

## CPP 24: Poster Session I

Topics: Biopolymers, Biomaterials and Bioinspired Functional Materials (24.1-24.9); Charged Soft Matter, Polyelectrolytes and Ionic Liquids (24.10-24.14); Crystallization, Nucleation and Self-Assembly (24.15-24.27); Electrical, Dielectrical and Optical Properties of Thin Films (24.28-24.33); Interfaces and Thin Films (24.34-24.37); Polymer Networks and Elastomers (24.38-24.42), Soft Matter and Nanocomposites - New opportunities with advanced neutron Sources (24.43-24.51).

Time: Monday 17:30–19:30

Location: P3

## CPP 24.1 Mon 17:30 P3

**Multivalent Cation-Induced Actuation of DNA-Mediated Colloidal Superlattices** — DEVLEENA SAMANTA<sup>1,3</sup>, ●AYSEUR ISCEN<sup>2</sup>, CHRISTINE R. LARAMY<sup>2,3</sup>, SASHA B. EBRAHIMI<sup>2,3</sup>, KATHERINE E. BUJOLD<sup>1,3</sup>, GEORGE C. SCHATZ<sup>1,3</sup>, and CHAD A. MIRKIN<sup>1,2,3</sup> — <sup>1</sup>Department of Chemistry — <sup>2</sup>Department of Chemical and Biological Engineering — <sup>3</sup>International Institute for Nanotechnology, Northwestern University, Evanston IL USA

Nanoparticles functionalized with DNA can assemble into ordered superlattices with defined crystal habits through programmable DNA “bonds”. Here, we examine the interactions of multivalent cations with these DNA bonds as a chemical approach for actuating colloidal superlattices. Multivalent cations alter DNA structure on the molecular scale, enabling the DNA “bond length” to be reversibly altered between 17 and 3 nm, ultimately leading to changes in the overall dimensions of the micron-sized superlattice. The identity, charge, and concentration of the cations each control the extent of actuation, with Ni<sup>2+</sup> capable of inducing a remarkable >65% reversible change in crystal volume. Molecular dynamics simulations provide insight into the conformational changes in DNA structure as the bond length approaches 3 nm and show that cations that screen the negative charge on the DNA backbone more effectively cause greater crystal contraction. Taken together, the use of multivalent cations represents a powerful strategy to alter superlattice structure and stability, which can impact diverse applications through dynamic control of material properties, including the optical, magnetic, and mechanical properties.

## CPP 24.2 Mon 17:30 P3

**Cross-scale characterization of the interaction of polymers on cellulose interfaces: Construction of a model surface of cellulose** — ●CASSIA LUX, THOMAS TILGER, OLAF SOLTWEDEL, and REGINE VON KLITZING — Department of Physics, Technische Universität Darmstadt, Darmstadt, 64289, Germany

As a functional material, cellulose based paper has a high importance in a variety of sectors, such as packaging, print media and speciality papers. This is especially crucial with regard to reducing plastic use and waste and replacing it with renewable and biodegradable resources.

The interactions of cellulose fibers with functional additives, such as the wet-strength increasing polymer PDADMAC, have been investigated in the past with respect to the mechanical properties of the resulting paper. Yet, a systematic understanding of the effects of the chemistry and structure of the polymer on the properties of the fibers is still missing and would lead to an exhaustive knowledge of the functionalization of paper.

For a detailed examination, model surfaces are prepared by dip and spin coating from both soluble carboxymethyl cellulose (CMC) and suspended microcrystalline cellulose (MCC) under the variation of extrinsic conditions such as concentration and pH value of the polyelectrolyte solutions and deposition time. Ellipsometry and AFM measurements allow for a comprehensive investigation of the influence of these conditions on features like thickness and roughness of the synthesized films.

## CPP 24.3 Mon 17:30 P3

**Development of a new paper-based test system using electrochemical reactions** — MARC RIEDEL<sup>1</sup>, ●OLIVER NAGEL<sup>2</sup>, WERNER WIRGES<sup>2</sup>, ROBERT NIEDL<sup>2</sup>, FRED LISDAT<sup>1</sup>, and CARSTEN BETA<sup>3</sup> — <sup>1</sup>Technische Hochschule Wildau — <sup>2</sup>Universität Potsdam — <sup>3</sup>Diamond Inventics

Paper-based sensors have reached a wide popularity in research and industry. Such systems are low cost in production and simple to fabricate. Furthermore, the benefit in analysis speed and availability made them attractive and easy to use as analytical tools. Paper is available in a wide range of thicknesses, it is biodegradable, and environmentally friendly. The hydrophilicity and porosity of the paper provide a nat-

ural substrate for the fabrication of microfluidic channels and can be operated without an external power source for fluid control. It is possible to easily print, coat, and link chemical reagents or (bio)molecules to the paper surface. This work will show a new paper-based test system consisting of a carbon and a silver electrode printed on the paper to detect electrochemical reactions on the chip. To test the  $\mu$ PAD (microfluidic paperbased analytical device), a peroxidase/ferrocene redox system was used for amperometric measurements.

## CPP 24.4 Mon 17:30 P3

**Folding kinetics within recombinant spider silk coatings** — ●MIRJAM HOFMAIER<sup>1,2</sup>, BIRGIT URBAN<sup>1</sup>, SARAH LENTZ<sup>3</sup>, THOMAS SCHEIBEL<sup>3</sup>, ANDREAS FERY<sup>1,2</sup>, and MARTIN MÜLLER<sup>4</sup> — <sup>1</sup>Leibniz Institute of Polymer Research Dresden, Institute of Physical Chemistry and Polymer Physics, Hohe Straße 6, D-01069 Dresden — <sup>2</sup>Technical University Dresden, Chair of Physical Chemistry of Polymeric Materials, 01069 Dresden — <sup>3</sup>University of Bayreuth, Chair of Biomaterials, Rüdiger-Bormann Str. 1, D-95447 Bayreuth — <sup>4</sup>Technical University Dresden, Chair of Macromolecular Chemistry, 01062 Dresden

The folding kinetics of the recombinant spider silk protein eADF4(C16) in thin films was analysed by in-situ ATR-FTIR spectroscopy. eADF4(C16) was cast from hexafluoroisopropanol solutions (1-50 mg/ml) to respective thin and thick films onto unidirectionally scratched silicon substrates (Si-sc). To quantify secondary structure portions, the Amide-I band was examined using line shape analysis (LSA). Five relevant components in the range between 1585 and 1730 cm<sup>-1</sup> were identified and assigned to typical secondary structures. Significant decrease of random coil and increase of beta-sheet content was recorded by ATR-FTIR measurements over 24 hours while treating the initial eADF4(C16) films with methanol vapour (MeOH-v) or liquid methanol (MeOH-l). The protein folding appears to be a two-state kinetic process. Received rate constants indicate folding kinetics of first order by MeOH-v treatment and both zero and first order by MeOH-l treatment. No dependence of folding kinetics on the layer thickness could be found.

## CPP 24.5 Mon 17:30 P3

**Structural properties and chain connectivity in squid-based biopolymer networks analysed by 1H time-domain NMR experiments** — ●LUCAS LÖSER<sup>1</sup>, HUIHUN JUNG<sup>2</sup>, MELIK DEMIREL<sup>2</sup>, and KAY SAALWÄCHTER<sup>1</sup> — <sup>1</sup>Inst. f. Physik - NMR, Martin-Luther-Universität Halle-Wittenberg, Halle — <sup>2</sup>Dep. of eng. science and mechanics, Pennsylvania State University, Pennsylvania

A variety of structural and topological factors is known to strongly influence the mechanical properties of a polymer network. Here, we focus on a molecular-engineered biopolymer network consisting of random coils and nano-sized  $\beta$ -sheet crystals (acting as physical crosslinks) that was obtained by modifying and expressing repetitive elements in the genetic code of squid-ring teeth proteins. Usage of different solvents and different chain lengths of the expressed biopolymer yields the possibility of variations in crystallinity and the amount of topological defects. Using 1H time-domain NMR experiments, namely free induction decay (FID) analysis and a double-quantum (DQ) experiment, we investigate the crystalline and mobile fraction, as well as the different chain connectivities being present in the network. Additionally, we investigate the segmental mobility along the elastic chain and show that a mobility gradient exists, which is possibly induced by confinement of the elastic chains due to the  $\beta$ -sheet crystals. We show that we can correlate  $\beta$ -sheet content and the crystallinity measured by FID analysis, and additionally we discuss a previously published entropic-elasticity model [1] in the context of our DQ-NMR results. [1] A. Pena-Francesch et. al., ACS Biomater. Sci. Eng. 2018, 4, 3, 884-891

## CPP 24.6 Mon 17:30 P3

**Ramanspectroscopic investigation of eco-friendly binder systems for carbon-bonded filters** — ●SIMON BREHM<sup>1</sup>, CAMELIU

HIMCINSCHI<sup>1</sup>, BENJAMIN BOCK<sup>2</sup>, CHRISTOS ANEZIRIS<sup>2</sup>, and JENS KORTUS<sup>1</sup> — <sup>1</sup>Institute of Theoretical Physics, TU Bergakademie Freiberg, Germany — <sup>2</sup>Institute of Ceramic, Glass and Construction Materials, TU Bergakademie Freiberg, Germany

Environmentally friendly binder systems for carbon-bonded filters based on lactose/tannin were investigated by Raman spectroscopy. In earlier samples, the carcinogenic material CarboresP was used as a binder [1], which is replaced by a lactose/tannin mixture in this work.

