

## CPP 33: Poster Session III

Topics: Wetting and Microfluidics (33.1-33.2), Soft Matter Physics: Emerging Topics, New Instruments and Methods (33.3-33.5), Functional Polymer Hybrids and Composites (33.6-33.12), Complex Fluids and Colloids (33.13-33.23), Confined Liquids (33.24-33.25), Droplets, Waves and Instabilities at Surfaces and Interfaces (33.26-33.28), Responsive and Adaptive Systems (33.29-33.31), Nanostructures, Nanostructuring and Nanosized Soft Matter (33.32-33.42).

Time: Tuesday 14:00–16:00

Location: Poster C

CPP 33.1 Tue 14:00 Poster C

**Microfluidic flow cell design based on additive manufacturing** — ●MAX MÄNNEL, RICARDO BERNHARDT, ANDREAS FERY, and JULIAN THIELE — Leibniz-Institut für Polymerforschung e.V., Dresden, Germany

Droplet-based microfluidics has undergone a rapid growth in recent years due to its potential in material design and biological applications. The most common technique for microfluidic flow cell fabrication is a combination of photo- and soft lithography. In this process, the widely used poly(dimethylsiloxane) (PDMS) is cured to replicate the microchannel structure, which is then bound to a glass slide. This multi-step process is time-consuming and arduous. A promising alternative technique is additive manufacturing utilizing stereolithography (SL). This 3D printing technique has drawn attention due to its low-cost fabrication and fast process time. It is based on a Digital Light Processor (DLP), which translates a digital image into a XY-illumination pattern. This way, a 3D CAD design of a micro flow cell can be printed layer-by-layer.

While the formation of double and higher-order emulsion droplets in planar flow cells generally requires spatially resolved microchannel wettability, we fabricated 3D-printed non-planar microchannels via SL with a resolution of 100  $\mu\text{m}$  for the first time to avoid the influence of wettability. Additionally, 3D-printed planar emulsion generators with a resolution of 20  $\mu\text{m}$  were fabricated. With that, we are able to fabricate micro flow cells with the same resolution as in conventional fabrication methods, but within much shorter process time.

CPP 33.2 Tue 14:00 Poster C

**Evolution of invading fluid interfaces at different wetting conditions and pore geometry** — ●LI WEIWEI<sup>1,2</sup>, MARTIN BRINKMANN<sup>1</sup>, HAGEN SCHOLL<sup>1,2</sup>, and RALF SEEMANN<sup>1,2</sup> — <sup>1</sup>Saarland University, Experimental Physics, D-66123 Saarbrücken, Germany — <sup>2</sup>Max Planck Institute for Dynamics and Self-Organization, D-37077 Göttingen, Germany

Wettability is an important factor that controls the front morphology during displacement of immiscible fluids. With the help of X-ray microtomography, we record the fluid front morphologies emerging during the fluid invasion into random piles of spherical beads. We identified two qualitatively different displacement regimes that are controlled by the advancing contact angle of the invading fluid. For the accurate characterization of the fluid front evolution, we considered several quantities related to the geometry of the interface. Extending our experiments to low contact angles and non-spherical grains, we found displacement patterns that differ substantially from those previously reported for spherical beads packs [1]. This result reveals the combined influence of wetting conditions and pore geometry on the global evolution of the fluid distribution.

[1] K. Singh, H. Scholl, M. Brinkmann, M. DiMichiel, M. Scheel, S. Herminghaus, and R. Seemann. *Sci. Rep.* 7: 444 (2017).

