

CPP 17: Poster Session I

Topics: Active Matter (17.1-17.3); Biopolymers, Biomaterials and Bioinspired Functional Materials (17.4-17.8); Charged Soft Matter, Polyelectrolytes and Ionic Liquids (17.9-17.17); Crystallization, Nucleation and Self-Assembly (17.18-17.22); Electrical, Dielectrical and Optical Properties of Thin Films (17.23-17.25); Glasses and Glass Transition (17.26-17.32); Interfaces and Thin Films (17.33-17.39); Physics of Self-Organization in DNA Nanostructures (17.40-17.42); Polymer Networks and Elastomers (17.43-17.44).

Time: Monday 17:30–19:30

Location: Poster B1

CPP 17.1 Mon 17:30 Poster B1

Translocation in Presence of Molecular Motors — ●IMAN ABDOLI, HIDDE VUIJK, and ABHINAV SHARMA — Leibniz Institute for Polymer Research

We study the assisted translocation of a polymer chain across a membrane nano-pore, on one side of which there are molecular motors. These motors can attach from the bulk on to the polymer, perform directed motion on the chain, and can undergo detachment. We model the directed motion of the motors using the Totally Asymmetric Random Process (TASEP) and the attachment/detachment using Langmuir Kinetics (LK). We study, analytically and computationally, how motors influence the rate of translocation of polymer chain across the membrane.

CPP 17.2 Mon 17:30 Poster B1

Fabrication of ellipsoidal microswimmers with controllable tip shape — ●YARA ALSAADAWI¹, FERNANDO VAZQUEZ LUNA², ANNA EICHLER-VOLF¹, MARTIN STEINHART², and ARTUR ERBE¹ — ¹Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany — ²Institute of Chemistry of New Materials and Center of Physics and Chemistry of New Materials, Universität Osnabrück, 49076 Osnabrück, Germany

Microswimmers are objects capable of converting applied energy into active motion, resulting in its propulsion in a medium. The shape and chemical compound of the microswimmer strongly influence its propulsion properties. Here we investigate a template-based approach for fabrication of particles with controlled composition, size, and shape, which can be used as fundamental units for the preparation of microswimmers. Polystyrene nanorods with different configurations of the tip shape were fabricated with an aspect ratio of 10:1. The ratio of length-to-width (i.e. aspect ratio) can be easily modified by controlling the surface properties of the template. The wettability transition of polystyrene was used to manipulate the morphology and entrapment of polymer nanostructures.

CPP 17.3 Mon 17:30 Poster B1

Modeling the interaction of magnetically capped colloidal particles — ●MAXIMILIAN NEUMANN¹, SIBYLLE GEMMING^{1,2}, GABI STEINBACH², and ARTUR ERBE¹ — ¹Institute of Physics, TU Chemnitz, D-09107 Chemnitz — ²Helmholtz-Zentrum Dresden - Rossendorf, D-01328 Dresden

Colloidal self-assembly bears significant potential for the bottom-up fabrication of advanced materials and micromechanical structures. A wide range of particles with different types of anisotropy have been recognized as promising precursors for controlled structure engineering. Here, we concentrate on particles that interact via polar fields, which are intrinsically anisotropic. More specifically, we focus on the assembly of micron-sized silica spheres which are partly covered by a thin ferromagnetic layer with an out-of-plane magnetic anisotropy. To study assemblies of such magnetic particles, we introduce a simple two-parameter model: The extended magnetization distribution is approximated by a current-carrying coil enclosed inside a hard sphere. The far field of that current reproduces the stray field of a point dipole model, the near field reflects an extended magnetization. Such a model employs only two parameters to describe the shape of the magnetization distribution: The radius and the position of the coil inside the sphere. We present stable assemblies as a function of both parameters. In the limit of very small coils the analytical solution for two particles with shifted point dipoles is correctly reproduced. By increasing the radius of the coil, we reproduce experimentally observed particle arrangements not covered by models based on single shifted dipoles.

CPP 17.4 Mon 17:30 Poster B1

Biopolymer templated titanium dioxide films prepared via spray coating — ●JULIAN HEGER¹, WEI CHEN¹, SEBASTIAN GROTT¹, XINYU JIANG¹, SIGRID BERNSTORFF², and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik-Department, LS für Funktionelle Materialien, 85748 Garching, Germany — ²Eletra-Sincrotrone Trieste S.C.p.A., Trieste, Italy

Nanostructured titanium dioxide films have great potential for application in photovoltaics, such as the inorganic counterpart in hybrid solar cells. For this purpose, the film morphology has crucial influence on the device performance, since a high surface-to-volume ratio is needed for efficient charge separation. So far, inorganic mesoporous matrices are successfully achieved by sol-gel chemistry in combination with block copolymer directed templating. As a novel approach, we use environmentally friendly biopolymers as tailoring agents. The whey protein β -Lactoglobulin was found to form different structures within denaturation, from fibrils to spheres. By combining heat denaturation at different pH and sol-gel chemistry, different nanosized structures are introduced into titanium dioxide. The resulting sol-gels are used as inks for film deposition via spray coating. After calcination to remove the biopolymer template, the film morphologies of the remaining titanium dioxide scaffolds are investigated by grazing incidence small-angle X-ray scattering (GISAXS). GISAXS measurements are supplemented by scanning electron microscopy.

CPP 17.5 Mon 17:30 Poster B1

Water-Mediated Protein-Protein Interactions at High Pressures are Controlled by a Deep-Sea Osmolyte — KARIN JULIUS¹, JONATHAN WEINE¹, NICO KÖNIG¹, MIMI GAO², JAN LATARIUS¹, ●MICHAEL PAULUS¹, MARTIN A. SCHROER³, METIN TOLAN¹, and ROLAND WINTER² — ¹Faculty of Physics/DELTA, TU Dortmund University, 44221 Dortmund, Germany — ²Faculty of Chemistry and Chemical Biology, TU Dortmund University, Otto-Hahn-Strasse 4a, 44227 Dortmund, Germany — ³European Molecular Biology Laboratory (EMBL) Hamburg c/o DESY, Notkestrasse 85, 22607 Hamburg, Germany

Living cells accumulate organic osmolytes to high concentrations as adaptive response towards external stressors such as dehydration, freezing, salinity or high hydrostatic pressure as encountered in the deep sea. The mechanisms of protein stabilization and the linkage to the intermolecular interactions between proteins in the cellular milieu at ambient as well as at elevated pressures are still largely terra incognita. Herein, we study the impact of natural osmolyte mixtures on the pressure dependent intermolecular pair-interaction potential of dense protein solutions by applying small-angle X-ray scattering in combination with a liquid-state theoretical approach. Particularly, the presence of the deep-sea osmolyte TMAO guarantees the sustainability of the native protein fold under harsh environmental conditions. Further, we find a strong interplay between water and osmolyte in controlling the water-mediated intermolecular interactions at high pressure, thereby preventing contact formation and hence aggregation of proteins.

CPP 17.6 Mon 17:30 Poster B1

Towards biomimetic carbon nanomembranes — ●RAPHAEL DALPKE¹, ANNA DREYER², THORSTEN SEIDEL², ANDRÉ BEYER¹, KARL-JOSEF DIETZ², and ARMIN GÖLZHÄUSER¹ — ¹Physics of Supramolecular Systems and Surfaces, Faculty of Physics, Bielefeld University, Universitätsstraße 25, 33615 Bielefeld, Germany. — ²Biochemistry and Physiology of Plants, Faculty of Biology, Bielefeld University, Universitätsstraße 25, 33615 Bielefeld, Germany.