With Raman spectroscopy, the size of the sp<sup>2</sup> carbon clusters using the intensity ratio of the D- and G-bands [2] and the -OH content can be qualitatively compared between different samples.

Temperature-dependent in-situ Raman measurements of the pure materials lactose and the tannin derivatives (tannic acid, gallic acid, ellagic acid) were performed.

Also two test series of the binder system were examined, one series was annealed to 1000°C and one was untreated. Both series consist of six samples, whereby the initial CarboresP portion of 20% is gradually replaced by a lactose/tannin mixture.

- [1] C. Himcinschi et al., J. Eur. Ceram. Soc. 38, 5580 (2018),  
[2] C. Röder et al., J. Raman Spectrosc. 45, 128 (2013)

CPP 24.7 Mon 17:30 P3

**Supermolecular ordering in monolayers of lipids with extended polymer head groups - DSPE-PEG** — ●HEIKO AHRENS, OLAF SOLTWEDEL, JENS-UWE GÜNTHER, and CHRISTIANE A. HELM — Institut für Physik, Uni-Greifswald, 17489 Greifswald

Depending on area per molecule, lipid monolayers - like Distearoylphosphatidyl-ethanolamine (DSPE) - at the air-water interface exhibit a phase transition from a liquid expanded to a condensed phase with tilted alkyl tails. On further compression the tilt angle decreases. Larger head groups increase the tilt angle and disturb the crystalline order.

DSPE with chemically attached short PEG (poly ethylene glycol) to the head group was investigated with GID and x-ray reflection. DSPE with longer PEG chains show a transition from fluid molecules to heterogeneous monolayer consisting of domains with condensed tilted lipid chains immersed in PEG chains adsorbed into the hydrophobic moiety of the lipid monolayer. These domains are then arranged in a hexagonal super structure with lattice constants up to 16 nm.

With a short PEG chain (8 monomers) an incompressible condensed phase with coherence length in the 10 nm range is found. The alkyl tails are strongly tilted - 39° - in a strongly distorted oblique lattice. Perpendicular to the tail axis they are arranged in the dense herring bone structure. Additional diffraction peaks due to an extended unit cell consisting of four alkyl tails were observed.

CPP 24.8 Mon 17:30 P3

**Studying the nanomechanical properties of functional organic and biologic macromolecules** — ●ILKA M. HERMES<sup>1</sup>, MINA HONG<sup>2</sup>, GERALD PASCUAL<sup>2</sup>, BYONG KIM<sup>2</sup>, and KEIBOCK LEE<sup>2</sup> — <sup>1</sup>Park Systems Europe, Mannheim, Germany — <sup>2</sup>Park Systems, Inc., Santa Clara, USA

As the functionality of organic and biologic macromolecules is often determined by their nanomechanical properties, visualizing the distribution of mechanical properties on the nanoscale provides crucial insights for soft matter research. Here, we present a study on structural and nanomechanical properties of functional organic and biologic macromolecules depending on the respective environment as well as external stimuli, such as temperature, ion concentration and pH. Force-distance measurements with atomic force microscopy (AFM) resolve adhesion and elasticity by pressing a nanometer-sized tip on the end of a cantilever onto the surface. However, the correlation of mechanical data from force-distance measurements to the local sample morphology additionally requires topographic sample information. Pin-Point nanomechanical imaging simultaneously acquires topographic and force-distance data within short amounts of time and is therefore ideally suited to investigate organic and biologic macromolecules.

CPP 24.9 Mon 17:30 P3

**Correlation between secondary structures and viscous properties of xanthan polymers** — ●JENNY FJODOROVA<sup>1</sup>, GERD HUBLIK<sup>3</sup>, VERA ORTSEIFEN<sup>2</sup>, KARSTEN NIEHAUS<sup>2</sup>, VOLKER WALHORN<sup>1</sup>, and DARIO ANSELMETTI<sup>1</sup> — <sup>1</sup>Experimental Biophysics and Applied Nanoscience, Bielefeld University, Germany — <sup>2</sup>Proteome and Metabolome Research, Bielefeld University, Germany — <sup>3</sup>Jungbunzlauer Austria AG, Pernhofen 1, 2064 Wulzeshofen, Aus-

tria

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 of the polysaccharide.

Using atomic force microscopy (AFM) imaging and rheological measurements, we analysed the structure of single xanthan polymers in different environments. We identified structures ranging from single-stranded coiled networks to branched double-strands. Viscosity measurements show a link between the microscopic structural features and the macroscopic viscosity. Thus, we will discuss a model, which describes a correlation between the secondary structure of the polymer with its shear-thickening properties.

CPP 24.10 Mon 17:30 P3

**Lithium Ion Transport in Block-Copolymer Electrolytes – A Molecular Dynamics Study** — ●LEN KIMMS, DIDDO DIDDENS, and ANDREAS HEUER — Institut für physikalische Chemie, Westfälische Wilhelms-Universität Münster, Corrensstraße 28/30, 48149 Münster, {len.kimms, d.diddens, andheuer}@uni-muenster.de

On this poster we will present insights into the ion transport in block-copolymer electrolytes with lamellar microstructure. Traditional solid polymer electrolytes (SPE) consist of salt accommodated in an amorphous poly(ethylene oxide) (PEO) melt. Subsequently other polymers have been tried in order to improve conductivity and safety. From a safety point of view rigid polymers are favored since they can suppress dendrite growth and provide mechanical stability. Unfortunately, those types of polymers exhibit decreased segmental dynamics which hinders the ion mobility. Block-copolymers provide the ability to tune the mechanical and ion-transport properties of the blocks independent from each other. Here we report results about the ion transport in block-copolymer electrolytes with lamellar microstructure which experimentally have displayed very high conductivities. In those observations the ionically conducting PEO domain consists of short PEO chains that can accommodate high salt concentrations. From the preparation of the lamellae there remains non-volatile Tetrahydrofuran (THF). We employ Molecular Dynamics (MD) simulations to understand the ion transport mechanism and compare our findings to earlier MD simulations of classical PEO-based SPEs. First conjectures on the role of the remaining THF are presented.

CPP 24.11 Mon 17:30 P3

**Fundamental principles of polyelectrolyte hydrogel pressure sensors and diodes from molecular simulations** — ●JOERG RÖTTLER<sup>1</sup>, VASILII TRIANDAFILIDI<sup>2</sup>, and SAVVAS HATZIKIRIAKOS<sup>2</sup> — <sup>1</sup>Dept. of Physics and Astronomy and Quantum Matter Institute, University of British Columbia, Vancouver BC Canada V6T 1Z1 — <sup>2</sup>Dept. of Chemical Engineering, University of British Columbia, Vancouver BC Canada V6T 1Z4

The function of many novel soft electronic materials arises from electrostatic effects at interfaces between polyelectrolyte networks. This talk uses coarse-grained molecular simulations to elucidate the molecular principles of two distinct effects: the emergence of a pressure gradient between two differently ionized gels that results in the buildup of a Nernst-Donnan potential, and the ability of a junction of two oppositely charged crosslinked networks to rectify an electric current. In both cases, the simulations are used to probe the regime of strong electrostatic coupling where counterion condensation becomes important. The Nernst-Donnan potential at the interface is found to scale linearly with temperature with the coefficient of proportionality given by the fraction of uncondensed counterions. Similarly, a Poisson-Boltzmann continuum electrostatic description of the gel diode interface is only applicable at weak electrostatic coupling, and modifications are developed to describe more strongly ionized gels.

CPP 24.12 Mon 17:30 P3

**Structure of Micelles Formed by Multi-responsive Triblock Terpolymers** — ●YANAN LI<sup>1</sup>, ATHANASIOS SKANDALIS<sup>2</sup>, VARVARA CHRYSOSTOMOU<sup>2</sup>, STERGIOS PISPAS<sup>2</sup>, and CHRISTINE M. PAPADAKIS<sup>1</sup> — <sup>1</sup>Physik-Department, Technische Universität München, Garching, Germany — <sup>2</sup>Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, Athens, Greece

Positively charged core-shell micelles are of interest for gene-transfer applications. Such systems may be formed by PDMAEMA-*b*-PLMA-*b*-POEGMA terpolymers. PDMAEMA is responsive to pH, ionic strength and temperature, whereas PLMA is strongly hydrophobic and POEGMA is permanently water-soluble and ensures biocompatibility. As a reference system, we investigate the simpler diblock copolymer PDMAEMA-*b*-PLMA as well. Detailed structural information is obtained from small-angle X-ray scattering.

