) films. These polymer-based batteries offer a promising alternative due to their thin, flexible nature and seamless integration into devices, coupled with cost-effectiveness. This study focuses on enhancing the conductivity of SPE films comprising a blend of biodegradable poly(ethylene oxide) (PEO) and poly(vinyl pyrrolidone) (PVP) as the host matrix, with varied lithium bis(trifluoromethane sulfonyl)imide (LiTFSI) dopant salt concentrations. Structural and optical characterization techniques, including X-ray diffraction (XRD), differential scanning calorimetry (DSC), Fourier transform infrared spectroscopy (FTIR), UV-Vis spectroscopy, and electrochemical analysis, were employed. Optimized lithium salt concentrations enabled functional device operation at ambient temper-

atures (20-60°C), with Impedance Spectroscopy revealing enhanced ionic conductivity. Furthermore, the incorporation of small metal additives further improved the ionic conductivity of the battery cell.

CPP 15.32 Mon 18:00 Poster C

Investigation of Li-ion dynamics at Hybrid Electrolyte Interfaces using M.D Simulations — ●GOURAV SHUKLA¹, DIDDO DIDDENS^{1,2}, and ANDREAS HEUER¹ — ¹Institut für physikalische Chemie, Universität Münster, Corrensstraße 28/30, 48149 Münster — ²Helmholtz Institute Münster, Corrensstraße 48, 48149 Münster

Several studies have been conducted to develop novel materials for use as electrolytes, aiming to enhance the performance of batteries in terms of ionic conductivity. Although polymers play a predominant role in electrolytes, the superior mechanical stability of solid electrolytes has spurred the development of hybrid electrolytes that combine the best attributes of both phases. In our work, we are investigating the interface between a Li-salt-containing polycaprolactone polymer and LLZO solid electrolyte, using molecular dynamics simulations. Experiments have shown that polycaprolactone (PCL) exhibits better conductivity when grafted onto solid electrolytes in hybrid systems, compared to non-grafted systems. These systems are studied by MD simulations to investigate the polymer structure and ion distribution as well as the dynamics near the interface. Furthermore, we varied the number of grafted polymer chains on the solid surface to compare the behavior of grafted and non-grafted interfaces. Different force field sets for the solid electrolytes have shown considerable impact on Li-ion migration both at the interface and within the solid phase at a constant temperature. Along with the charge scaling of salt ions for faster dynamics, we also explored the ion migration at different grafted and ungrafted regions.

CPP 15.33 Mon 18:00 Poster C

Investigation of Li-ion dynamics at Hybrid Electrolyte Interfaces using MD Simulations — ●GOURAV SHUKLA¹, DIDDO DIDDENS^{1,2}, and ANDREAS HEUER¹ — ¹Institut für physikalische Chemie, Universität Münster, Corrensstraße 28/30, 48149 Münster — ²Helmholtz Institute Münster, Corrensstraße 48, 48149 Münster

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CPP 15.34 Mon 18:00 Poster C

Simulation of pH-Responsive Hydrogel Formation — ●DAVID BEYER¹, PETER KOŠOVAN², and CHRISTIAN HOLM¹ — ¹Institute for Computational Physics, University of Stuttgart, D-70569 Stuttgart, Germany — ²Department of Physical and Macromolecular Chemistry, Charles University, 128 00 Prague 2, Czechia

Motivated by recent experiments investigating pH-responsive, electrostatically triggered hydrogel formation (Mons et al., in preparation), we investigate the interaction between permanently charged sulfonate chains and charge-regulating carboxybetaine chains. Through simulations integrating a state-of-the-art Monte Carlo method for charge-regulating systems with a free energy approach, we obtain the potential of mean force between these chains for different pH-values. Our simulations reveal a substantial charge-regulation effect, elevating the stability of the complex to pH-values beyond what the Henderson-Hasselbalch equation would suggest. A comparative study between fully functionalized and 75% functionalized betaines reveals a further significant enlargement of the pH-stability window in the latter scenario. Overall, our simulations provide a comprehensive explanation

for the observed stability at much higher pH-values than naively expected, emphasizing the combined impact of these two effects.