Cell membranes are a prerequisite for life. Incorporated membrane proteins facilitate the transfer of substances. To explore the mechanisms of vectorial transport across cell membranes, an ultrathin, biomimetic system is desirable which allows the controlled integration of proteins. Here, we present different strategies to immobilize proteins with high

affinity on carbon nanomembranes (CNMs). Covalently bonded aromatic precursor molecules form self-assembled monolayers (SAMs) on metal surfaces. After the irradiation with low energy electrons (100 eV) these cross-link to mechanically stable, chemically inert, and permeable CNMs with a typical thickness of around 1 nm which can be transferred onto any arbitrary substrate for further usage [1]. In particular, we discuss functionalization strategies for reversible as well as for irreversible protein immobilization. The basis of the reversible type is the non-covalent interaction of streptavidin and biotin which can be released by d-desthiobiotin. The irreversible type is based on the maleimide coupling chemistry, where a stable thioether bond is formed.

[1] A. Turchanin and A. Götzhäuser, Carbon Nanomembranes, *Advanced Materials*, 2016, 28 (29), pp. 6075-6103.

CPP 17.7 Mon 17:30 Poster B1

Biomimetical Surfaces for Pollutant Separation — ●SEBASTIAN STELZNER¹, DAGMAR VOIGT², BERNHARD ALEXANDER GLATZ¹, and ANDREAS FERY¹ — ¹Leibniz-Institut für Polymerforschung, Dresden, Germany — ²Institut für Botanik, Technische Universität Dresden, Germany

The cuticula is a main part of the evolutionary progress of terrestrial plants. It consists of an insoluble polymer fraction and a soluble lipid (wax). Those waxes are crystalloid micro- and nanostructures with a high structural and morphological diversity and can rearrange in a self-organized manner. The platelets, tubules, filaments etc. are forming based on their chemical composition and share the ability to regenerate. In order to utilize those properties, structured polymer substrates are produced with the target of adhesion and recrystallization of vaporized plant waxes. By tuning the chemical properties of the waxes as well as the surficial ones of the substrates, the shape and orientation of the crystals can be manipulated to the intended usage. In this project, environmental pollutant adhesion is targeted. The influence of surface-structured polymers on the wax crystallization is compared to flat substrates and the difference in grade of adhesion is analyzed and quantified. The aim is to generate an optimized material adhesion system. By separation and regeneration of the waxes or by the use of embedded catalysts, harmful air contaminants are sought to be decimated.

CPP 17.8 Mon 17:30 Poster B1

Secondary structure analysis of xanthan using atomic force microscopy — ●JENNY FJODOROVA¹, JULIA VOSS², GERD HUBLIK³, VERA ORTSEIFEN², KARSTEN NIEHAUS², VOLKER WALHORN¹, and DARIO ANSELMETTI¹ — ¹Experimental Biophysics and Applied Nanoscience, Bielefeld University, Germany — ²Proteome and Metabolome Research, Bielefeld University, Germany — ³Jungbunzlauer Austria AG, Pernhofen 1, 2064 Wulzeshofen, Austria

Xanthan is an extracellular polysaccharide, secreted by the bacterium *Xanthomonas campestris*. Due to its unique viscosifying properties over a wide range of salt concentrations, xanthan has numerous industrial applications e.g. in food, cosmetic or oil industry. Therefore, the optimisation of xanthan production and its rheological properties is of particular interest. Targeted genetic modification of the *Xanthomonas* metabolism and subsequent change of salt concentrations can be a powerful tool to optimise the shear-thickening potency and to improve the xanthan production efficiency.

Using atomic force microscopy (AFM) imaging and single molecule force spectroscopy (SMFS), we analysed the structure and the elastic characteristics of single xanthan polymers, which were produced by different *Xanthomonas* strains. We identified structures ranging from single-stranded coiled networks to branched double-strands. Taking into account the varying ability to form double-strands and differences in the bending stiffness, we observed a correlation between the formation of secondary structures and its resulting different viscosifying properties.

CPP 17.9 Mon 17:30 Poster B1

Structure of Ionic Liquid Mesophases inside Nanopore Confinement — ●ANDRE ULTES¹, JULIAN MARS^{1,2}, KATHRIN SENTKER³, MILENA LIPPMANN⁴, FORIAN BERTRAM⁴, PATRICK HUBER³, and MARKUS MEZGER^{1,2} — ¹Max Planck Institute for Polymer Research, Mainz — ²Institute of Physics, Johannes Gutenberg University Mainz — ³Institute of Materials Physics and Technology, Hamburg University of Technology — ⁴DESY Photon Science, Hamburg

Ionic liquids composed of cations with long aliphatic side chains exhibit so-called microphase separation leading to structural hetero-

geneities on the nanometer length scale. Depending on their molecular structure, short range order as well as thermodynamically metastable and stable liquid crystalline (LC) mesophases have been observed [1]. Interfaces can strongly affect their phase stability and relative orientation [2]. In this work, the orientation and phase behavior of $[C_{22}C_{1}im]^{+}[NTf_{2}]^{-}$ inside anodized aluminum oxide (AAO) nanopores was investigated by X-ray scattering. Here, confinement can stabilize phases not observed in bulk. Depending on pore diameter and surface functionalization different orientations of the LC director relative to the pore axes were observed.

[1] H. Weiss et al., *J. Phys. Chem. B*, 121, 620 (2017).

[2] J. Mars et al., *Phys. Chem. Chem. Phys.*, 19, 26651 (2017).

CPP 17.10 Mon 17:30 Poster B1

Influence of hydrocarbons on the bulk and surface structure of ionic liquids — ●JULIAN MARS^{1,2}, HENNING WEISS¹, VEIJO HONKIMÄKI³, BRIDGET MURPHY^{4,5}, MARKUS BIER^{6,7}, and MARKUS MEZGER^{1,2} — ¹Max Planck Institute for Polymer Research, Mainz — ²Institute of Physics and MAINZ Graduate School, Johannes Gutenberg University Mainz — ³ESRF The European Synchrotron, Grenoble — ⁴Institute of Experimental and Applied Physics, Kiel University — ⁵Ruprecht Haensel Laboratory, Kiel University — ⁶Max Planck Institute for Intelligent Systems, Stuttgart — ⁷University of Applied Sciences Würzburg-Schweinfurt

In supported ionic liquid (IL) phase catalysis, knowledge of the interfacial structure is essential to understand diffusion of reactants and products across IL/vapor interfaces. ILs composed of cations with long aliphatic side chains exhibit mesoscopic order and liquid crystalline mesophases. The solvate affinity to the ionic- and aliphatic domains of such ILs can strongly affect their structures adjacent to IL/vapor interfaces. We employ X-ray scattering techniques to investigate the bulk and near surface structure on the molecular length scale. For increasing alkane concentrations, we observe a shift of the first sharp diffraction peak to lower q -values. Originating from the mesoscopic order, this signature indicates aggregation of the non-polar alkanes in the aliphatic domains. Simultaneously, ionic liquid crystal transition temperatures decrease. At the surface, we observe the formation of adsorbate layers and surface induced smectic order.