CPP 24.13 Mon 17:30 P3

**Adsorption of Dodecyl Sulfonate Surfactants and Alkali Ions at Extended and Nanoscopic Oil/Water Interfaces** — •DANA GLIKMAN, ERIC WEISSENORN, and BJÖRN BRAUNSCHWEIG — Institute of Physical Chemistry and Center for Soft Nanoscience, Corrensstr. 28/30, 48149 Münster, Germany

Emulsions find many applications in different everyday life and industrial applications. However, a complete molecular-level understanding of the soft oil/water interface inside emulsions is still missing, but is prerequisite for targeted manipulation of emulsions. In this contribution, we report on the influence of anionic dodecyl sulfate (DS<sup>-</sup>) surfactants and their counter ions (Li<sup>+</sup>, Na<sup>+</sup>, Cs<sup>+</sup>) at the extended- and nanoscopic hexadecane/water interface. In order to study the oil/water interface as a function of surfactant concentration and ionic strength on different length scales, we have applied a thin-film pressure balance and the captive bubble method for extended surface, but also recorded the zeta-potential and second-harmonic light scattering (SHS) profiles from nanoscopic oil drops. Due to the higher affinity of DS<sup>-</sup> to oil, the surface pressure is higher at the oil/water interface than at the air/water interface. Nevertheless, we find similar trends for the alkali cations at the oil/water interface as for the air/water interface: in dependence on the counter ion, the maximal surface excess of DS<sup>-</sup> decreases with decreasing ion size (Cs<sup>+</sup> > Na<sup>+</sup> > Li<sup>+</sup>). In addition, the zeta-potential of nanoemulsions is for NaDS more negative than for CsDS, which is corroborated by SHS experiments that can address the double-layer potential directly.

CPP 24.14 Mon 17:30 P3

**Influence of added salt on the foam film properties of NaPSS/C<sub>14</sub>TAB-mixtures** — •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 in personal care products and in food technology.

To understand the properties of macroscopic foam, it is essential to investigate foam films - the framework of foams.

Due to the formation of highly surface-active complexes, mixtures of oppositely charged polyelectrolytes and surfactants are widely used in many industrial applications. There exist many studies that focus on a big variety of surfactant-polyelectrolyte mixtures. However, the influence of the ionic strength - especially on the foam films - is still unclear.

In this work, a thin film pressure balance (TFPB) is used to study foam films of NaPSS/C<sub>14</sub>TAB-mixtures in terms of disjoining pressure, surface potential and foam film stability. We add NaBr (the combination of the two counterions) to get insights on the influence of the ionic strength on the foam film properties. Our current investigation shows an unexpected increase in foam film stability with added NaBr which might be explained by a change of the conformation of NaPSS at the air/water interface. To study the effects of the presence of NaBr in detail, the NaBr concentration is further varied.

CPP 24.15 Mon 17:30 P3

**Hierarchical assembly of non-spherical colloids by critical Casimir forces** — •TIMO KNIPPENBERG, JAKOB STEINDL, TIAN LI, and CLEMENS BECHINGER — FB Physik, Universität Konstanz

Recent experiments demonstrated the use of critical Casimir forces in the context of spherical colloidal aggregation processes. Such forces arise due to the geometrical confinement of a critical mixture. Critical Casimir induced particle assembly essentially takes advantage of the fact, that the strength of such forces strongly depends on the temperature of the fluid and the adsorption preference of the colloidal particles. Here, we experimentally study the aggregation of semi-disk like particles under the influence of critical Casimir forces. We observe a preferential attraction between the flat facets of the particles which leads to their assembly into disk-shaped aggregates. At larger particle densities, the assembled disks form a hexagonal lattice. This hierarchical assembly process is explained by the strong curvature dependence

of critical Casimir forces which leads to a strong alignment of non-spherical particles. This alignment strongly depends on the particle thickness which has been systematically varied in our experiments.

CPP 24.16 Mon 17:30 P3

**Packing polydisperse colloids into crystals: when charge-dispersity matters** — •LUCAS GOEHRING<sup>1</sup>, GUILLAUME BAREIGTS<sup>2</sup>, PREE-CHA KIATKIRAKAJORN<sup>3</sup>, JOAQUIM LI<sup>4</sup>, ROBERT BOTET<sup>5</sup>, MICHAEL SZTUCKI<sup>6</sup>, BERNARD CABANE<sup>4</sup>, and CHRISTOPHE LABBEZ<sup>2</sup> — <sup>1</sup>Nottingham Trent University — <sup>2</sup>University Bourgogne — <sup>3</sup>Max Planck Institute for Dynamics and Self-Organisation — <sup>4</sup>ESPCI Paris-Tech — <sup>5</sup>University Paris-Sud — <sup>6</sup>ESRF-The European Synchrotron

Here we show that even modest amounts of polydispersity can dramatically change how colloidal crystallization occurs. Monte-Carlo simulations, fully constrained by experimental parameters, are found to agree well with a measured phase diagram of aqueous dispersions of nanoparticles with a moderate size polydispersity over a broad range of salt concentrations,  $c_s$ , and volume fractions,  $\phi$ . Upon increasing  $\phi$ , the colloids freeze first into coexisting compact solids then into a body centered cubic phase (bcc) before they melt into a glass forming liquid. The surprising stability of the bcc solid at high  $\phi$  and  $c_s$  is explained by the interaction (charge) polydispersity and vibrational entropy.

CPP 24.17 Mon 17:30 P3

**Crystallization kinetics in colloidal hard spheres by confocal microscopy** — •SAHANA KALE and HANS-JOACHIM SCHOEPE — University of Tuebingen, Germany

We study the homogeneous crystallization of meta-stable colloidal hard sphere fluids using laser scanning confocal microscopy. Direct imaging in three dimensions offers the unique possibility to observe crystal nucleation and growth on the particle level.

We present nucleation rate densities for various volume fraction in comparison with previous data from light scattering and simulation. In addition, we analyse the temporal evolution of the local structure of the crystallizing clusters.

CPP 24.18 Mon 17:30 P3

**Modeling epitaxial film growth of C<sub>60</sub>** — •WILLIAM JANKE and THOMAS SPECK — Institut für Physik, Johannes Gutenberg-Universität Mainz, Deutschland

Epitaxial films evolve on time and length scales that are inaccessible to atomistic computer simulation methods like molecular dynamics (MD). To numerically predict properties for such systems, a common strategy is to employ kinetic Monte Carlo (KMC) simulations, for which one needs to know the transition rates of the involved elementary steps. The main challenge is thus to formulate a consistent model for the set of transition rates and to determine its parameters. We revisit a well-studied model system, the epitaxial film growth of the fullerene C<sub>60</sub> on an ordered C<sub>60</sub> substrate(111). We implement a systematic multiscale approach in which we determine transition rates through MD simulations of specifically designed initial configurations. These rates follow Arrhenius' law, from which we extract energy barriers and attempt rates. We discuss the issue of detailed balance for the resulting rates. Finally, we study the morphology of submonolayer and multilayer film growth and compare simulation results to experiments.

CPP 24.19 Mon 17:30 P3

**Machine learning for DNA self-assembly: a numerical case study** — •JÖRN APPELDORN, ARASH NIKOUBASHMAN, and THOMAS SPECK — Inst. für Physik, Universität Mainz, Germany

We study the spontaneous self-assembly of single-stranded DNA fragments using the coarse-grained oxDNA2 implementation [1]. A successful assembly is a rare event that requires to cross a free energy barrier. To employ advanced numerical algorithms like forward-flux sampling or Markov state modeling one needs to identify one or more collective variables (order parameters) that faithfully describe the transition towards the assembled state. Formulating appropriate order parameters typically relies on physical insight, which is then verified, e.g., through a committer analysis. Here we explore the use of machine learning to automatize this process and to find suitable collective variables based on structural information. For this step one still needs to map configurations onto structural descriptors, which is a non-trivial task. Specifically, we investigate the latent space of EncoderMap [2] and how it changes with the amount of information contained in the descriptor.

[1] - Snodin et al., J. Chem. Phys.(2015), 142, 234901 [2] - T. Lemke

and C. Peter, *J.Chem.TheoryComput.* (2019), 15, 1209\*1215

CPP 24.20 Mon 17:30 P3

**Characterisation of the Free Energy Landscape of Syndiotactic Polyesterene** — ●ATREYEE BANERJEE, TRISTAN BERAU, and JOSEPH F. RUDZINSKI — MPIP

Syndiotactic polyesterene (sPS) is known to crystallise in distinct forms, commonly known as polymorphs [1]. Traditional molecular dynamics simulations are powerful tools for characterizing the molecular mechanism of transition between polymorphs, but require extreme computational resources due to the strong metastability of the polymorph states. Enhanced sampling methods have the potential to largely remedy this problem, but require prior knowledge of collective variables (CVs) that can resolve the relevant transition pathways, typically identified through physical or chemical expertise. CVs are also often used for constructing a kinetic model to better characterise the transition pathways of the characteristic long timescale processes of the system. A huge interest has grown to apply neural networks to automate the discovery of a low-dimensional representation [2]. Autoencoders are potentially powerful tools to identify good CVs, since the technique forces an information compression in the bottleneck region. A specialised autoencoder architecture, the Gaussian mixture variational autoencoder (GMVAE), performs dimensionality reduction and clustering within a single unified framework, and can identify the inherent dimensionality of the system by enforcing physical constraints in the latent space. In contrast to manually constructed CVs, we apply the GMVAE approach to accurately characterise the pathways of transition between polymorphs in sPS.