CPP 15.35 Mon 18:00 Poster C

Injectable hydrogels from thermoresponsive tri- and tetrablock terpolymers investigated using scattering methods — ●FEIFEI ZHENG¹, PABLO ALVAREZ HERRERA¹, WENQI XU¹, EIRINI MELAMPANAKI¹, JOACHIM KOHLBRECHER², ANNA P. CONSTANTINOU³, THEONI K. GEORGIIOU³, and CHRISTINE M. PAPADAKIS¹ — ¹TUM School of Natural Sciences, Technical University of Munich, Garching, Germany — ²Paul Scherrer Institut, Villigen PSI, Switzerland — ³Department of Materials, Imperial College London, London, UK

Thermogels are an exciting class of stimuli-responsive materials with many promising applications, e.g. in 3D bioprinting. The mechanical properties in the gel state strongly depend on the architecture of the polymer. Here we address an ABC triblock terpolymer and a BABC tetrablock terpolymer consisting of the hydrophilic OEGMA (A), the hydrophobic BuMA (B), and the thermoresponsive DEGMA (C). The results from dynamic light scattering on dilute solutions indicate that the hydrodynamic radii of the micelles formed by both, ABC and BABC, increase strongly above 25 °C, and the solutions feature a cloud point, i.e. aggregation of the micelles sets in. By small-angle neutron scattering, we found that ABC forms spherical core-shell micelles, that transform into cylinders at high temperatures, and then become a more compact structure upon further heating. In contrast, the core-shell micelles formed by BABC stay spherical and form small fractal aggregates at higher temperatures, that form a less dense network structure in comparison to those formed by ABC.

CPP 15.36 Mon 18:00 Poster C

Photoswitchable Molecules: Impact on Swelling in Thermoresponsive Polymer Films under UV Irradiation — ●DAVID P. KOSBAHN¹, JULIJA REITENBACH¹, MORGAN LE DÜ¹, LUKAS V. SPANIER¹, RENÉ STEINBRECHER^{2,3}, ANDRÉ LASCHEWSKY^{2,3}, ROBERT CUBITT⁴, THOMAS SAERBECK⁴, CHRISTINE M. PAPADAKIS¹, and PETER MÜLLER-BUSCHBAUM^{1,5} — ¹TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — ²Institut für Chemie, Universität Potsdam, 14476 Potsdam-Golm, Germany — ³Fraunhofer Institut für Angewandte Polymerforschung, 14476 Potsdam-Golm, Germany — ⁴Institut Laue-Langevin, 38000 Grenoble, France — ⁵MLZ, TUM, 85748 Garching, Germany

In this study, we investigated the swelling characteristics of p(AzAm-co-DMAm) and p(AzPyAm-co-DMAm) thin films in both isomer states of the photoswitchable molecules azobenzene (Az) and azopyrazole (AzPy). The influence of UV-irradiation on the swelling behavior in water vapor was explored, aiming to control water uptake, expansion, and morphology on the nanoscale. These materials hold promise for applications such as light sensors, photo-actuators, and drug-delivery systems. Utilizing in situ time-of-flight neutron reflectometry measurements with high temporal resolution at the D17 instrument at ILL, we obtained depth-resolved data about the water distribution during swelling, drying, and irradiation in the dry and swollen states. Our results reveal insights into how photoswitchable molecules affect the microscopic properties of thin polymer films.

CPP 15.37 Mon 18:00 Poster C

Phase behavior of thermo- and photoresponsive diblock copolymers for non-invasive schizophrenic switching — ●PEIRAN ZHANG¹, RENÉ STEINBRECHER², ANDRÉ LASCHEWSKY², DMYTRO SOLOVIOV³, PETER MÜLLER-BUSCHBAUM¹, and CHRISTINE M. PAPADAKIS¹ — ¹Technical University of Munich, TUM School of Natural Sciences, Garching, Germany — ²University of Potsdam, Institute of Chemistry, Potsdam-Golm, Germany — ³European Molecular Biology Laboratory, c/o DESY, Hamburg, Germany

Stimuli-responsive diblock copolymers (DBCPs) are of interest as carriers due to their change of properties upon exposure to external stimuli, such as temperature and light. In this study, we present the phase behavior of a series of DBCPs comprising thermo-responsive blocks, one of which is functionalized with a photoactive group. Thus, the DBCP will feature a fixed cloud point (CP) due to the singly responsive block and a tunable CP due to the doubly responsive block. This way, the DBCPs can self-assemble in aqueous solution into micelles and inverse micelles, achieving "schizophrenic switching". Dynamic light scattering indicates that all DBCPs under investigation show a single CP in dilute aqueous solution, namely the one of the singly thermoresponsive block. Small angle X-ray scattering reveals that the DBCPs are ex-

panded chains below this CP and are collapsed at temperatures above, forming large aggregates. Switching the photoactive group by UV irradiation does not have an effect on this behavior, which points to a very high CP of the doubly responsive block.