CPP 17.11 Mon 17:30 Poster B1

Hydration forces on mica-electrolyte interfaces and their ion specificity — SIMONE VAN LIN¹, IGOR SIRETANU¹, ●KARA K. GROTZ², NADINE SCHWIERZ², and FRIEDER MUGELE¹ — ¹Physics of Complex Fluids Group and MESA+ Institute, Faculty of Science and Technology, University of Twente, Enschede, The Netherlands — ²Department of Theoretical Biophysics, Max Planck Institute of Biophysics, Frankfurt am Main, Germany

Hydration forces play a fundamental role for a wide range of biological, chemical, and physical phenomena as they control the formation or prevention of direct contact between any kind of dissolved molecules or suspended particles in water. Here, we study the hydration of mica surfaces in contact with pure water as well as with aqueous alkali chloride salt solutions. Using molecular dynamics simulations in combination with atomic force microscopy experiments, we demonstrate that hydration forces generally consist of both a monotonically decaying and an oscillatory part, each with unique dependence on the specific cation. In measurements, the monotonic hydration force gradually decreases in strength with decreasing ion size, leading to a transition from an overall repulsive (Li^{+}) to an overall attractive (Cs^{+}) total force. In simulations, the presence of strongly hydrated cations (Li^{+}) hardly disturbs the water structure, whereas weakly hydrated cations (Cs^{+}) suppress the pronounced layering of water at the interface, as well as the oscillatory part of the measured hydration force.

CPP 17.12 Mon 17:30 Poster B1

Correlated ion motion in lithium bis(trifluoromethanesulfonyl)imide – glyme solvate ionic liquids: Atomistic insights from molecular dynamics simulations — ●ANDREAS THUM¹, DIDDO DIDDENS², and ANDREAS HEUER¹ — ¹Institut für Physikalische Chemie, Westfälische Wilhelms-Universität Münster, Corrensstraße 28/30, 48149 Münster, Germany — ²Helmholtz-Institut Münster (IEK-12), Forschungszentrum Jülich GmbH, Corrensstraße 46, 48149 Münster, Germany

Motional coupling of ions strongly influences the ionic conductivity of electrolyte solutions and ionic liquids (ILs). In both, the overall anticorrelated motion of like-charged ions reduces the conductivity compared to the ideal Nernst-Einstein conductivity. In electrolyte so-

lutions, the overall correlated motion of opposite-charged ions lowers the conductivity, too. Contrary, in ILs this motional coupling is overall anticorrelated and enhances the conductivity.

To see how dynamic ion correlations evolve in time and space, we performed molecular dynamics simulations of mixtures of lithium bis(trifluoromethanesulfonyl)imide with glymes. These mixtures are known to form solvate ionic liquids (SILs) if mixed in a 1:1 molar ratio. The mixtures investigated here had molar ratios of 2:1, 3:2, 1:1, 1:2, 1:4 and 1:8, covering highly concentrated solutions, SILs and conventional solutions. We found that regarding the motional ion coupling the 2:1, 3:2, 1:1 and 1:2 mixtures behave like conventional ILs, whereas the 1:4 and 1:8 mixtures behave like conventional electrolyte solutions.

CPP 17.13 Mon 17:30 Poster B1

A mechanistic understanding of lithium ion transport in ternary electrolyte systems — ●ALINA WETTSTEIN¹, DIDDO DIDDENS², and ANDREAS HEUER^{1,2} — ¹Institut für Physikalische Chemie, Corrensstraße 28-30, 48149 Münster, Germany — ²Helmholtz-Institut Münster (HI MS), Corrensstraße 46, 48149 Münster, Germany

With regard to methodologically enhancing the electrolyte functionality, and hence the ionic conductivity as a crucial indicator, a profound understanding of the correlated ion motion is essential. For binary ionic liquid systems it has been shown that the motional coupling between ions is determined to a large extent by the conservation of momentum, concurring with simple theoretical relations for transference numbers that serve as a guideline for optimizing the electrolyte [1,2]. Inspired by this work, we perform Molecular Dynamics (MD) simulations to unravel the complex, and rather counterintuitive, interplay of dynamical electrostatic correlations in a ternary ionic liquid - lithium salt mixture, which contribute to the overall conductivity. From systematic analysis of a variety electrolyte compositions we try to identify key parameters that quantify the microscopic transport properties and serve as a constructive optimization concept.

[1] H. Kashyap et al., J. Phys. Chem. B, 2011, 115 (45), pp 13212-13221

[2] D. Diddens, V. Lesch and A. Heuer, Correlated Motion in Ionic Liquids. To be submitted., 2018

CPP 17.14 Mon 17:30 Poster B1

Foam film properties of NaPSS/C₁₄TAB-mixtures: Effect of added Salt — ●KEVIN GRÄFF, LARISSA BRAUN, and REGINE VON KLITZING — Technische Universität Darmstadt, Soft Matter at Interfaces, Darmstadt, Germany

The properties of foams are of interest in many applications such as food technology, firefighting and in personal care products. To understand the properties of macroscopic foams it is important to investigate the single building blocks of it the so-called foam films, which separate the air bubbles from each other. Mixtures of oppositely charged polyelectrolytes and surfactants are widely used in industrial applications as they form highly surface active complexes. Many studies focus on different surfactant, different polyelectrolytes and their ratios. However, the influence of the ionic strength - especially on the foam films - is still unclear. In this work, we use a thin film pressure balance (TFPB) to study the foam films of NaPSS/C₁₄TAB-mixtures in terms of the disjoining pressure inside the foam films, the surface potential at the air/water interface and the foam film stability. We add NaBr (the combination of the two counterions) to get insights on the effect of the ionic strength on the foam film properties.

CPP 17.15 Mon 17:30 Poster B1

Incorporating chemical reactivity into classical molecular dynamics simulations — ●MYRA BIEDERMANN¹, DIDDO DIDDENS^{1,2}, and ANDREAS HEUER^{1,2} — ¹Institute of Physical Chemistry, University of Münster — ²Helmholtz-Institut Münster

We aim at developing a simulation method that incorporates chemical reactivity in a simple but realistic manner while retaining the time and length scales of standard molecular dynamics (MD) simulations. Our methodological approach is inspired by work of Takenaka et al. [1]. There, reactive steps in form of Monte Carlo (MC) steps are introduced in addition to the standard MD steps in order to model chemical reactions within the system. Our specific realisation of those reactive steps differs from those in [1] inasmuch as it also uses information about the kinetics of the reactions (e.g. reaction rates) instead of only thermodynamic informations (e.g. reaction enthalpies). We use extensive ab initio molecular dynamics simulations to validate our approach as well as to estimate the required reaction rates which are used in the

reactive molecular dynamics simulations.

This work is motivated by research on lithium ion batteries, more specifically by investigations regarding the molecular transport and reaction processes at the interface between electrode and electrolyte which lead to the initial formation of a Solid Electrolyte Interphase (SEI) and the formation of dendrites.