CPP 33.3 Tue 14:00 Poster C

**Density determination of liquids in the pressure range up to 5000 bar** — JULIA NASE, MIREN BÜYÜKASIK, MIRKO ELBERS, MICHAEL PAULUS, PAUL SALMEN, CHRISTIAN STERNEMANN, ●GÖRAN SURMEIER, and METIN TOLAN — Fakultät Physik/DELTA, TU Dortmund, 44221 Dortmund, Germany

The knowledge of the density of liquids is of high importance in many fields of research. Densities need to be known e.g., for the exact analysis of Terahertz spectroscopy data or X-ray scattering data. Exact values are also needed to verify theoretical density models and as parameter for Molecular Dynamics simulations of liquids. Densities of liquids are typically measured in a vibrating tube densitometer (VTD) with high accuracy, however limited to a small range of temperature and pressure. Notably, the pressure can be increased to several 100 bar only. From the increasing interest in high hydrostatic pressure condi-

tions in the last years, the need for density data in the kbar regime was arising. We present a setup to determine densities of liquid samples from X-ray absorption measurements at pressures up to 5000 bar. Comparing to numerical simulations and data from a VTD, we show that relative density changes can be determined reliably in the whole pressure range. Trimethylamine-*N*-oxide, urea, and salt solutions were examined. Experiments were performed at beamline BL8 of DELTA (Dortmund, Germany).

CPP 33.4 Tue 14:00 Poster C

**Temperature evolution of the density disturbance in water on attosecond timescale** — ●MIRKO ELBERS<sup>1</sup>, NOZOMU HIRAOKA<sup>2</sup>, YURY FOROV<sup>1</sup>, SUSANNE DOGAN<sup>1</sup>, CHRISTOPHER WEIS<sup>1</sup>, CHRISTIAN STERNEMANN<sup>1</sup>, and METIN TOLAN<sup>1</sup> — <sup>1</sup>Fakultät Physik/DELTA, Technische Universität Dortmund, 44227 Dortmund, Germany — <sup>2</sup>National Synchrotron Radiation Research Center, 30076 Hsinchu, Taiwan

Water is one of the key components of life on this planet. Its unique properties and anomalies make it highly relevant for many processes in physics, biology and chemistry. In order to investigate those processes, ultrafast techniques such as pump-probe experiments gained in importance during the last years, leading to a better understanding of e.g. the hydrogen bond dynamics in bulk water. We used a different approach, introduced by Abbamonte et al. (*Phys. Rev. Lett.* 92, 237401, 2004), to image the dynamics of the electron density disturbance in liquid water. This ultrafast imaging method utilizes inelastic x-ray scattering to map the electron density disturbance on an attosecond timescale with an atomic spatial resolution. This is achieved by inverting the energy loss function, accessible in the experiment for a wide range of momentum and energy transfers, into time and space. In this study we take a closer look on the electron dynamics in water at various thermodynamical conditions i.e. different temperatures and pressures, reaching a time resolution below 9 as. The experiments were performed at beamline BL12XU of SPring-8 (Koto, Japan).

CPP 33.5 Tue 14:00 Poster C

**Application of adaptive resolution simulations: free energy calculation in liquids and proteins** — ●RAFFAELE FIORENTINI<sup>1</sup>, AOIFE FOGARTY<sup>1</sup>, RAFFAELLO POTESTIO<sup>2</sup>, and KURT KREMER<sup>1</sup> — <sup>1</sup>Max Planck Institute for Polymers, Mainz, Germany — <sup>2</sup>Department of Physics of the University of Trento, Trento, Italy

A fully atomistic modelling of many biophysical and biochemical processes at biologically relevant length- and time-scales is beyond our reach with current computational resources. One approach to overcome this difficulty is the use of multiscale simulation techniques in which different system components are simultaneously modelled at different levels of resolution. In the case of biomolecules, functionally relevant parts of the system are modelled at as high a level of detail as necessary, while the remainder of the system is represented using less expensive models. Such a multiscale simulation can employ an Adaptive Resolution Simulation (AdResS) methodology, in which the simulation box is divided into atomistic and coarse-grained regions with solvent particles smoothly changing their resolution on-the-fly as they move between regions. In this talk I will discuss how the AdResS approach can be applied to the calculation of thermodynamical properties of biomolecules, and employ it for the first time in combination with Thermodynamic Integration to calculate free energies.