CPP 15.38 Mon 18:00 Poster C

PNIPAM microgel-stabilized aqueous Pickering foams — ●JOANNE ZIMMER, GAËTAN BARTH, LUCA MIRAU, and REGINE VON KLITZING — Technische Universität Darmstadt, Department of Physics, Soft Matter at Interfaces, Hochschulstraße 8, 64289 Darmstadt

Particle-stabilized foams (Pickering foams) are gaining increasing attention due to their high long-term stability and possible stimuli-responsiveness. Suitable stabilizers for generation of these foams are PNIPAM microgels (MG) as they possess a high adsorption energy at the water-air-interface compared to classical surfactants. In addition, they show a temperature-dependent reversible volume phase transition which allows for generation of switchable foams, that can be destroyed on demand.

In this work MG stabilized Pickering foams were generated by sparging gas through a PNIPAM MG dispersion. For this purpose, the Teclis Foam Scan device is used, which measures foam properties like foam volume over time, liquid fraction and bubble size and bubble size distribution. A special focus was set on identifying device and sample parameters for generation of foams with a homogenous bubble size distribution. This is essential for a quantitative comparison of the foam properties and investigation of foam destabilization processes. In addition, it must be noticed, that addition of NaCl to the MG dispersion is required to increase the electrical conductivity and allow for determination of the foam liquid content. Thus, the influence of the NaCl concentration on the foaming properties was also subject of this study.

CPP 15.39 Mon 18:00 Poster C

Consistent description of Electrostatic Interactions in Nano-Confinement: from Ab-Initio to Coarse-Grained Models —

●PHILIPP STÄRK¹, ZHIWEI JIN¹, HENRIK STOOSS¹, and ALEXANDER SCHLAICH^{1,2} — ¹SC Simtech, Universität Stuttgart — ²ICP, Universität Stuttgart

The electrode/electrolyte interface is crucial for applications like energy storage and production or electrocatalysis. To describe the microscopic effects, usually the electronic structure (ESP) problem needs to be solved, strongly restricting the accessible length- and time-scales. We combine ESP calculations with semi-classical models that allow for enhanced grand canonical sampling schemes within atomistic simulations of fluids confined between nano-porous electrodes. We derive coarse-grained models that yield the experimentally relevant information like the differential capacitance from the fundamental properties of the electrode/electrolyte interface. Importantly, using this approach allows us to study systematically the influence of the electrode electronic degrees of freedom on the behavior of the confined fluid.

CPP 15.40 Mon 18:00 Poster C

Friction Measurements of Single Pinning Defects Using Droplet Probe Microscopy — ●DIEGO CORTES¹, MICHAEL KAPPL¹, HANS-JÜRGEN BUTT¹, and TOMAS CORRALES² — ¹Max Plank Institute, Mainz, Germany — ²Universidad Tecnica Federico Santa Maria, Valparaiso, Chile

Friction of drops sliding over solid surfaces depends on several effects. By scaling down the size of drops, dissipation at the contact line becomes more and more dominant and can be isolated from other dissipation processes. Here, we measure the energy dissipation of pico liter drops sliding over hydrophobic surfaces using Atomic Force Microscopy. This novel technique allow us to test the wetting behavior of hydrophobic material on sub-micrometer scale.

CPP 15.41 Mon 18:00 Poster C

Electrochemical potential study of the electric double layer in dynamic wetting of electrolyte drops — ●JAMILA RZAYEVA¹, MANUEL BRINKER^{1,2}, and PATRICK HUBER^{1,2} — ¹Institut für Material- und Röntgenphysik, Technische Universität Hamburg, Denickestraße 15, 21073 Hamburg, Deutschland — ²Deutsches Elektronen-Synchrotron DESY, Center for X-Ray and Nano Science CXNS, 22607 Hamburg, Deutschland

Our study aims to investigate the dynamic variations in electrochemical potential within the electric double layer (EDL) of electrolyte's drops. The behaviour of the EDL is investigated during drying and

wetting at the interface of the liquid and a conductive gold surface. Understanding the EDL is paramount for fundamental electrochemical processes, especially in dynamic environments where electrolyte drop changes occur. In this work, besides spontaneous evaporation of the liquid, the drop is also deliberately altered by changing its volume. Here, vitally, the advancing and receding contact angle impacts both the wetting and the potential. The experiments combine drop shape analyser measurements with open circuit potentiometry to yield a comprehensive picture of the link between electrochemistry and wetting of drops on a conductive surface. All of these measurements are conducted with different types of electrolyte and concentration, while also varying the relative humidity of the surrounding atmosphere.