[1] N. Takenaka, Y. Suzuki, H. Sakai und M. Nagoaka, The Journal of Physical Chemistry C, pp. 10874-10882, 2014

CPP 17.16 Mon 17:30 Poster B1

Protein condensation in the presence of lanthanide metal ions: relating local structure at the metal centres to phase behaviour — ●OLGA MATSARSKAIA¹, SIN-YUEN CHANG², FELIX ROOSEN-RUNGE³, STEPHEN PARRY², GIANNANTONIO CIBIN², FAJUN ZHANG¹, SVEN L. M. SCHROEDER⁴, and FRANK SCHREIBER¹ — ¹Universität Tübingen, Germany — ²Diamond Light Source Ltd, Didcot, UK — ³Lund University, Sweden — ⁴University of Leeds, UK

Multivalent salts, e.g. YCl₃, have been shown to induce a liquid-liquid phase separation with a lower critical solution temperature (LCST-LLPS) in aqueous solutions of bovine serum albumin (BSA), providing an intriguing experimental framework for a comprehensive study of LLPS in proteins. Here, we attempt to connect the different levels of the description of LCST-LLPS from molecular-level to macroscopic. To this end, we examine the local chemical environment of the Y³⁺ cations using extended X-ray absorption fine-structure (EXAFS) spectroscopy. The EXAFS data show that the Y³⁺ coordination number (CN) decreases with increasing protein concentration and temperature due to the partial substitution of hydration water molecules around the Y³⁺ cations by protein carboxyl groups upon Y³⁺ coordination by the protein. The results of this study thus provide molecular-level evidence that hydration effects are key to LCST-LLPS in systems of BSA and multivalent salts.

CPP 17.17 Mon 17:30 Poster B1

Thermophoresis of a single colloidal particle — ●DANIEL BENJAMIN MAYER and THOMAS FRANOSCH — Institut für Theoretische Physik, Leopold-Franzens Universität, Technikerstraße 21A, A-6020 Innsbruck, Austria

We want to address the problem of a single charged colloid immersed in an electrolyte solution. In the presence of a temperature gradient, electrical body forces are no longer counter balanced by pressure gradients, thereby inducing solvent flow and a directed motion of the colloidal particle. In the limit of small temperature gradients, we numerically solve the associated field equations, including the non-linear Poisson-Boltzmann equation for the electrical potential and the steady Stokes equation governing the fluid flow.

The aim to calculate the thermal mobility is accompanied by difficulties since it appears as a boundary condition in the governing electrokinetic equations. However a decomposition of the problem into two auxiliary ones simplifies this task considerably. Furthermore we also examine the dependence of the thermal mobility on the surface potential and the Soret coefficient of the different ions in the electrolyte.

CPP 17.18 Mon 17:30 Poster B1

Nano-confinement on chain alignment and crystallization of conjugated polymers P3HT and PffBT4T-2OD by printed mesoporous TiO₂ photoanodes — ●NIAN LI, LIN SONG, NITIN SAXENA, WEI CAO, XINYU JIANG, and PETER MÜLLER-BUSCHBAUM — TU München, Physik-Department, LS Funktionelle Materialien, James-Frank-Str. 1, 85748 Garching

Control of n-type inorganic morphology, chain orientation and crystallization of the donor polymers is of significance in hybrid solar cells. Here, we use slot-die printing combined with wet chemistry to fabricate controllable mesoporous TiO₂ nanostructures in large scale. Subsequently, the mesoporous TiO₂ films with different pore size are backfilled with P3HT and PffBT4T-2OD, respectively, using two different ways of infiltration. TiO₂ film morphology is investigated by scanning electron microscopy (SEM) and grazing incidence small-angle X-ray scattering (GISAXS). In order to investigate the effect of TiO₂ pore size on the crystalline properties of the conjugated polymers P3HT and PffBT4T-2OD, e.g. lattice distance, crystal size or orientation, grazing incidence wide-angle X-ray scattering (GIWAXS) is applied to probe the hybrid films. Both P3HT and PffBT4T-2OD crystals with a denser packing of polymer chains exist in the large pore size of TiO₂ films. For backfilling with PffBT4T-2OD, the face-on to edge-on ratio also prefers in the large-pore active layer.

CPP 17.19 Mon 17:30 Poster B1

Time-resolved X-ray scattering for the study of colloidal thin films — ●CHRISTOPHER GREVE¹, MICHAEL BUCHHORN¹, DINESH KUMAR², GUILLAUME FREYCHET², ALEXANDER HEXEMER², LUTZ WIEGART³, and EVA M. HERZIG¹ — ¹Universität Bayreuth, Universitätsstr. 30, 95447 Bayreuth, Germany — ²ALS, Lawrence Berkley National Lab, 1 Cyclotron Road, Berkeley CA 94270, USA — ³NSLSII, Brookhaven National Lab, Brookhaven Avenue, Upton NY, USA

X-Rays are a useful tool to investigate the dynamics and the morphology of hard and soft condensed matter. Synchrotron radiation makes it possible to probe short length scales (< 100 nm) and long time scales (>10⁻⁴ s). To obtain information about the underlying dynamics, during thin film formation, time-resolved measurements are investigated. We investigate slot-die coated thin films in situ in grazing incident geometry to gain insights into the underlying processes of thin film formation. For printing, an up-scalable printer setup is used and as a model system a drying colloidal suspension is examined. Such suspensions are widely used to investigate lattice growth, which is a technologically important research topic (e.g. programmable matter). As a model system, silica nanospheres are used. These feature under solvent evaporation a Kirkwood-Alder transition from amorphous to crystalline FCC thin films via an intermediate glass phase. In addition, a known Bain transition from FCC to BCC can take place under annealing. Using different experimental settings, we systematically study the effect of multiple scattering on the extracted dynamics of drying thin films to investigate the mentioned transitions.

CPP 17.20 Mon 17:30 Poster B1

Stabilization of tubular J-aggregates by silica coating for use in dry environment — ●KATHERINE HERMAN, HOLM KIRMSE, JÜRGEN P. RABE, and STEFAN KIRSTEIN — Humboldt Universität zu Berlin, Institut für Physik

The amphiphilic cyanine dye C8S3 is known to self-assemble in aqueous solution into tubular J-aggregates with a diameter of 13 nm and lengths exceeding microns. Their optical spectra are dominated by exciton bands which are very sensitive to structural changes. A major disadvantage of these aggregates is their low stability during drying. Here we use a coating of a thin layer of silica to stabilize these aggregates. In earlier work [1] shells of silica with controlled and homogeneous thickness of a few nanometer were synthesized around these aggregates without disrupting their optical spectra and hence their J-aggregate character. It is demonstrated here that these silica coatings mechanically and chemically stabilize the C8S3 J-aggregates and allow them to survive not only drying under ambient, but also under vacuum conditions of an electron microscope. Transmission electron microscope images confirm that the thickness of the silica coatings is 5 nm or less and energy dispersive X-ray spectroscopy confirms the presence of true silica. Emission spectra of dried silica coated samples indicate that the molecular structure of the aggregates is preserved and photobleaching under ambient conditions is significantly reduced.

[1] Y. Qiao, F. Polzer, H. Kirmse, S. Kirstein, and J.P. Rabe, Chem. Commun. 51, 11980 (2015)

CPP 17.21 Mon 17:30 Poster B1

Crystallization kinetics in colloidal hard spheres via real space analysis using Confocal microscopy — ●SAHANA KALE and HANS JOACHIM SCHÖPE — Institut für Angewandte Physik, Universität Tübingen, Germany

The nucleation rate densities from experimental and theoretical data diverge by several orders of magnitudes and the curves are qualitatively different. One of our research goals is to find the underlying reason for this discrepancy, if there is any.