A further multiscale simulation method is the dual resolution approach in which the biomolecule has a dual fixed resolution: atomistic and Coarse Grained part. In this case, the dual-resolution model is employed to compute the protein's free energy landscape.

CPP 33.6 Tue 14:00 Poster C

**Soft X-ray analysis of microgels and polymer-based microcontainers in aqueous environment** — ●ANDREAS SPÄTH<sup>1</sup>, GEORGE TZVETKOV<sup>2</sup>, GAIO PARADOSSI<sup>3</sup>, and RAINER H. FINK<sup>1</sup> — <sup>1</sup>Friedrich-

Alexander Universität Erlangen-Nürnberg, Lehrstuhl für Physikalische Chemie II and ICMM, Erlangen, Germany — <sup>2</sup>University of Sofia, Department of Inorganic Chemistry, Sofia, Bulgaria — <sup>3</sup>Universita di Roma Tor Vergata, Dipartimento di Scienze e Tecnologie Chimiche, Rome, Italy

Polymer-based microgel and core-shell particles are versatile containers for the transport of drugs, theranostic gases or catalytically active molecules. They are in many cases biodegradable and fully compatible to in-vivo applications. During recent years we have investigated a broad range of such hybrid materials ranging from gas filled microballoons and thermoresponsive microgel networks to magneto-responsive particles with embedded iron nanoparticles and core-shell systems filled with theranostic gases or catalytically active fluids. Soft X-ray microscopy is an excellent tool to study those systems in-situ in aqueous matrix with high-resolution and chemical sensitivity. We have analyzed shell thicknesses, swelling behaviors and temperature response to contribute better understanding on release mechanisms and have developed procedures to derive high-resolution 3D representations of the particles from 2D transmission micrographs. The project is funded by the BMBF (05K16WED).

CPP 33.7 Tue 14:00 Poster C

**Study on inner structure and carrier dynamics of colloidal quantum dots solids** — ●WEI CHEN and PETER MÜLLER-BUSCHBAUM — TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching

Colloidal quantum dots (CQDs) have attracted a lot of research interests in both optoelectronics and photovoltaics due to their unique properties, including tunable band-gap, solution processability and the high monodispersity. Due to the intensive investigations on their surface engineering, CQDs based homo-junction solar cells have achieved similar power conversion efficiency (PCE) as compared to top-class bulk heterojunction (BHJ) organic solar cells. The surface engineering is working on not only decreasing the trap states of CQDs\* surface, but also optimizing the positions of each CQDs among the array, which is supposed to be the key factor to achieve higher charge mobility. We use inorganic and organic iodide ions sources to proceed the ligands exchanges on the surface of CQDs during the solids forming by spin coating in a layer by layer fashion. We use grazing incidence small angle x-ray scattering to confirm the inner structure changes of the films, including the inner dot spacing and the structures in larger scale, of CQDs solids under different ambient conditions. Moreover, the femtosecond pump-probe transient absorption spectroscopy (TA) is used to study the carrier dynamics of CQDs solids.

CPP 33.8 Tue 14:00 Poster C

**Morphology phase diagram of printed titania films derived from block copolymer assisted sol-gel templating** — ●NIAN LI, BO SU, SENLIN XIA, and PETER MÜLLER-BUSCHBAUM — TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching

Printing, a simple and low-cost technique for producing films on an industrial scale, is employed to fabricate mesoporous titania thin films. Titanium(IV)isopropoxide (TTIP) is used as precursor and a diblock copolymer polystyrene-block-polyethylene oxide (PS-b-PEO) as the structure-directing template. The amphiphilic block copolymer PS-b-PEO undergoes phase separation and self-assembly due to a good-bad pair solvent, 1,4-dioxane and hydrochloric acid (HCl), respectively. By adjusting the weight fraction of 1,4-dioxane, HCl and TTIP, the titania films with different morphologies are obtained after evaporation and calcination processes. The surface morphology is probed via scanning electron microscopy (SEM) and atomic force microscopy (AFM), and the inner morphology is detected by grazing incidence small-angle X-ray scattering (GISAXS). A high degree of crystallinity of anatase titania is proved by X-ray diffraction (XRD) through optimizing the calcination temperature. The optical properties are examined with UV/Vis spectroscopy.