CPP 24.21 Mon 17:30 P3

**Self-Assembly of Polymers in Presence of Solvent Evaporation** — ●GREGOR IBBEKEN and MARCUS MÜLLER — Georg-August Universität, Göttingen, Deutschland

Integral asymmetric polymer membranes are promising functional macromolecular systems which have numerous applications, like water purification and protein separation. Since their synthesis requires high control over kinetic pathways, a description in terms of statistical physics and exploiting computer simulations will help improve understanding and production. Here we tackle a process combining self-assembly of asymmetric diblock copolymers and non-solvent induced phase separation using continuum descriptions of self-assembling polymer systems. First, model B for the Ohta-Kawasaki free energy functional, which successfully describes dynamics of diblock copolymers, is phenomenologically altered to feature space and time dependent parameters. This mimics the impact of solvents. In a second step the impact of solvents is explicitly investigated using the Uneyama-Doi functional, a model capable of describing arbitrary polymer mixtures. Appropriate parameter regions and thus corresponding kinetic pathways in which the copolymers form ideal standing cylinders, later functioning as pores, are identified. Finally, bridging the gap between simulation and experiment, the parameters are mapped to experimental ones, such as mobilities and Flory-Huggins parameters.

CPP 24.22 Mon 17:30 P3

**Unraveling kinetically driven self-assembly of nanoplatelets** — ●NANNING PETERSEN, REBECCA MOMPER, MARTIN GIRARD, ANDREAS RIEDINGER, and OMAR VALSSON — Max Planck Institute for Polymer Research, Ackermannweg 10, D-55128 Mainz

CdSe can form thin rectangular semiconductor nanoparticles. These nanoplatelets are remarkably uniform in thickness and size [1]. To make use of their extraordinary properties the colloidal particles have to be collectively orientated in solid state films. Previous experiments in our group have demonstrated that effective control over the collective orientation can be gained by exploiting kinetic effects in the self-assembly process. This yields well defined monolayer films with controlled nanoplatelet orientation. Through variation of the solvent, the temperature or the partial pressure the evaporation rate can be tuned, yielding monolayers with nanoplatelets either orientated "face-down" or "edge-up". However, the mechanism behind the kinetically driven self-assembly is not well understood.

Recently there have been major efforts to understand self-assembly processes in different nanoparticle systems. Molecular simulations have been proven to be a promising strategy to get a microscopic understanding of these processes. For nanoplatelets we have taken the first steps in this direction by employing coarse-grained molecular dynamics simulations using the MARTINI force field. Here we present our initial results on model nanoplatelet systems.

[1] A. Riedinger *et al.*, *Nat. Mater.* 16, 743-748 (2017)

CPP 24.23 Mon 17:30 P3

**In-situ investigation of sputter deposition of electrodes for non-fullerene organic photovoltaics application** — ●XINYU JIANG<sup>1</sup>, SIMON J. SCHAPER<sup>1</sup>, MATTHIAS SCHWARTZKOPF<sup>2</sup>, STEPHAN V ROTH<sup>3</sup>, JONAS DREWES<sup>4</sup>, OLEKSANDR POLONSKYI<sup>4</sup>, THOMAS STRUNSKUS<sup>4</sup>, and PETER MÜLLER-BUSCHBAUM<sup>1</sup> — <sup>1</sup>Technische Universität München, Physik-Department, Lehrstuhl für Funktionelle Materialien, James-Franck-Str. 1, Garching, Germany — <sup>2</sup>DESY, Notkestr. 85, 22607 Hamburg, Germany — <sup>3</sup>KTH, Department of Fibre and Polymer Technology, SE-100 44 Stockholm, Sweden — <sup>4</sup>Christian Albrechts-Universität zu Kiel, Materialverbunde Lehrstuhl, Materialwissenschaft Institut, Kaiserstr. 2, D-24143 Kiel, Germany

Electrode quality of photovoltaic devices plays a very important role in device performance. The metal growth process directly influences the material density, electrical conductivity and interface contact of the electrode. Electrodes of aluminum are widely used in organic photovoltaic devices. For understanding the mechanism of Al cluster growth on non-fullerene organic solar cells, we use in-situ grazing incidence small angle X-ray scattering (GISAXS) to observe detailed information during the sputter process. We find that the early stages of Al cluster growth on the non-fullerene active layers determine the later stages and strongly influence the percolation threshold. Furthermore, the cluster growth varies for active layers with an additional electron blocking layer. These findings are of great importance for improving the performance of the photovoltaic devices.

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**Versatile approach to well-defined conjugated oligomers and polymers with narrow molecular weight distribution for fundamental studies on structure-property relationships** — ●FRANK-JULIAN KAHLE<sup>1</sup>, JULIA WOLLMANN<sup>2</sup>, IRENE BAUER<sup>2</sup>, ANNA KÖHLER<sup>1</sup>, and PETER STROHRIEGL<sup>2</sup> — <sup>1</sup>Soft Matter Optoelectronics, University of Bayreuth, Germany — <sup>2</sup>Macromolecular Chemistry I, University of Bayreuth, Germany

In this work, we present a versatile approach to achieve well-defined conjugated polymers and oligomers from a single standard synthesis route via preparative Size Exclusion Chromatography. Using a special recycle mode and well-defined end-cappers, we are able to prepare pure oligomers with three to eight repeat units and high molecular weight polymers with dispersity D as low as 1.06 in just one preparation step with reasonable yield. To demonstrate the capabilities of our method, we conducted a fundamental spectroscopic study on the influence of chain length and molecular weight distribution on electronic properties and aggregation behavior of a series of fluorene based oligo- and polymers. Due to the well-defined nature of the investigated compounds we consistently find a first-order phase transition and an increase of the critical transition temperature from amorphous to  $\beta$ -phase as function of the number of repeat units in accordance with the Sanchez model on coil-globule transitions.

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**Thermophoretic Trapping of Single Amyloid Fibrils** — MARTIN FRÄNZL<sup>1</sup>, ●TOBIAS THALHEIM<sup>1</sup>, JULIANE ADLER<sup>1</sup>, DANIEL HUSTER<sup>1</sup>, JULIANE POSSECKARDT<sup>2</sup>, MICHAEL MERTIG<sup>2,3</sup>, and FRANK CICHOS<sup>1</sup> — <sup>1</sup>Leipzig University, Germany — <sup>2</sup>Kurt-Schwabe-Institut für Mess- und Sensortechnik e.V. Meinsberg, Germany — <sup>3</sup>TU Dresden, Germany

The formation of aggregates of peptides is responsible for a number of neurodegenerative diseases. The individual steps of this aggregation from single soluble monomers or oligomers to highly ordered, insoluble amyloid fibrils, however, are commonly hidden in the ensemble average of common measurement techniques. The heterogeneity of the ensemble at all stages of the aggregation process hides the growth details such as secondary nucleation processes or fibril fragmentation. I will present on my poster a method that is able to trap single amyloid fibrils freely diffusing in solution relying on thermophoresis. This thermophoretic trap allows us to extract a lot of properties of the individual fibrils, like their Soret coefficients as well as the translational and rotational diffusion coefficients over time periods of at least several 10 minutes up to even hours. Repeating the measurement for several single fibrils permits us to measure a length dependence of the translational and rotational diffusion coefficients. Due to the high sensitivity of the rotational diffusion coefficient on length changes, we are furthermore able to study the growth of single fibrils down to a few 10 nm in

the presence of monomers or monitor secondary nucleation events and fragmentation which have not been seen directly before.

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**Effect of entanglements on the morphology and crystallinity of semi-crystalline polymer** — ●ZEFAN WANG, MAREEN SCHÄFER, ALBRECHT PETZOLD, THOMAS THURN-ALBRECHT, and KAY SAAL-WÄCHTER — Institute for Physics, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle (Saale), Germany

Recent simulation work indicates that the thickness of crystalline lamellae in the semi-crystalline polymer might be controlled by the entanglement density of the crystallizing melt. However, experimental evidence of how the morphology and the crystallinity of the semi-crystalline polymer is influenced by the topological restriction of entanglement density is scarce. By diluting high molecular weight polycaprolactone (PCL) with its own oligomer, a series of PCL samples with different entanglement density in equilibrium were prepared. The reduced entanglement density in the melt state was confirmed by rheological measurements. In addition, after crystallization, the semicrystalline morphology was characterized by SAXS and solid state NMR. At low crystallization temperatures the long chain polymer and the oligomer cocrystallize. SAXS data indicate that the lamellar thickness remains constant while the thickness of the amorphous regions decreases with decreasing entanglement density in the melt state. NMR measurements confirmed the corresponding increase of the crystallinity. These observations suggest that the thickness of the amorphous regions and therefore also the of semicrystalline polymers is controlled by the entanglement density in the melt state.