Crystallization of meta-stable colloidal hard sphere suspensions is studied in real space using laser scanning confocal microscopy. Direct imaging in three dimension offers the unique possibility to observe crystal nucleation and growth on particle level giving detailed information about the fluid to crystal phase transformation

Keywords: Colloids, Confocal microscopy, Nucleation, Crystallization

CPP 17.22 Mon 17:30 Poster B1

Surface Preparation of Ice Single Crystals — ●MARKUS BATZER^{1,2}, JENÉE CYRAN¹, MARC-JAN VAN ZADEL¹, ELLEN H. G. BACKUS^{1,3}, and MARKUS MEZGER^{1,2} — ¹Max Planck Institute for Polymer Research, Mainz — ²Institute of Physics, Johannes Gutenberg University Mainz — ³Department of Physical Chemistry, University of Vienna

Experiments in surface science often require samples made of high quality single crystals with surfaces containing little defects. However, at temperatures of around -10 °C, ice is a comparatively ductile material, making surface preparation challenging. We studied the near surface structure of ice single crystals prepared by different protocols using high resolution X-ray diffraction. Analysis of the diffraction data revealed that mechanical treatment can introduce distortions ranging up to several millimeters inside the bulk ice.

CPP 17.23 Mon 17:30 Poster B1

Post-treatment of thermoelectric polymer thin films to influence their thermoelectric properties — ●ANNA-LENA OECHSLE, NITIN SAXENA, and PETER MÜLLER-BUSCHBAUM — TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany

Thermoelectric materials are of great interest in terms of waste heat recovery and the use of solar thermal energy. Especially thermoelectric polymers are attractive, as they own some advantages over so far used inorganic thermoelectric materials, such as low cost, high mechanical flexibility, low or no toxicity, light weight and intrinsically low thermal conductivity. A way to evaluate the thermoelectric property of a material is the power factor $PF=S^2\sigma$. This parameter depends on the Seebeck coefficient S and the electrical conductivity σ , which again are affected by the electronic and morphological features of the polymer. In order to investigate ways to influence these features and improve the power factor, we fabricate thin semi-conducting polymer films and post-treat them in different ways. With measurements of the Seebeck coefficient, the electrical conductivity, UV-Vis, layer thickness changes and determination of the structure we attempt to find a morphology-function relation.

CPP 17.24 Mon 17:30 Poster B1

Electrically conductive multilayer films created from carbon nanotubes and polyelectrolytes — ●SVEN NEUBER, ANNEKATRIN SILL, HEIKO AHRENS, and CHRISTIANE A. HELM — Institute of Physics, University of Greifswald, 17489 Greifswald, Germany

Films built from polyelectrolytes PSS, PDADMAC in 0.1 Mol/L NaCl and carbon nanotubes are investigated. Multilayer built-up was carried out by sequential adsorption of oppositely charged polyelectrolytes. Carbon nanotubes were modified with a volume/volume acid mixture (HNO₃ (60-68%) and H₂SO₄ (98%)) to make them water soluble and negatively charged. AFM-images revealed a horizontal orientation of carbon nanotubes on the surface of the multilayer. Also, UV-vis, QCM and ellipsometry measurements were used to determine surface coverage and thickness on nm-scale. Sheet resistance decreases monotonously with the number of carbon nanotube layers. Choosing the multilayer architectures allows to tune its sheet.

CPP 17.25 Mon 17:30 Poster B1

A new wafer scale deposition concept for 2D photoactive Bismuth/Bismuth(hydr)oxide multilayers for energy harvesting and environmental sensors — ●SEBASTIAN RUNDE, CHRISTIAN VON SAVIGNY, and CHRISTIANE A. HELM — Institute of Physics, Universität Greifswald, Felix-Hausdorff-Str. 6, 17489 Greifswald

We present a transparent and photoactive multilayer consisting of ultrathin Bismut/Bismuth(hydr)oxide (Bi/BiOxHy) layers, prepared on glass substrates by induced break-up after forced wetting. A 3 nm thick monolayer is electrically isolating, transparent and laterally homogeneous. Multilayers are photoactive. The electric conductivity increases spontaneously with light intensity, it depends weakly on temperature and relative humidity. Thus, the sheet resistance can be tuned between 10 and 350 kΩ. To test long-term stability, the electric conductivity of the multilayer was measured in dependence of the local solar radiation. Fast-Fourier-Transformation of this time dependent sheet resistance shows a dominating cycle duration of ca. 24h.

CPP 17.26 Mon 17:30 Poster B1

Dynamics upon arrest in protein solutions with LCST phase behavior — ●ANASTASIA RAGULSKAYA¹, NAFISA BEGAM¹, ANITA GIRELLI¹, HENDRIK RAHMANN², FAJUN ZHANG¹, CHRISTIAN GUTT², THOMAS ZINN³, and FRANK SCHREIBER¹ — ¹Universität Tübingen — ²Universität Siegen — ³ESRF

Dynamically arrested states can occur as a result of an interplay of liquid-liquid phase separation (LLPS) and glass formation in protein and colloidal systems. We use a model system of bovine serum albumin (BSA) with YCl₃ which shows LLPS and a lower critical solution tem-

perature (LCST) phase behavior [1]. Following a temperature jump (T-jump) the protein-rich phase undergoes an arrested spinodal decomposition. Growth kinetics of a characteristic length as a function of time, observed using ultra-small angle X-ray scattering, shows a transition to an arrested state at high temperatures. Here, we investigate the dynamics of LLPS approaching the arrested state using X-ray photon correlation spectroscopy (XPCS). The analysis of two-time correlation functions obtained from XPCS shows compressed exponential dynamics in the temperature range $\sim 45 - 50^\circ\text{C}$, with further transfer to stretched dynamics beyond 52.5°C . This may be treated as a transition from a superdiffusive to an intermittent dynamics of a glassy state. The dramatic jump of the characteristic relaxation time τ constant with q indicates the emergence of an arrested state above 52.5°C , but below thermal denaturation (60°C). For each T-jump, τ first increases, then becomes faster again before the system gets arrested.

[1] O.Matsarskaia et. al., *Phys. Chem. B*, **120**, 5564, 2016.

CPP 17.27 Mon 17:30 Poster B1

Heterogeneous dynamics in an arrested state in a protein system — ●ANITA GIRELLI¹, NAFISA BEGAM¹, ANASTASIA RAGULSKAYA¹, HENDRIK RAHMANN², FABIAN WESTERMEIER³, CHRISTIAN GUTT², FAJUN ZHANG¹, and FRANK SCHREIBER¹ — ¹Universität Tübingen, Germany — ²University of Siegen, Germany — ³Petra III, DESY, Germany

In protein solutions, the interplay between LLPS and glass formation can lead to an arrested state. So far, little is known about the dynamic properties of the arrested state. Here we show the collective dynamics using XPCS for a protein-PEG system. The protein employed here is γ -globulin. PEG (polyethylene glycol) permits the attraction between the protein through depletion. The system has an upper critical solution temperature (UCST), and in a previous study the coarsening kinetics after quenching was studied with USAXS and USANS [1]. The results show that the size of the domains remains constant with time at very low temperatures (below glass transition) indicating that the system enters an arrested state. Here we find that the system close to the arrest shows lower relaxation times compared to the one where a complete phase separation occurs. The dynamics in the arrested state shows strong heterogeneity which increases with the quench depth. The results indicate the presence of cooperative domain motion, suggesting that the enhancement of cooperativity leads to the arrest at low temperatures.

[1] Da Vela et al., *Soft Matter*, **13**, 8756, 2017

CPP 17.28 Mon 17:30 Poster B1

Effect of shear on relaxation dynamics in glass-forming systems close to the glass transition — ●LAWRENCE SMITH, DARIO MAUTH, GERHARD WILDE, and ANDREAS HEUER — Westfälische Wilhelms-Universität, Münster, Germany

In ongoing experimental work on bulk metallic glasses, it has been observed that deformed samples may exhibit a higher relaxation enthalpy than an undeformed reference sample as measured by differential scanning calorimetry.