CPP 33.9 Tue 14:00 Poster C

**Magnetic Nanoparticles in Diblock Copolymer Matrix** — ●KALYAN BISWAS<sup>1</sup>, SENLIN XIA<sup>1</sup>, SARA LAFUERZA<sup>2</sup>, PIETER GLATZEL<sup>2</sup>, MATTHIAS OPEL<sup>3</sup>, and PETER MÜLLER-BUSCHBAUM<sup>1</sup> — <sup>1</sup>TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — <sup>2</sup>ESRF, Grenoble, France — <sup>3</sup>Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching

Fabrication of nanostructured films composed of a polymer matrix and

inorganic functional nanoparticles is highly desirable due to its interesting physical properties in the areas of magnetic sensors. Hybrid films of the diblock copolymer polystyrene-b-(ethylene oxide) (PS-b-PEO) and surface-functionalized magnetic nanoparticles (Fe<sub>3</sub>O<sub>4</sub> with hydrophobic coating) are prepared via spin coating. Both real-space and reciprocal-space techniques are employed to characterize the obtained nanocomposite films. The micro- and nanostructures of the magnetic films as a function of the nanoparticle concentration are probed using optical microscopy, scanning electron microscopy, atomic force microscopy, and grazing incidence small-angle X-ray scattering (GISAXS). The observed structures are explained in the framework of microphase separation and confinement. By using superconducting quantum interference device (SQUID) magnetometer, the magnetic property of the hybrid films like superparamagnetism is explored. The electronic and magnetic structures of the hybrid films are studied by resonant inelastic X-ray scattering and X-ray magnetic circular dichroism (RIXS-XMCD).

CPP 33.10 Tue 14:00 Poster C

**Nanostructured titania templated by amphiphilic diblock copolymer for lithium-ion battery anodes** — ●SHANSHAN YIN, LIN SONG, and PETER MÜLLER-BUSCHBAUM — TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching

Lithium-ion batteries (LIBs) have been widely used in many aspects of modern life. Compared with conventional graphite anodes, titania possesses higher capacity and better operation safety, which makes it a promising substitute to the commonly used graphite anodes. However, problems such as gradual capacity decay and relative high intercalation potential hinder its practical application. It has been reported that nanostructured titania can efficiently improve the electrochemical performance. Therefore, in this work titania nanostructures are prepared via sol-gel synthesis in combination with the amphiphilic diblock copolymer poly(styrene-block-ethylene oxide) (PS-b-PEO) as structure-directing agent. The morphology of the obtained titania nanostructures is studied with optical microscopy (OM) and scanning electron microscopy (SEM), while the optical properties are investigated with UV/Vis spectroscopy and Photoluminescence (PL).

CPP 33.11 Tue 14:00 Poster C

**Orientation of Halloysite nanotubes embedded in a polymer matrix** — ●OLIVER LÖHMANN<sup>1</sup>, OLIVIER FELIX<sup>2</sup>, YURI LVOV<sup>3</sup>, GERO DECHER<sup>2</sup>, and REGINE VON KLITZING<sup>1</sup> — <sup>1</sup>Technische Universität Darmstadt — <sup>2</sup>Institut Charles Sadron — <sup>3</sup>Louisiana Tech University

Halloysites are inorganic, biocompatible nanotubes consisting of aluminosilicates with a length of 0.5 - 2 microns and a diameter of 50 - 80 nm. [1] The surface of the inner lumen is predominated by alumina with a positive surface charge and therefore available for adsorption and protection of small molecules. The nanotubes have an overall negative surface potential at moderate pH due to predomination of silica at the outside. That opens the possibility to embed them into positively charged polyelectrolytes. Zhao et al. showed that Halloysites orientate parallel to each other at the liquid-substrate contact line during solvent evaporation. [2] Based on this we built up multilayers of orientated halloysite over a larger area by controlled spraying method.