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**Strain induced polymer crystallization** — ●RAJDEEP SINGH PAYAL<sup>1</sup> and JENS-UWE SOMMER<sup>1,2</sup> — <sup>1</sup>Leibniz Institute for Polymer Research, Hohe Str. 06, Dresden, Germany — <sup>2</sup>Institut für Theoretische Physik, Technische Universität Dresden, Zellescher Weg 17, 01062 Dresden, Germany

Crystallization behavior of polymers is known to be influenced by the processing conditions. Lamellar thickness and crystallinity can be enhanced by the application of strain. Here, we have utilized molecular dynamics simulations and primitive path analysis to establish a direct correspondance between the thermo-mechanical history of the molten state and crystallization behavior. Within linear extension regime, crystalline behavior is governed by the mixture of thermodynamic and topological effects. Partial disentanglement of the polymer chains due to applied force results in higher lamellar thickness and crystallinity. Furthermore, predicted behavior cannot be accounted using the kinetic theory of polymer crystallization.

CPP 24.28 Mon 17:30 P3

**Controllable Au Nanoparticle Plasmonic Effects via Sputter Deposition on TiO<sub>2</sub> Templates** — ●SUZHE LIANG<sup>1</sup>, WEI CHEN<sup>1</sup>, SHANSHAN YIN<sup>1</sup>, MATTHIAS SCHWARTZKOPF<sup>2</sup>, STEPHAN V. ROTH<sup>2</sup>, and PETER MÜLLER-BUSCHBAUM<sup>1</sup> — <sup>1</sup>Lehrstuhl für Funktionelle Materialien, Physik-Department, TU München, 85748 Garching, Germany — <sup>2</sup>Deutsches Elektronen-Synchrotron (DESY), 22607 Hamburg, Germany

Due to the localized surface plasmon resonances (LSPR) effect, plasmonic metal nanostructures exhibit unique optical properties and have been applied in various fields, such as plasmon-enhanced sensing and chemistry, biotechnologies, and lighting harvesting for solar energy. Generally, plasmonic mantle nanostructures can be fabricated by colloid chemical methods, electron-beam lithography, and laser ablation. The wavelength of LSPR can be tuned from the ultraviolet to the infrared regions by changing the structure size and shape. In this work, we have introduced a facile and scalable method to obtain plasmonic nanoparticle array, with uniformed size and inter-distance distribution, by sputtering gold on TiO<sub>2</sub> template. The sputtering measurement is realized by a unipolar reactive pulsed DC magnetron sputtering device. The uniform distribution of gold nanoparticles can be controlled by sputtering time and the customized TiO<sub>2</sub> templates with designable morphologies. The growth dynamics of gold nanoparticles are studied by GISAXS. Combined with SEM and UV-vis spectroscopy measurements, the relationship between gold nanoparticles distribution and LSPR effects is established and explained.

CPP 24.29 Mon 17:30 P3

**Hybrid Energy Harvester based on Solar Cell and Triboelectric Nanogenerator** — ●TIANXIAO XIAO<sup>1</sup>, WEI CAO<sup>1</sup>, WEI

CHEN<sup>1</sup>, SVEN-JANNIK WÖHNERT<sup>2</sup>, STEPHAN V. ROTH<sup>2</sup>, and PETER MÜLLER-BUSCHBAUM<sup>1</sup> — <sup>1</sup>Lehrstuhl für Funktionelle Materialien, Physik-Department, Technische Universität München, James-Frank-Str. 1, 85748 Garching, Germany — <sup>2</sup>Deutsches Elektronen-Synchrotron (DESY), Notkestr. 85, 22607 Hamburg, Germany

Developing clean energy plays a central role in the sustainable development of human society. Solar energy is one of the most promising energy sources in replacement of conventional used fossil fuels. However, the daily and seasonal fluctuations in weather limit solar cell's applications. Integrating the solar cell with other kinds of energy harvesters in one device is a possible solution. Triboelectric nanogenerator (TEENG) originating from Maxwell's displacement current is a new type of energy harvesters. Due to its advantages of light-weight, low-cost, and easily fabricated, TEENG attracts worldwide attention in the past years. In the present work, a flexible hybrid energy harvester is designed and fabricated based on quantum dots (QDs). This device consists of a PbS-QD solar cell part and a polydimethylsiloxane (PDMS) based TEENG part, which can harness both, solar and mechanical energy from ambient environment to generate electricity. GISAXS measurements are used to characterize the bending stability and morphology changes of the mesoscale structure.

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**A surface treatment recipe for significantly enhancing thermoelectric PEDOT:PSS films** — ●SUO TU and PETER MÜLLER-BUSCHBAUM — Physik-Department, Lehrstuhl für Funktionelle Materialien, Physik Department, Technische Universität München, James-Frank-Str. 1, 85748 Garching, Germany

Organic semiconductors have attracted intense attention because of their potential use in mechanically flexible, lightweight, and inexpensive electronic devices. Especially, PEDOT:PSS is the most studied conducting polymer system due to their intrinsically high electrical conductivity, low thermal conductivity, and high mechanical flexibility in thermoelectric devices. The energy conversion efficiency of a TE material is evaluated by a dimensionless figure of merit ZT. However, it is generally considered that it is difficult to obtain a high ZT value of TE materials, due to the fact that the parameters are interdependence as a function of carrier concentration and hard to be optimized simultaneously. Mostly methods employing film treatment or both film treatment and additives in the solution show better conductivity than the mere additives in the PEDOT:PSS aqueous solution. Herein, a facile multi-step surface treatment was applied to enhance TE properties of pristine PEDOT:PSS thin films. Subsequently, the surface morphology and the inner morphology were probed using atomic force microscopy and grazing-incidence wide/small-angle X-ray scattering, respectively. Additionally, UV-Vis spectroscopy, Raman spectroscopy and X-ray photoelectron spectroscopy were employed to investigate the mechanism behind for TE performance improvement.

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**DC and AC conductivity of ultra-thin carbon nanotube/polycation multilayers in air and different aqueous solutions** — ●SVEN NEUBER, PETER NESTLER, HEIKO AHRENS, and CHRISTIANE A. HELM — Institute of Physics, University of Greifswald, 17489 Greifswald, Germany

To prepare implants covered by an electrically conductive film it is necessary to control the device surface and properties. Electrically conductive multilayers were built by the layer-by-layer technique, sequential adsorption of oppositely charged chemically modified carbon nanotubes and polycations. Quartz crystal microbalance, atomic force microscopy and ellipsometry measurements were used to determine surface coverage, thickness and roughness on nm-scale. Also, frequency-dependent conductivity (kHz range, DC and AC) measurements at ambient conditions (20°C), at different humidities (r.h. between 0 \* 100%) and in physiological solutions were investigated to get an overview of the multilayer capability for cell stimulation. It was found that the electrical conductivity depends on the environment. For PDADMA/CNT films (7 layer pairs) in air a current of 22.4 mA was obtained, in 100 mM NaCl solution 20.8 mA and in deionized water 10.5 mA. Also no phase change occurred during the frequency shift up to 100 kHz, indicating an ohmic behavior. The results are discussed in terms of film swelling, electron conductivity through the film and ionic conductivity through the solution.

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**Dispersion Relations of Metal/Organic Hybrid Structures caused by Strong Coupling between Plasmons and Excitons**

— ●MAXIMILIAN RUDLOFF<sup>1</sup>, MAXIMILIAN RÖDEL<sup>1</sup>, THOMAS STARK<sup>2</sup>, JOCHEN MANARA<sup>2</sup>, and JENS PFLAUM<sup>1,2</sup> — <sup>1</sup>Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — <sup>2</sup>Bavarian Center for Applied Energy Research (ZAE Bayern), 97074 Würzburg

Light-matter interaction in the vicinity of a metal surface is an intensely researched topic motivated by the possibility of tuning the optical properties of thin film devices on sub-wavelength scales [1]. By extending this concept to organic semiconductors on top of a metal surface, new hybrid states appear, labelled plexcitons. In our contribution we analyze the dispersion relations of plexcitons emerging by the coupling of localized excitons in ZnPc molecular layers and the collective electronic excitations at gold surfaces by means of a surface plasmon resonance setup. The resulting coupling strength is in the order of  $\approx 100$  meV and is interpreted by the characteristics inherent to the individual systems. In addition we discuss the influence of the morphology on the plexcitonic dispersion branches, which provides an additional degree of freedom upon implementing this concept in future opto-electronic devices.

[1] V. Kolb, Opt. Express 25 (2017) 6678

CPP 24.33 Mon 17:30 P3

**The Gradient Contribution to Light Scattering in an Interface Layer** — ●REINHARD SIGEL — 88677 Markdorf

The effect of the refractive index gradient in an interface layer on the diffuse interface scattering is investigated theoretically. An extension of the transfer matrix method for a layered interface profile by small fluctuations in the layers provides predictions for diffuse interface light scattering. While the s-polarization follows the conventional wave equation, there is an extra term with a first order derivative in the wave equation for p-polarization. Within the transfer matrix method there are step-like gradients located at the layer boundaries. The gradient term in p-polarization produces an extra scattering contribution at the layer boundaries. It becomes significant for an evanescent wave illumination with an angle of incidence close to the critical angle and can be used for a new approach to depth resolution in interface scattering experiments. A comparison to the Distorted Wave Born Approximation (DWBA) which is highly celebrated within the X-ray community is discussed.