We investigate this effect using molecular dynamics (MD) simulations of a mixture of binary Lennard-Jones particles. The deformation of this model glass former is known to exhibit a stress overshoot and shear-bands as observed in experimental bulk metallic glasses and is therefore appropriate to qualitatively reproduce these results and shed light on the underlying mechanisms.

The analysis of the underlying potential energy landscape of small systems has been shown to yield quantitative information on the systems dynamics in MD simulations in equilibrium. We use these same methods to investigate the relaxation from a deformed sample and an undeformed non-equilibrium sample close to the glass transition, and observe a crossing in the potential energy curves during relaxation.

Any anisotropy in the deformed sample vanishes before significant relaxation processes take place, ruling it out as a major factor on the relaxation. In larger samples we find a long lived local density modulation that may enable different mechanisms for the relaxation to take place in deformed and undeformed samples.

CPP 17.29 Mon 17:30 Poster B1

How coupled elementary units determine heterogeneity in macroscopic glass-forming systems — ●LAWRENCE SMITH and ANDREAS HEUER — Westfälische Wilhelms-Universität, Münster, Germany

Elementary units of a binary Lennard-Jones glassformer can be iden-

tified through quantitative analysis of its underlying potential energy landscape. These units can be fully understood within the continuous time random walk formalism and are found to contain the complete information concerning thermodynamics and diffusivity, while displaying finite size effects with respect to relaxation times and spacial correlations [1].

Previous research has shown that it is possible to identify major contributions to the non-Gaussian parameter as arising from the moments of the waitingtime distribution for jumps between metabasins of the potential energy landscape [2].

We investigate the impact of a coupling between elementary units on the non-Gaussian parameter (NGP) to gain insight into mechanisms underlying the emergence of dynamic heterogeneity as measured in the NGP and four-point correlation functions in the stochastic model as well as in molecular dynamics simulations.

[1] C. Rehwald, A. Heuer, *Phys. Rev. E* **86**, 051504 (2012)

[2] C. Schröder, A. Heuer, *Phys. Rev. Lett.* **110**, 067801 (2013)

CPP 17.30 Mon 17:30 Poster B1

Impact of incorporating ultrastable glass layers on device efficiency and stability of organic light-emitting diodes — ●ELISABETH BIRGIT SCHWARZ¹, PAUL-ANTON WILL¹, JOAN RÀFOLS-RIBÉ², CHRISTIAN HÄNISCH¹, MARTA GONZALEZ-SILVEIRA², SIMONE LENK¹, JAVIER RODRÍGUEZ-VIEJO², and SEBASTIAN REINEKE¹ — ¹Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute for Applied Physics, Technische Universität Dresden, Germany — ²Group of Nanomaterials and Microsystems, Universitat Autònoma de Barcelona, Spain

For current and future applications of organic-light emitting diodes (OLEDs), high device efficiency and stability are required. Additionally, to keep the process of making OLEDs competitive in the real production, simple device architecture and reproducibility are crucial. In this work, we present the incorporation of ultrastable glass layers in OLEDs as a concept that does not require material refinement or changes in stack architecture and is hence suggested to be generally applicable. At the same time, it allows to increase both, external quantum efficiency and lifetime of the OLEDs, by more than 15% compared to reference devices. This enhancement is achieved by fabricating several of the functional organic layers as ultrastable glasses through adjusting the substrate temperature and hence the growth conditions during physical vapor deposition. Ultrastable glasses appear as thermodynamically most favorable state and, thus, most stable molecular conformation in disordered solids achievable nowadays. We present detailed studies for OLEDs with four different phosphorescent emitters.

CPP 17.31 Mon 17:30 Poster B1

Multiple Glassy Dynamics of an Asymmetric PVME/PS Blend Investigated by Broadband Dielectric and Specific Heat Spectroscopy — ●PAULINA SZYMONIAK, SHERIF MADKOUR, and ANDREAS SCHÖNHALS — Bundesanstalt für Materialforschung und prüfung (BAM), Berlin, Germany

Over the past decades research on the molecular dynamics of miscible polymer blends is of topical interest in the literature, to understand the segmental mobility of individual components, as it is affected by blending. In general, miscible polymer blends exhibit a complex dynamic behavior. For an A/B blend the relaxation times of component A and component B are affected by the spatial local compositional heterogeneity, present in binary systems on a microscopic level, regardless of the macroscopic homogeneity. Here, a combination of broadband dielectric and specific heat spectroscopy was employed to study the dynamically asymmetric PVME/PS blend with seven different compositions, focusing on samples with high PS contents. Considering that PS is dielectrically invisible, BDS is a powerful technique to study the response of PVME, as it is affected by PS segments. Here, three separate relaxation processes were found by dielectric investigations, related to confined or constrained PVME segments due to the spatial local compositional heterogeneities, which is in contrary to the previous literature findings [1]. Moreover, the dielectric data was compared with results obtained by specific heat spectroscopy, where a fourth relaxation process was found, due to the cooperative fluctuations of PVME and PS. [1] Colmenero, J., Arbe, A. *Soft Matter*, 2007, 3, 1474.

CPP 17.32 Mon 17:30 Poster B1

Tunable surprising glassy dynamics in MAPLE deposited nanostructured polymer — ●MITHUN CHOWDHURY¹, XAVIER MONNIER², YUCHENG WANG³, DANIELE CANGIALOSI², and RODNEY PRIESTLEY³ — ¹Metallurgical Engineering and Materials Science, IIT

Bombay, Mumbai 400076, India — ²Centro de Fisica de Materiales, CSIC-UPV/EHU, San Sebastian 20018, Spain — ³Chemical and Biological Engineering, Princeton University, NJ 08544, USA

In this study we characterize glassy dynamics of Matrix Assisted Pulsed Laser Evaporation (MAPLE) deposited poly (methyl methacrylate) (PMMA) films. For that, we exploit fast scanning calorimetry to investigate the molecular mobility and the vitrification kinetics in terms of the thermodynamic state attained after a given cooling rate. We found in general any MAPLE deposited glass is thermodynamically more stable than bulk polymer standard glass, as indicated by lower fictive temperature in comparison to standard glass. Intriguingly, MAPLE deposited glasses exhibits at the same time faster molecular mobility. For a standard glass, the opposite behavior is generally found. Furthermore, by heating (aging and annealing) and controlling MAPLE deposition temperature, the amorphous state can be tuned. This still significantly deviates from the standard PMMA. We tentatively conclude that MAPLE deposited glasses are formed following a distinguished kinetic path, leading to an amorphous state well different from that of glasses formed in the conventional way, that is, by cooling through its glass transition temperature from melt.

CPP 17.33 Mon 17:30 Poster B1

Growth Kinetics and Molecular Mobility of Irreversibly Adsorbed Layers in Thin Polymer Films — ●MARCEL GAWEK, ANDREAS HERTWIG, and ANDREAS SCHÖNHALS — Bundesanstalt für Materialforschung und -prüfung, Unter den Eichen 87, 12205 Berlin

In well-annealed thin polymer films, with non-repulsive polymer/substrate interactions, an irreversibly adsorbed layer is formed. These adsorbed layers have shown enormous potential for technological applications. The growth kinetics and molecular dynamics of these buried layers in thin films are still not fully investigated due to the hard accessibility. Here, the irreversibly adsorbed layers of homopolymer thin films are revealed by solvent-leaching experiments. The growth kinetics of these layers is investigated as a function of original film thickness and annealing times. The thickness, topography and quality of the adsorbed layer is determined with Atomic Force Microscopy (AFM) and spectroscopic ellipsometry. Additionally, the molecular mobility of the adsorbed layer is investigated with Broadband Dielectric Spectroscopy (BDS). A recently developed nanostructured capacitor (NSC) is employed to measure the adsorbed layers with a free surface layer depending on annealing and solvent-leaching time. The results are quantitatively compared and discussed with respect to recently published work.