Here, we show that halloysites can be orientated by grazing incident spray coating. [3] Multilayers of Halloysites and polyelectrolytes are built up by alternating spray coating. Topology as well as mechanical properties of composites with different layer numbers and compositions measured with Atomic force microscopy will be presented.

[1] Lvov et al., Prog Polym Sci 38 (2013) 1690 - 1719

[2] Zhao et al., J Colloid Interf Sci 440 (2015) 68 - 77

[3] Blell et al., ACS Nano 11 (2017) 84 - 94

CPP 33.12 Tue 14:00 Poster C

**Novel Boehmite-embedded organic/inorganic hybrid nanocomposite: cure behaviour, morphology and thermal properties** — ●IEVGENIIA TOPOLNIAK<sup>1</sup>, VASILE-DAN HODOROABA<sup>1</sup>, SIGRID BENEMANN<sup>1</sup>, DIETMAR PFEIFER<sup>2</sup>, and HEINZ STURM<sup>1</sup> — <sup>1</sup>Federal Institute for Materials Research and Testing (BAM), Unter den Eichen 87, 12205 Berlin, Germany — <sup>2</sup>Federal Institute for Materials Research and Testing (BAM), Richard-Willstätter-Strasse 11, 12489 Berlin, Germany

Hybrid materials have attracted growing interest during the last decade, particularly due to their extraordinary properties. Cycloaliphatic-epoxy oligosiloxane (CEO) resin was shown to be a good candidate as a barrier material for the encapsulation purposes. Incorporation of nanoparticles such as Boehmite (BA) into polymers

was observed to modify their specific characteristics, in particular, thermal, thermo-oxidative and barrier ones. In this work, novel BA-embedded organic inorganic hybrid nanocomposite material was engineered by combining the advantageous properties of hybrid polymers and nanoparticle enhancement effect. Impacts of particles on the photocuring kinetics, degree of crosslinking and the resultant changes in the thermal properties of the cured films were investigated. CEO synthesis via condensation reaction was confirmed by  $^1\text{H}$  and  $^{29}\text{Si}$  NMR. The particle distribution within the films was verified by SEM including transmission mode coupled with EDX elemental analysis. Photocuring kinetics and thermal properties of the films were studied by *in situ* FTIR spectroscopy and DSC with TGA, respectively.

CPP 33.13 Tue 14:00 Poster C

**Comparison of different measurement techniques for optical contrast factors for ternary mixtures** — ●MARCEL SCHRAML, THOMAS TRILLER, ROMAN REH, and WERNER KÖHLER — Institute of Physics, University of Bayreuth, 95440 Bayreuth, Germany

Non-isothermal diffusion in ternary mixtures is extensively studied both on ground and under microgravity conditions on the International Space Station ISS (ESA/Roscosmos, DCMIX3). In most cases are optical, contactless techniques the method of choice. These methods have the disadvantage that the measured data need to be transformed from the refractive index space into the concentration space. Therefore the contrast factor matrix  $a_{ij} = (\partial n_i / \partial c_j)_{p,T,c_k \neq j}$  has to be inverted. We are using self-designed experiments which are based on refraction or interferometry, because commercial refractometers are not accurate enough or can not provide data in a broad temperature range and at wavelengths covering the entire visible spectrum up to the near IR. On the poster we will explain the difficulty of the contrast factor determination and discuss the different measurement methods.