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**Protein adsorption at the solid-liquid interface tuned by the choice of trivalent cations** — ●NINA CONZELMANN, MADELEINE FRIES, FAJUN ZHANG, and FRANK SCHREIBER — University of Tübingen, Germany

In biological processes, such as cell adhesion, protein adsorption at solid-liquid interfaces plays a crucial role since it is often observed as one of the first steps. Our study focuses on the effect of trivalent cations ( $\text{La}^{+3}$ ,  $\text{Y}^{+3}$ ) on globular proteins such as bovine serum albumin (BSA) which exhibits a rich phase behavior including reentrant condensation between two critical salt concentrations ( $c^*$ ,  $c^{**}$ ) and liquid-liquid phase separation [1]. Ellipsometry and quartz crystal microbalance were used to investigate the effect of increasing amounts of salt on the protein-interface system. The interaction of BSA with net-negatively charged surfaces like  $\text{SiO}_2$  is dominated by electrostatic repulsion and minimum protein adsorption. First, an increasing amount of adsorbed protein on the surface was observed while increasing salt concentration. Then, in the regime II, the thickness of adsorbed protein reaches a maximum. At high salt concentrations, the adsorbed layer first decreases and then approaches a constant value. This behavior can be explained by using the ion-activated patchy interactions model [2]. Both salts used show the same overall adsorption trend, yet the absolute adsorbed amount in regime II ( $c^* < c < c^{**}$ ) differs. The difference in regime II for  $\text{LaCl}_3$  and  $\text{YCl}_3$  is caused by  $\text{LaCl}_3$  having weaker effective attractive protein-protein interactions.

[1] Matsarskaia et al, PCCP (2018); [2] Fries et al, PRL (2017)

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**Real-time observations of alkali metal doped 6-Phenacene films** — ●MATTHIAS ZWADLO, MARTIN HODAS, ALEXANDER GERLACH, NADINE RUSSEGGER, BERTHOLD REISZ, and FRANK SCHREIBER — Institut für Angewandte Physik, Universität Tübingen, Germany

The characterization of growth and structure formation in molecular and hybrid systems is an important topic in fundamental organic semiconductor research. In order to study and influence this process different real-time methods have to be used [1]. A promising strat-

egy for tuning the properties of these materials is alkali metal doping, which for example, can lead to superconductivity under specific circumstances [2]. In this work, the growth and structure formation of 6-Phenacene doped with potassium has been investigated. Thin films of pure 6-Phenacene have been grown in ultra-high vacuum (UHV) and investigated with x-ray, AFM and optical methods. Furthermore, grazing incidence wide angle scattering (GIWAXS) measurements of thin films of 6-Phenacene with potassium doping were performed in-situ during growth at PETRA 3 (beamline P03) in Hamburg. First results show small distortions in crystal structure after potassium doping. The results allow us to get a better understanding on the structural behavior and growth process in theory and experiment.

[1] Hosokai, T., Gerlach, A., Hinderhofer, A., Frank, C., Ligorio, G., Heinemeyer, U., \* Schreiber, F. Appl. Phys. Lett., 97(6), 9 (2010) doi:10.1063/1.3478450

[2] Mitsuhashi, R., Suzuki, Y., Yamanari, Y. et al. Nature 464, 76 (2010) doi:10.1038/nature08859

CPP 24.36 Mon 17:30 P3

**Gold Sputter Deposition on Polystyrene Thin Films: Influence of Template Thickness and Molecular Weight** — ●VIVIAN WACLAWEK<sup>1,2</sup>, MATTHIAS SCHWARTZKOPF<sup>2</sup>, MARC GENSCH<sup>2,5</sup>, PALLAVI PANDIT<sup>2</sup>, MICHAEL RÜBHAUSEN<sup>1,3</sup>, and STEPHAN V. ROTH<sup>2,4</sup> — <sup>1</sup>Universität Hamburg, Luruper Chaussee 149, D-22761 Hamburg — <sup>2</sup>DESY, Notkestr. 85, D-22607 Hamburg — <sup>3</sup>Center for Free Electron Laser Science (CFEL), Luruper Chaussee 149, D-22761, Hamburg — <sup>4</sup>KTH, Teknikringen 56-58, SE-10044 Stockholm — <sup>5</sup>Lehrstuhl für Funktionelle Materialien, Physik Department, Technische Universität München, James-Frank-Str.1, D-85748 Garching

Nanostructured noble metal films on polymer layers promise various potentials applications in solar cells, biosensors, reflective or antireflective coatings. Moreover, such material combinations have recently gained importance for stabilizing thin polymer films during annealing above glass temperature. In order to study the effect of polymer film thickness  $d_{PS}$  and molecular weight  $M_W$  we combine sputter deposition with grazing incidence X-ray scattering (GISAXS) to investigate in-situ the growth kinetics of Au on polystyrene thin films with different thin (3-80nm) thicknesses and two different  $M_W$ s (4 and 270kDa). We analyze quantitatively the metal nanoparticle layer growth and compare our results within the different polymer thicknesses. It is mandatory to understand the influence of the growth kinetics on the metal film morphology during sputter deposition for understanding the influence of  $M_W$  and  $d_{PS}$  on Au cluster growth. For future studies the results could be compared with different homopolymers.

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**Influence of Wavy-Interface on the Dynamics of Drop-Interface Coalescence** — ●KUNTAL PATEL — Indian Institute of Technology, Bombay, India

In drop-interface type coalescence, when a droplet is placed gently on a liquid pool, it will try to merge with the liquid pool (by draining the liquid within the droplet into the pool), which may result in either partial or complete coalescence. It primarily depends on the relative competition among the surface tension, viscous resistance, and gravity [1]. In present work, we perform numerical simulations using the ghost-fluid method based sharp-interface level-set method [2] to study the coalescence dynamics of an ethanol droplet (of diameter 1.07 mm) with a wavy pool of ethanol (surrounded by air).

Numerical experiments show that the dual coalescence-cascade pattern observed with a planar ethanol pool gets altered in the case of a wavy pool. This deviation in the coalescence dynamics is attributed to the complex interaction between two different capillary waves, one originated due to the coalescence, and other from the waviness of the ethanol pool. We demonstrate the transition from dual coalescence-cascade to single and zero coalescence-cascade (i.e., complete coalescence) for different waviness (defined here using amplitude and frequency) of ethanol pool.

[1] B. Ray, et al., Journal of Fluid Mechanics 655, 72-104 (2010).

[2] J. Shaikh, et al., Chemical Engineering Science 176, 77-95 (2018).

CPP 24.38 Mon 17:30 P3

**The Aging Mechanism of Silicone Molds for Vacuum Casting** — ●NATALIE FRESE<sup>1</sup>, MARTIN WORTMANN<sup>2</sup>, ALEXANDER HEIDE<sup>2</sup>, JOHANNES BRIKMANN<sup>2</sup>, ELMAR MORITZER<sup>3</sup>, BRUNO HÜSGEN<sup>2</sup>, and ARMIN GÖLZHÄUSER<sup>1</sup> — <sup>1</sup>Bielefeld University, Bielefeld, Germany — <sup>2</sup>Bielefeld University of Applied Sciences, Bielefeld, Germany — <sup>3</sup>Paderborn University, Paderborn, Germany

The use of silicone casting molds in the vacuum casting process for the production of prototypes made of polyurethane is state of the art. Although the process is widely used for prototype replication, it is rarely considered for an extensive use in small batch production. With this, the gap in plastic processing between very small (rapid prototyping) and very large quantities (injection molding) might one day be closed. We present an in-depth investigation of the aging effects in silicone casting molds for vacuum casting processes. Their lifetime is limited to a few production cycles due to contamination with the diisocyanate component of the polyurethane casting resin. By using a wide variety of characterization methods, the chemical and physical mechanisms of the aging process have been identified. It has been shown that an anomalous diffusion process of diisocyanate into the silicone surface leads to the formation of interpenetrating polymer networks of polyurea derivatives in the poly(dimethylsiloxane) matrix. This has been proven by extracting and analyzing polyurea of low molecular weights from the silicone.