CPP 17.34 Mon 17:30 Poster B1

Structure and morphology in tetracene-C60 blends — ●KATJA SCHICK, CLEMENS ZEISER, and KATHARINA BROCH — Institut für Angewandte Physik, Universität Tübingen, Deutschland

Although C60 is one of the classical acceptors in organic solar cells [1], the mechanisms of its structure formation in blends are not fully understood. However, since the mixing behaviour or the length scales of phase separation are affecting device performance [2], an understanding of the underlying mechanisms is important. Phase separating systems can exhibit interesting kinetic effects as demonstrated, e.g. in blends of C60 and diindenoperylene (DIP), for which a thickness-dependent domain size has been observed [3].

In order to study how the length of the co-evaporated molecule influences the thickness-dependent phase separation and island size, we use tetracene (TET) which is shorter than DIP. To analyse the thickness-dependent structure and morphology of the TET:C60 films we use X-ray diffraction, AFM and SEM and discuss our findings in view of the steric compatibility of the two molecules.

- [1] N. Martín et al. *Chemical Review*. 98(1998)
- [2] S. Oosterhout et al. *Nature Materials*. 8(2009)
- [3] R. Banerjee et al. *Physical Review Letters*. 110(2013)

CPP 17.35 Mon 17:30 Poster B1

Structural and optical properties of pentacene and tetracene blends — ●DANIEL LEPPLE, CLEMENS ZEISER, and KATHARINA BROCH — Universität Tübingen

Optoelectronic devices based on organic semiconductors (OSCs) have found industrial applications, e.g. as light-weight and flexible displays [1]. In many devices, the active layer is composed of mixtures of two OSCs where one acts as a donor and the other one as an acceptor. As the device performance is strongly affected by the structural and optical properties of the mixed film, an understanding of structure-

property relations is not only interesting from the viewpoint of fundamental research but also important for further device optimization. A prototypical class of OSCs to study the processes of structure formation and their impact on photophysical properties are acenes, especially tetracene and pentacene [2]. Although their properties have been studied extensively, there remain open questions due to the complex photophysics of these two molecules [3]. Here, we report on the structural and steady-state optical properties of blends of tetracene and pentacene, which we use as a model system for the study of structure-property relations in weakly interacting, structurally compatible systems.

- [1] J. H. Koo et al. *Adv Funct. Mater.* 28 (2018)
- [2] J. Anthony et al. *Chemical Review*. 106 (2006)
- [3] D. Beljonne et al. *Physical Review Letter*. 110 (2013)

CPP 17.36 Mon 17:30 Poster B1

Optical Investigation of Charge Transfer States in Tetracene/F6-TCNNQ Blends — ●CHRISTOPH THEURER¹, CLEMENS ZEISER¹, NICO HOFEDITZ², WOLFRAM HEIMBRODT², MARTIN KOCH², and KATHARINA BROCH¹ — ¹Eberhard Karls Universität Tübingen, Institut für Angewandte Physik, Auf der Morgenstelle 10, 72076 Tübingen — ²Philipps Universität Marburg, Physikalisches Institut, Renthof 5, Laborbau II, 35032 Marburg

Organic semiconductors have a huge potential for large area, cost and energy efficient optoelectronic devices like organic solar cells or OLED displays [1]. The majority of functional devices rely on charge transfer interactions between acceptor and donor molecules.

F6-TCNNQ is one of the strongest organic acceptor molecules known and is widely used for doping and studying charge transfer effects [2]. We have mixed it with tetracene, a member of the family of acenes, which exhibit interesting optical properties and effects like singlet fission [3]. Although tetracene is already intensively studied, little is known about charge transfer interactions in blends with acceptors [4]. We study the photophysics of the observed charge-transfer states and discuss our findings based on the structural and morphological properties of tetracene/F6TCNNQ blends with different mixing ratios. This serves as starting point for further time-resolved investigations of this fundamentally interesting system.

[1] Forrest, S. R., *Nature* 428 (2004) [2] Koech, P. K., et al., *Chemistry of Materials* 22 (2010) [3] Smith, M. B., and Michl, J., *Chemical Reviews* 110 (2010) [4] Hu, P., et al., *CrystEngComm* 19 (2017)

CPP 17.37 Mon 17:30 Poster B1

Analysis of metal nanostructure evolution on polymer surfaces by in-situ GISAXS during sputter deposition — ●VALENTIN MUNTEANU¹, SIMON J. SCHAPER¹, VOLKER KÖRSTGENS¹, MATTHIAS SCHWARTZKOPF², PALLAVI PANDIT², ALEXANDER HINZ³, OLEKSANDR POLONSKYI³, THOMAS STRUNSKUS³, FRANZ FAUPEL³, STEPHAN V. ROTH⁴, and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — ²DESY, 22607 Hamburg — ³CAU zu Kiel, Institut für Materialwissenschaft, LS Materialverbunde, 24143 Kiel — ⁴KTH, Department of Fibre and Polymer Technology, SE-100 44 Stockholm, Sweden

A good understanding of the fabrication process of reproducible functional metal-polymer interfaces is of high importance for their use in organic electronics. Sputter deposition offers the ability to precisely control and tailor the fabrication of metal-polymer interfaces. During sputter deposition, the evolution of the metallic layer morphology is monitored in-situ with time-resolved grazing-incidence small-angle X-ray scattering (GISAXS). The resulting in-situ scattering data is processed and analyzed using the DPDAK software package. By fitting the processed data, structure parameters can be extracted whose temporal evolution reveals the mode of metal growth on polymer surfaces. Simulations with BornAgain lead to a deeper understanding of the growth mechanism of sputter deposited metal-polymer interfaces.

CPP 17.38 Mon 17:30 Poster B1

Self-assembly of large nanoparticles in ultrahigh molecular weight linear diblock copolymer films — ●WEI CAO¹, SENLIN XIA¹, XINYU JIANG¹, MICHAEL APPOLD², MATTHIAS OPEL³, MARKUS GALLEI², MATTHIAS SCHWARTZKOPF⁴, STEPHAN V. ROTH^{4,5}, and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — ²TU Darmstadt, Ernst-Berl-Institute for Technical and Macromolecular Chemistry, 64287 Darmstadt — ³Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching — ⁴DESY,

Notkestrasse 85, 22603 Hamburg — ⁵KTH Royal Institute of Technology, SE-100 44 Stockholm, Sweden

The preparation of block copolymer nanocomposite films that consist of nanoparticles (NPs) with diameters (D) of more than 10 nm is a challenging task. Herein, ultrahigh molecular weight (UHMW) linear polystyrene-block-poly(methyl methacrylate) (PS-*b*-PMMA) diblock copolymer was spin-coated as a template for the self-assembly of large iron oxide NPs (D = 28.5 nm), and the morphology of hybrid nanocomposites was governed by the concentration (C) of the iron oxide NPs. Via hydrogen bonding between the carboxylic acid groups on iron oxide and the PMMA side chains of the diblock copolymers, the NPs were selectively incorporated inside the PMMA cylinders. Due to the rearrangement of the PMMA chains for accommodating the NPs, well-ordered cylindrical nanostructure were readily generated at low NP concentrations (C = 0.5 wt%). Most interestingly, a chain-like network appears inside the hybrid films at a high NP loading.