CPP 33.14 Tue 14:00 Poster C

**Isotropic-nematic phase transition in a 3D lattice model of hard rods with sticky attractions** — ●PAUL QUIRING, MIRIAM KLOPOTEK, and MARTIN OETTEL — University of Tübingen, Germany

We investigate the isotropic-nematic phase transition in a 3D lattice model of  $1 \times 1 \times 8$ -sized hard rods with nearest-neighbor attractions via grand canonical Monte Carlo simulations. It appears that below a critical-like temperature the transition between an isotropic gas state and a nematic liquid state is strongly first order. Above that temperature, the isotropic-nematic transition appears to be weakly first order, as in the corresponding system with no attractions. We also implemented successive umbrella sampling [1] to resolve the transition better. We compare the phase diagram to that calculated with classical Density Functional Theory [2], which overestimates the strength of the transition.

[1] R. L. C. Vink, S. Wolfsheimer, and T. Schilling. Isotropic-nematic interfacial tension of hard and soft rods: Application of advanced grand canonical biased-sampling techniques. *The Journal of Chemical Physics*, 123(7):074901, 2005.

[2] M. Mortazavifar and M. Oettel. Phase diagrams for sticky rods in bulk and in a monolayer from a lattice free-energy functional for anisotropic particles with depletion attractions. *Physical Review E*, 96(3), 2017.

CPP 33.15 Tue 14:00 Poster C

**A new approach to evaluate the phase gradient in diffusion measurements by digital interferometry** — ●DANIEL SOMMERMANN, THOMAS TRILLER, and WERNER KÖHLER — Institute of Physics, University of Bayreuth, 95440 Bayreuth, Germany

In order to get a better understanding of thermodiffusion in ternary mixtures, the so called DCMIX experiments (Diffusion Coefficients in MIXtures) were performed on the International Space Station (ISS) using the SODI-interferometer (Selective Optical Diagnostics Instrument) under microgravity conditions. This Mach-Zehnder-Interferometer measures the Soret effect by applying a vertical temperature gradient to the system and using digital interferometry with laser phase stepping for readout.

Information about mass diffusion coefficients is obtained by an evaluation of the phase of the interferogram which is done by temporal phase shifting using five pictures in a row. Unfortunately, the readout laser in the DCMIX3 microgravity experiments suffered from instabilities and phase fluctuations. Usual temporal phase shifting algorithms are expecting a constant change in phase and are therefore unable to evaluate part of the data.

In this work a new spatial evaluation method is introduced which can handle the problem of nonconstant phase stepping by analysing all pictures individually, thereby reconstructing the phase gradient.

CPP 33.16 Tue 14:00 Poster C

**Network formation and clustering in a simple Monte Carlo model for protein solutions** — ●FRANK HIRSCHMANN, MARC HABINGER, MALTE LÜTJE, JOHANNES BLEIBEL, and MARTIN OETTEL — Institut für angewandte Physik - Computational Soft Matter and Nano-Science, Universität Tübingen, Germany

Recent experimental investigations of globular proteins in solutions with three-valent salt ions show interesting phase behavior as well as the formation of extended clusters for a specific parameter range. This can be explained by condensation of salt ions to the surface groups of the proteins, thus leading to aggregation by forming ion bridges via short-range Coulombic attraction.

In order to analyze these results theoretically, we introduce a "patchy particle" model, realized by a non-additive, binary mixture, consisting of hard sphere-like "particles" representing proteins and "floating bonds" representing "bridging ions". By using Brownian-like dynamics simulations, we analyse the emerging network structure and clustering properties both in the spatial and temporal domain.

CPP 33.17 Tue 14:00 Poster C

**Halloysite nanotubes surface manipulation by catalyst to control physico-chemical properties of Pickering emulsions** — ●SEBASTIAN STOCK<sup>1</sup>, DMITRIJ STEHL<sup>1</sup>, REGINE VON KLITZING<sup>1</sup>, YURI LVOV<sup>3</sup>, TOBIAS POGRZEBA<sup>2</sup>, and REINHARD SCHOMÄKER<sup>2</sup> — <sup>1</sup>TU Darmstadt, Hochschulstraße 6-8, 64289 Darmstadt — <sup>2</sup>TU-Berlin, Straße des 17 Juni 124, 10623 Berlin — <sup>3</sup>Louisiana Tech University, 911 Hergot Ave, Ruston, LA 71272, USA