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**Measuring Diffusion Coefficients of Methylene Diphenyl Diisocyanate in Polymeric Coatings on Poly(dimethylsiloxane)** — ●MARTIN WORTMANN<sup>1</sup>, RICHARD PETKAU<sup>1</sup>, WALDEMAR KEIL<sup>2</sup>, NATALIE FRESE<sup>3</sup>, ELMAR MORITZER<sup>2</sup>, ARMIN GÖLZHÄUSER<sup>3</sup>, ANDREA EHRMANN<sup>1</sup>, CLAUDIA SCHMIDT<sup>2</sup>, and BRUNO HÜSGEN<sup>1</sup> — <sup>1</sup>Bielefeld University of Applied Sciences, Bielefeld, Germany — <sup>2</sup>Paderborn University, Paderborn, Germany — <sup>3</sup>Bielefeld University, Bielefeld, Germany

Methylene diphenyl diisocyanate (MDI), as a common constituent of polyurethane, is the most frequently produced isocyanate and therefore of vital industrial importance. The diffusivity of MDI in polymeric materials is relevant i.a. due to its health hazardous properties but also due to its use in technical processes. In this work, the diffusion coefficients of MDI in eight different amorphous polymers were determined by means of a newly proposed test methodology. For this purpose, the polymers were dissolved in various volatile solvents and coated by solvent casting on individually pretreated poly(dimethylsiloxane) (PDMS) samples. By measuring the mass transfer rate and the MDI concentrations on both sides of the coating, the diffusivity could be calculated with the stationary Fickian diffusion equation. To determine the MDI concentrations, nuclear magnetic resonance spectroscopy (NMR) was used. DOSY NMR was used to determine the concentration of MDI in the liquid state and a combination of 1H MAS solid-state NMR and thermogravimetric analysis was used to determine the MDI concentration in the PDMS substrate.

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**Development of a process to characterize an elastomer-metal contact with the aim of leakage prediction** — ●FELIX SENF<sup>1</sup>, MARIUS PÄTZOLD<sup>1</sup>, ROBIN FONK<sup>2</sup>, SEAN SCHNEEWEISS<sup>2</sup> und OTHMAR MARTI<sup>1</sup> — <sup>1</sup>Institut für Experimentelle Physik, Ulm — <sup>2</sup>Ulmer Zentrum für wissenschaftliches Rechnen, Ulm

The following investigation describes the connection between surface structures, elastomers and tightness of critical leakage systems. In technical applications the sealing of hardware components is described with leakage rates based on different boundary conditions of the system. In general, physical rules state that an absolutely sealed system is not possible. Different parameters like materials, surface structures, roughness parameters, closing forces and not least the design of the sealing system influence the function of the sealing joint. The research program investigates the alignment between elastomers and metal surface structures and the resulting open volumes. The theory of contact problems, FEA simulation tasks and compression experiments help us to describe this alignment. An experimental set-up for leakage measurements and the combination with CFD simulations are the main tool to understand the leakage nature more in detail. Out of this toolbox we create a new process to describe leakage cases in a time efficient manner. Filter methods like morphological filters and Voronoi diagrams help us to work out the process.

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**Analysis of liquid distribution in micro-channel systems using the electro-hydraulic analogy** — ●MARIUS PÄTZOLD<sup>1</sup>, FELIX SENF<sup>1</sup>, CARL KRILL<sup>2</sup> und OTHMAR MARTI<sup>1</sup> — <sup>1</sup>Institut für Experimentelle Physik, Ulm — <sup>2</sup>Institut für funktionelle Nanosysteme, Ulm

The research program investigates the calculation of leakages in hydraulic systems by modelling the systems using electric resistor networks as an alternative to simulations using computational fluid dynam-

ics. Based on a rigid geometry, describing a network of channels with rectangular cross sections of constant height, the hydraulic properties of the network are examined. The system is then modelled using an electric resistor network using these hydraulic properties. For a given pressure drop between the in- and outlets the model can be solved and the leakages can be calculated using the modified nodal analysis. The results show that modelling the geometry this way can be an alternative to simulations using computational fluid dynamics within the requirements set by the electric-hydraulic analogy. Modelling hydraulic networks that are not within these requirements, like those with very short channels or highly complex channel networks, results in errors spreading through the network resulting in significant differences between the modelling and simulation approach.

CPP 24.42 Mon 17:30 P3

**Studies on the Effect of Stoichiometric Changes on Thermo-mechanical Properties of Anhydride-cured Epoxy Resin** — ●FARNAZ EMAMVERDI — BAM, Berlin, Germany

Introducing boehmite nanoparticles (BNPs) to anhydride-cured epoxy networks can improve the mechanical properties of the polymer. Understanding of the interaction between BNPs and the epoxy system is crucial since previous studies reveal that the interaction between the BNPs and the epoxy induces changes in the curing reaction locally. AFM-based studies revealed that the anhydride molecule has a preferential interaction with the BNP. It is hypothesized that such preferential absorption disturbs the curing reaction and causes a stoichiometric imbalance at the interphase in the epoxy matrix. To explain this behavior, we prepared off-stoichiometric samples where ratio between epoxy and anhydride were systematically altered. Previous studies have failed to focus on stoichiometric changes of epoxy-anhydride system. The effect of stoichiometric imbalance on the thermomechanical properties like the shear modulus and Tg is the focus of this study. The characterization for rich-hardener, poor-hardener and standard samples were done by FT-IR, TGA, DMA and DSC. Brown discoloration occurred in poor hardener sample. TGA results showed that all samples are thermally stable up to 200°C where the poor-hardener sample is the most stable one. DMA measurements show a post-curing effect for all samples, which is most pronounced in rich-hardener sample where G\* dropped by 28%. Poor-hardener sample shows the highest Tg and crosslinking density.

CPP 24.43 Mon 17:30 P3

**From flower-like micelles to bridged networks: Thermo-responsive block-polymers in solution studied by small-angle neutron scattering.** — ●ALBERT PRAUSE<sup>1</sup>, MICHELLE HECHENBICHLER<sup>2</sup>, BENJAMIN VON LOSPICH<sup>1</sup>, ANDRÉ LASCHEWSKY<sup>2,3</sup>, and MICHAEL GRADZIELSKI<sup>1</sup> — <sup>1</sup>Technische Universität Berlin, Department of Chemistry, Berlin, Germany — <sup>2</sup>Universität Potsdam, Department of Chemistry, Karl-Liebknecht-Str. 24-25, 14476 Potsdam, Germany — <sup>3</sup>Fraunhofer Institute for Applied Polymer Research IAP, Geiselbergstr. 69, 14476 Potsdam, Germany

Mediation between hydrophilic and hydrophobic phases is necessary for almost every application or process, e.g. cleaning, solubilization and stabilization. Best known for this purpose are amphiphilic molecules like surfactants. Usually, it is important to be able to control and adjust rheologic properties like the viscosity of a solution, wherefore polymers were commonly used to obtain the desired rheologic behavior. With this, inducing the possibility of a distinct temperature response to a rheologic property can become highly favorable for applications where temperature can be used to manipulate the rheology. To combine these properties, in this work hydrophobically modified thermo-responsive block-polymers are characterized between 20°C and 60°C in D<sub>2</sub>O. The block-polymers are built of a permanently hydrophilic and a hydrophilic/hydrophobic temperature switchable block with a lower critical solution temperature (LCST). Used monomers are *N*-dimethylacrylamide (DMA) and monomers with LCST like *N*-isopropylacrylamide (NiPAm), respectively.

CPP 24.44 Mon 17:30 P3

**Phase transition kinetics in a doubly thermo-responsive poly(sulfobetaine)-based block copolymer thin film** — ●LUCAS P. KREUZER<sup>1</sup>, TOBIAS WIDMANN<sup>1</sup>, LORENZ BIESSMANN<sup>1</sup>, RAPHAEL MÄRKL<sup>1</sup>, JEAN-FRANCOIS MOULIN<sup>2</sup>, VIET HILDEBRAND<sup>3</sup>, ANDRÉ LASCHEWSKY<sup>3</sup>, CHRISTINE M. PAPADAKIS<sup>1</sup>, and PETER MÜLLER-BUSCHBAUM<sup>1</sup> — <sup>1</sup>TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — <sup>2</sup>HZG at MLZ, 85747 Garching —

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Thermo-responsive polymers show a strong change in volume towards slight changes of their surrounding temperature. While this behavior is well understood for polymers in solution, less is known about the underlying mechanisms in thin film geometry. In our work, we investigate the phase transition kinetics upon increasing temperature in a thermo-responsive block copolymer thin film, that shows both, upper and lower critical solution temperature (UCST and LCST) behavior. Time-of-flight neutron reflectometry (ToF-NR) is used to follow the phase transition kinetics with high time resolution. At temperatures, below the UCST, the polymer film is first swollen in D<sub>2</sub>O atmosphere to increase the mobility of the polymer chains. Subsequent, temperature is increased to an intermediate regime (between UCST and LCST) and high regime (above LCST). In addition ToF grazing incidence small angle neutron scattering (GISANS) measurements are performed at the beginning and in between the kinetic processes to gain detailed information about the thin film morphology at different temperatures.

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**Kinetics of shell collapse and aggregation in thermoresponsive PMMA-*b*-PNIPAM micelles revealed by time-resolved small-angle neutron scattering and fast pressure jumps** — ●GEETHU P. MELEDAM<sup>1</sup>, CHIA-HSIN KO<sup>1</sup>, SHU-HSIEN HUANG<sup>1</sup>, BART-JAN NIEBUUR<sup>1</sup>, LEONARDO CHIAPPISI<sup>2</sup>, ALFONS SCHULTE<sup>3</sup>, and CHRISTINE M. PAPADAKIS<sup>1</sup> — <sup>1</sup>TU München, Physik-Department, Garching, Germany — <sup>2</sup>Institut Laue-Langevin, Grenoble, France — <sup>3</sup>University of Central Florida, Orlando, U.S.A.