CPP 15.42 Mon 18:00 Poster C

Core-shell nanoparticles for wet-coated surface-enhanced raman scattering (SERS) application — ●JUNGUI ZHOU¹, YINGJIAN GUO^{1,2}, SUO TU², ANURADHA BHOGRA¹, SARATHAL KOYILOTH VAYALIL¹, DANIEL SÖDERBERG⁵, PETER MÜLLER-BUSCHBAUM^{2,3}, PENG ZHANG⁴, and STEPHAN V. ROTH^{1,5} — ¹Deutsches Elektronen-Synchrotron, Hamburg, Germany — ²Technical University of Munich, Garching, Germany — ³Heinz Maier-Leibnitz Zentrum, Garching, Germany — ⁴Sun Yat-sen University, Guangzhou, China — ⁵KTH Royal Institute of Technology, Stockholm, Sweden

Plasmonic nanoparticles (NPs) are extensively used in various applications, in particular, SERS, which has been widely used in viral molecular detection. Virus Raman detection is mainly focused on the detection of viral nucleic acid and bases, but the detection of viral proteins is rare. In addition, there is limited knowledge about the interaction between virus proteins and core-shell NPs. Thus, understanding the relationship between the behaviour of viruses and the Raman signal can lead to the development of advanced NPs for virus detection. Here, spraying water-based cellulose nanofiber (CNF) and core-shell NPs solutions is used for the fabrication of sensors. In-situ small-angle grazing incidence X-ray scattering (GISAXS) technique is used to investigate the self-assembly of CNF and NPs during deposition. After the fabrication of sensors, some measurements will be taken, such as Raman, AFM and XPS et al. Moreover, the relationship between NPs, sensor performance, and virus behaviour is explored and constructed to lay solid foundations for the fabrication of sensors for virus detection.

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CPP 15.43 Mon 18:00 Poster C

Knot diagrams for 3-periodic entanglements. — ●TOKY ANDRIAMANALINA¹, MYEAWY EVANS¹, and SONIA MAHMOUDI² — ¹University of Potsdam, Germany — ²Tohoku University, Japan

Polymers, DNA origami crystals, and many other biological and chemical structures present features of entanglement, arranging in a 3-periodic fashion. As the topology of those structures have influence on their physical properties, some knot invariants have been extended into measures, such as the periodic linking number or the periodic Jones polynomials, to quantify the entanglement. This project aims to give a new mathematical diagrammatic description based on Knot theory for 3-periodic entangled structures. To do so, we project a unit cell of the structure onto a square with periodic boundaries. To the projected curves, we add crossing information, and we introduce new symbols to capture the periodic boundary conditions of the unit cell. The new diagrams require a set of new moves added to the three usual Reidemeister moves.

CPP 15.44 Mon 18:00 Poster C

The neutron time-of-flight spectrometer TOFTOF and its application to soft condensed matter physic — ●MARCELL WOLF and CHRISTOPHER GARVEY — Heinz Maier-Leibnitz Zentrum, Technische Universität München, Germany

TOFTOF is a direct geometry disc-chopper time-of-flight spectrometer. A cascade of seven fast rotating disc choppers is used to prepare a monochromatic pulsed beam which is focussed onto the sample by a converging super-mirror section. The scattered neutrons are detected by 1000 He detector tubes with a time resolution up to 50 ns. The detectors are mounted at a distance of 4 m and cover 0.75 sr. The high rotation speed of the chopper system together with a high neutron flux in the wavelength range of 1.4 -14 Å allows free tuning of the energy resolution between 3 meV and 2 µeV. The fast neutron background is suppressed by the s-shaped primary neutron guide. This enables the investigation of weak signals. Here we will discuss the value of neutron spectroscopy for different applications in soft condensed matter physics. We will show different sample environments which can be used for sample manipulation.

CPP 15.45 Mon 18:00 Poster C

Deep learning based method for speeding up the extraction of morphological parameters in GISAXS data — ●SHACHAR DAN¹, ELДАР ALMAMEDOV², STEPHAN V. ROTH^{1,3}, MATTHIAS SCHWARZKOPF¹, SVEN J. WÖHNERT¹, ANDRE ROTHKIRCH¹, and VOLKER SKWAREK² — ¹DESY, Hamburg, Germany — ²HAW, Hamburg, Germany — ³KTH, Stockholm, Sweden

In situ grazing incidence small angle X-ray scattering (GISAXS) is a powerful tool for accessing nanoscale structure formation in real time with high time resolution and high statistical relevance. Nevertheless, the analysis is clearly time consuming and challenging task, necessitating the need for strategies to speed up the process. In this context we introduce our two-step method that incorporates a pre-processing

of GISAXS simulations, which are employed to train a neural network (NN). The NN is subsequently utilized to predict the average cluster radius and distance of the model system gold on silica. There are multiple aspects of the method that require detailed characterization. Here we focus on the effects of using intensity thresholds in the pre-processing step and on the relationship between the network architecture and the distribution of results. As part of ongoing research, we are investigating different configurations and examining their direct impact on the predictive capabilities of the NN. This iterative refinement process aims not only to improve the effectiveness of the approach for the specific system, but also to lay the foundation for its applicability to broader material systems in the field of GISAXS data analysis.