CPP 17.39 Mon 17:30 Poster B1

Thermal Oscillations in Homopolymer Blends — •LOUIS PIGARD and MARCUS MÜLLER — Institute for Theoretical Physics, University of Göttingen, Germany

Immiscible homopolymer blends are binary mixtures that exhibit macroscopic phase-separation of their constituents A and B in equilibrium. The immiscibility of A and B is commonly characterized by the interaction parameter χ_N . For sufficiently high χ_N the blend demixes into two macroscopic A- and B-rich domains that are spatially separated by a single interface.

We study how this behaviour is altered if the temperature of the system and thus χ_N is oscillating in time. We model the dynamics by the Cahn-Hilliard equation and, additionally, verify our results with Monte-Carlo simulation of a soft, coarse-grained particle model that mimics Rouse dynamics.

For suitable values for the amplitude and period of the oscillation we observe the emergence of new metastable states with three interfaces and four domains in a thin-film geometry, i.e., the oscillation of incompatibility qualitatively changes the behavior from macro- to microphase separation in a thin film geometry.

We study the dependence of this microphase-separated state on the strength and frequency of the oscillation and explore the (meta)stability of the new, oscillation-induced state.

CPP 17.40 Mon 17:30 Poster B1

Free energy of interaction between polymers and Guanine-Quadruplexes using Molecular Dynamics Simulations — •SANWARDHINI PANTAWANE and STEPHAN GEKLE — Biofluid Simulation and Modeling Group, Theoretische Physik VI, Universität Bayreuth, 95440 Bayreuth Germany

In this investigation, free energy calculations on a system consisting of Poly(3-hexylthiophene-2,5-diyl) (P3HT) chains and Guanine-Quadruplex DNA molecule, immersed in water are carried out. Such a polymer-DNA assembled system can be used to construct DNA biosensors, but has yet not been accomplished due to the lack of understanding of their conformational and thermodynamical stability. We construct a system with a four repeat G-Quadruplex molecule sitting over a planar surface of five collaterally arranged P3HT chains with 20 repeats each and apply umbrella sampling to pull the DNA molecule away from the P3HT polymer surface. We carry out the free energy calculations derived from a series of umbrella sampling simulations using a Weighted Histogram Analysis Method (WHAM), which would give an insight on determining the probability of the DNA molecule to attach to the conjugated polymers. An additional study on the effect of oxidation on such a G-quadruplex structures is also presented here.

CPP 17.41 Mon 17:30 Poster B1

Modelling DNA-strand displacement reactions in the presence of base-pair mismatches — •PATRICK IRMISCH and RALF SEIDEL — Molecular Biophysics group, Peter Debye Institute for Soft Matter Physics, University of Leipzig, 04103 Leipzig, Germany

Toehold-mediated strand displacement is the most abundantly used method to achieve dynamic switching in DNA-based nanotechnology. A single-stranded 'invader' strand binds to the 'toehold' overhang of a target strand and replaces a target-bound 'incumbent' strand. Hereby, complementarity of the invader to the single-stranded toehold provides the energetic bias of the reaction.

The aim of this work is to obtain a quantitative description of the kinetics of strand displacement reactions in the presence of mismatches

using simple biophysical modelling. This would allow for predicting strand-displacement rates when setting up strand-displacement reaction networks. We model the strand-displacement rate as the mean-first-passage time of a random walk within a simplified 1D energy landscape. In case of single invader mismatches, our model successfully describes the displacement kinetics as function of the mismatch position and the toehold length using a minimal set of parameters. Most importantly, our model is able to predict the kinetics of strand displacement reactions in presence of multiple invader mismatches as well as incumbent mismatches. Comparisons with experimental data confirm the model prediction and thus the general applicability of our approach.

CPP 17.42 Mon 17:30 Poster B1

Nano-electronic components built from DNA templates — •JINGJING YE and RALF SEIDEL — 1Peter Debye Institute for Soft Matter Physics, Universität Leipzig, Germany

DNA Origami takes advantage of base complementarity of individual short oligonucleotides, to fold a long scaffold strand into almost any continuous 2D or 3D shape. We recently introduced a new concept of DNA origami mold-based particle synthesis that allows the synthesis of inorganic nanoparticles with a programmable shape. We demonstrated the concept by fabricating a 40 nm long rod-like gold nanostructure with a quadratic cross-section. We expanded the capabilities of the mold-based particle synthesis to demonstrate the synthesis of uniform μm long conductive gold nanowires with 20-30 nm diameters. With conductance characterization, metallic conducting wires were demonstrated. Here the concept is further expanded by designing mold monomers with different geometries and interfaces. We can fabricate more complex mold-superstructure in an addressable and flexible way like lego bricks.

CPP 17.43 Mon 17:30 Poster B1

Anomalous Diffusion in Reversible Networks — •KIRAN SURESH KUMAR^{1,2}, JENS-UWE SOMMER^{1,2}, and MICHAEL LANG¹ — ¹Leibniz-Institut für Polymerforschung Dresden, Institut Theorie der Polymere, Hohe Strasse 6, 01069 Dresden, Germany — ²Institute für Theoretische Physik, Technische Universität Dresden, Zellescher Weg 17, 01069 Dresden, Germany

Recent experiments and simulation studies find an anomalous super diffusive regime in reversible networks by analyzing Forced Rayleigh Scattering (FRS) data [1-3]. The molecular origin of this super diffusive regime is not yet fully understood. In our contribution, we approach this problem by computer simulations of FRS experiments in reversible networks based upon the Bond Fluctuation Model and additional stochastic simulations. We analyze the dynamics of individual molecules and correlate these with bond association and dissociation times. We further discuss the dependence of collective observables as accessible in FRS experiments with molecular parameters of the reversible gel.

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[3] Ramirez, J.; Dursch, T. J.; Olsen, B. D. *Macromolecules* 2018, 51, 2517-2525.

CPP 17.44 Mon 17:30 Poster B1

Investigation of swelling of coatings and the change of their mechanical properties at different air humidity — •HANNES SCHEDLBERGER¹, BERNHARD STRAUSS², and SABINE HILD¹ — ¹Institute of Polymer Science, Johannes Kepler University Linz, Altenberger Str. 69, 4040 Linz, Austria — ²Voestalpine Stahl GmbH, voestalpine-Straße 3, 4020 Linz, Austria

To protect steel surfaces against corrosion thin layer of organic coatings are applied. When used, water may be absorbed in the coatings and diffused through the layers. This can cause a variety of damages. Although this is a well known effect, the process of migration within the coatings and its consequences are still not clear. Therefore it is of utmost importance to investigate the amount of absorbed water, the adsorption kinetics and the correlation of the water absorption with the chemical structure and the mechanical properties of the coatings.

Atomic Force Microscopy (AFM) provides the possibility to observe the changes at the surface and to analyse the changes in the mechanical properties of the coatings as well. The swelling of the organic coating applied on a steel substrate were observed for 24 hours at various air humidity concentrations within a humidity cell at the AFM. To

obtain the various air humidity concentrations, different salt solutions like potassium hydroxide or potassium nitrate were inserted into the humidity cell, followed by the analysis of the coatings. The changes

of the mechanical properties of the coatings were analysed performing force distance curves.