The amphiphilic diblock copolymer, poly(methyl methacrylate)-*b*-poly(N-isopropylacrylamide) (PMMA-*b*-PNIPAM) self-assembles into core-shell micelles in aqueous solution, and the thermoresponsive PNIPAM shell collapses upon heating through its cloud point. Here, we explore the kinetics of structural modifications and intermicellar interactions in PMMA-*b*-PNIPAM micelles during its phase transition by performing time-resolved small-angle neutron scattering (SANS) in combination with millisecond pressure jumps. Because of the fast equilibration in a pressure jump, we are able to observe different stages of micellar shell collapse and aggregation while undergoing phase transition. At high pressures, the micellar shell stays rather hydrated and the growth proceeds via diffusion-limited aggregation. On the contrary, at low pressures, a hydrophobic-driven micellar aggregation occurs due to the strong dehydration of the PNIPAM shell. In general, the strategy of combining time-resolved SANS with rapid pressure jump experiments provides an exclusive possibility to probe the initial stages of phase transitions in macromolecules.

CPP 24.46 Mon 17:30 P3

**Dehydration process of thermoresponsive molecular brushes with copolymer side chains** — ●JIA-JHEN KANG<sup>1</sup>, JUNPENG ZHAO<sup>2</sup>, LESTER C. BARNESLEY<sup>3</sup>, FABIAN KOHLER<sup>1</sup>, HENDRIK DIETZ<sup>1</sup>, STERGIOS PISPAS<sup>2</sup>, and CHRISTINE M. PAPADAKIS<sup>1</sup> — <sup>1</sup>TU München, Physik-Department, Garching, Germany — <sup>2</sup>National Hellenic Research Foundation, Theoretical and Physical Chemistry Institute, Athens, Greece — <sup>3</sup>FZ Jülich, JCNS at MLZ, Garching, Germany

Molecular brushes are densely grafted polymers composed of a backbone and side chains attached to virtually every monomer of the backbone. In the present study, we investigate molecular brushes with PEO-*ran*-PPO or PEO-*block*-PPO copolymer side chains in aqueous solution. Both PEO, poly(ethylene oxide), and PPO, poly(propylene oxide), exhibit lower critical solution temperature (LCST) behavior with very different cloud points. Their structural evolution upon heating from ambient temperature to temperatures above the corresponding cloud points is resolved using dynamic light scattering (DLS) and small-angle neutron scattering (SANS). The results reveal that the vastly different dehydration process strongly affects the side chain conformation, and thus the overall brush conformation as well as the collapse and the aggregation behavior.

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**Increase of the diffusion constant of polyanion PSS in polyelectrolyte multilayers on approach to the glass transition temperature in dependence of salt concentration and pH** — ●ANNEKATRIN SILL, SVEN NEUBER, and CHRISTIANE A. HELM — University Greifswald, Institute of Physics, Germany

Using neutron reflectivity, the vertical diffusion of polyanion PSS within polyelectrolyte multilayers is probed. We used a slab archi-

ture with selective polyanion deuteration. The temperature-, salt- and pH-dependent change of the diffusion constant was determined. The films were measured as prepared and after annealing for different times (i) in 1 M NaCl solution at different temperatures approaching the glass transition at 55°C, (ii) at 40°C and different NaCl concentrations of the annealing solution and (iii) in 100 mM NaCl solution with different pH values. As the temperature of the annealing solution increases, the diffusion constant increases by five orders of magnitude. If the salt concentration in the annealing solution is reduced, the diffusion constant becomes smaller by two orders of magnitude. Preliminary measurements show that the diffusion constant decreases as the pH of the annealing solution increases. We conclude that for a large diffusion constant not only electrostatic monomer/monomer bonds need to be replaced by monovalent/ion bonds, but the most important effect is the increased mobility of the water molecules on approach to the glass transition temperature.

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**Polyelectrolyte Microemulsion Complexes (PEMECs) Studied by Scattering Methods** — ●MICHAEL GRADZIELSKI<sup>1</sup>, MIRIAM SIMON<sup>1</sup>, LAURENCE NOIREZ<sup>2</sup>, EMMANUEL SCHNECK<sup>3</sup>, and HOFFMANN INGO<sup>4</sup> — <sup>1</sup>Stranski Laboratorium für Physikalische Chemie, Technische Universität Berlin, Germany — <sup>2</sup>Laboratoire Leon Brillouin (LLB) Saclay, France — <sup>3</sup>MPI für Kolloide und Grenzflächen, Golm/Potsdam, Germany — <sup>4</sup>Institut Laue-Langevin (ILL), 38000 Grenoble, France

Charged oil-in-water microemulsion droplets one can form polyelectrolyte/microemulsion complexes (PEMECs), where colloidal stability and structure are controlled by the properties of the individual components. In our experiments we varied systematically Mw and type of the polyelectrolyte as well as size and charge density of the microemulsion droplets and determined the phase behaviour and mesoscopic structure by means of static and dynamic light scattering, and small-angle neutron scattering (SANS). The formed structures are typically elongated but elongation and total size depend strongly on the mixing ratio, the Mw of the PE and its persistence length - and show and interesting pH response. Further dynamic experiments with PFG-NMR and neutron spin-echo (NSE) showed a remarkably high internal dynamics of these systems. In summary, PEMECs are an interesting and so far only little explored colloidal system that is a well-defined model system suitable for fundamental investigations but also highly relevant for formulations in cosmetics and pharmacy, due to their high loading with hydrophobic components.

CPP 24.49 Mon 17:30 P3

**New insights of the gold nanoparticle growth: Simultaneous SAXS/SANS study** — ●EZZELDIN METWALLI<sup>1</sup>, KLAUS GÖTZL<sup>1</sup>, TOBIAS ZECH<sup>1</sup>, CHRISTIAN BÄR<sup>1</sup>, ANNE MARTEL<sup>2</sup>, LIONEL PORCAR<sup>2</sup>, and TOBIAS UNRUH<sup>1</sup> — <sup>1</sup>ICSP, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — <sup>2</sup>Institut Laue-Langevin, 71, Avenue des Martyrs, Grenoble, 38042, France

Exploiting small angle X-ray and neutron scattering SAXS/SANS methods on the same sample volume at the same time offers a unique possibility to obtain complementary nanoscale structural information at two different contrast situations. A custom-made portable SAXS system has been designed, constructed and installed at D22-ILL for simultaneous SAXS/SANS experiments. For the first time, the temporal structural cross-correlation between organic stabilizing agent (cetyltrimethylammonium bromide; CTAB micelles) and gold seeds, which cooperate in the formation of different size/shape of large stabilized gold nanoparticles [1], has reliably been determined on the same sample. Compared with an independent experimental approach, the current experimental approach ensures the exactness of the probed samples, especially for time-resolved studies. This novel nano-analytical method at ILL will answer yet unresolved scientific questions allowing real time investigations of a wide range of innovative materials such as smart self-assembling nanomaterials and multifunctional materials as well as enabling comprehensive in situ studies on biological systems. [1] T. Schmutzler, et al., ACS Applied Nano Materials 2, 3206 (2019).

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**Grazing incidence scattering for the study of buried interfaces** — ●MAX WOLFF — Department for Physics and Astronomy, Uppsala University

Neutrons can penetrate deeply into matter and are sensitive to light elements. If applied under grazing incidence beam geometry they of-



fer surface sensitivity and the opportunity to address highly relevant scientific challenges on solid-liquid boundaries, like e.g. the hydrodynamic boundary condition. From specular reflectivity the density profile, along the normal of the interfaces, of a liquid close to a solid substrate can be extracted.

Lateral correlations, parallel to an interface, are accessible by off-specular ( $\mu\text{m}$ ) or grazing incidence scattering (nm length scale). Moreover, by using time of flight (TOF) methods a range of  $Q$  (momentum transfers) vectors and related penetration depth can be addressed. In turn the measurements are flux hungry and demanding with respect to brilliance of the source. This in combination with the low absorption of the neutrons in the liquid limits the achievable depth resolution. A combined approach of further improved instrumentation and sample design may allow to overcome this limitations by careful control of the wave amplitude using reference layers and resonators.

CPP 24.51 Mon 17:30 P3

**RheoNSE for the study of topological interactions in poly-**

**mers** — ●MAX WOLFF — Department for Physics and Astronomy, Uppsala University

Entangled polymers show unique flow behaviors, since the relaxation processes occur on time scales relevant for our daily lives, ranging from milliseconds to hours or even days. Yet, due to experimental limitations, the nonlinear rheological behavior of complex fluids is only modestly understood. We investigate the microscopic structure and dynamics of highly entangled polymers under shear with small angle neutron scattering (SANS) and neutron spin echo (NSE), respectively.

The viscoelastic properties of materials are typically investigated by rheology. If such measurements are done in shear rate controlled mode, the formation of a stress plateau can be observed above a critical shear rate. It is known that for these systems the measured stress shows a plateau when investigated under controlled shear rate. At these shear rates the polymer might disentangle resulting in a change in the topological interactions between the chains. This transition can only be observed in the dynamics of the chains studied with NSE.