An emulsion with water and oil has a natural tendency to separate in two phases very fast. The high surface energy is minimized by minimizing the surface between the oil and the water phase. To prevent this process and stabilize the emulsion nanoparticles can be used. Suitable particles for this are the Halloysite nanotubes (HNTs). In opposite to common spherical nanoparticles HNTs are multiwall tubes based on aluminosilicate. They are around 50 nanometers in diameter and can be up to 1 micrometer long. HNTs have the ability to adsorb at the oil/water interface, change the interface properties this way and stabilize the emulsion. These particle stabilized emulsions are named Pickering emulsions (PEs). Different factors influence the PEs structure. The variation of the PEs HNT and salt (NaCl) concentration and HNT surface modifications by the Rh-catalyst were studied. In order to evaluate the PEs properties, the droplet size and the zeta potential are determined.

CPP 33.18 Tue 14:00 Poster C

**Modification of polymer particles with Rh-catalyst for stabilization of Pickering emulsions in catalysis** — ●SANDRA FORG, DMITRIJ STEHL, and REGINE VON KLITZING — Institut für Festkörperphysik, Technische Universität Darmstadt, Alarich-Weiss-Straße 10, D-64287 Darmstadt

Particle stabilized oil-in-water emulsions, so called Pickering emulsions, are useful for many applications, i.e. the liquid/liquid catalysis. To create such emulsions nanoparticles accumulate at the interface of the two liquids to prevent them to coalesce. The benefit of these emulsions is the increase of the surface area available for catalytic reactions, which enhances the efficiency of these reactions. Besides, the stabilized Pickering emulsions should make it easier to recover the catalyst.

Due to this reason, emulsions stabilized both with Poly(N-isopropylacrylamide) (PNIPAM) and with Polystyrene-NH<sub>2</sub> (PS-NH<sub>2</sub>) will be used during this work. Both particles will have a positive charge and thus, the negatively charged Rh-catalyst will adsorb on them. By modification of the ratio between particles and catalyst, the hydrophobicity will be changed. Furthermore, PNIPAM has the benefit that it is temperature-responsive. Due to this temperature-dependence, the diameter of PNIPAM and its chemical affinity to water can be easily affected by changing the temperature. This will result in changes in the stability of the emulsion. A main goal of this work will also be the improvement of knowledge of Pickering emulsions with respect of different properties such as their stability, their structure or the immobilization of the catalyst on the particles.

CPP 33.19 Tue 14:00 Poster C

**Structure properties of biaxial phases formed by mixtures composed of uniaxial liquid crystal particles.** — ROBERT SKUT-

NIK, •LOUIS LEHMANN, SERGEJ PÜSCHEL-SCHLOTTHAUER, and MARTIN SCHOEN — Stranski-Laboratorium für Physikalische und Theoretische Chemie, Technische Universität Berlin, Sekr. C7, Straße des 17. Juni 135, Berlin 10623, Germany

Liquid crystals consist of organic molecules of anisotropic shapes. With respect to their shape, they can be classified as disc- and rod-like particles. Both types of particles undergo an isotropic-nematic phase transition. In the nematic phase, the particles align parallel to each other and exhibit thereby a long-range orientational order. In mixtures of discotics and rods, the favored configuration of two separate disc-like particles or two rod-like particles remains parallel. However, rod-like particles align perpendicularly to the disc-like particles with respect to their symmetry axes. In order to study the phase transition of such mixtures, we perform isothermal-isobaric Monte Carlo simulations where the interparticle interactions are modeled by an orientation-dependent Lennard-Jones potential. Here we present a phase diagram of a binary mixture including a biaxial nematic phase as well as a mixture of a uniaxial nematic phase and an isotropic phase with reduced degrees of freedom. We use finite-size scaling theory to identify the phase transition temperatures and use different order parameters to analyze the structure of the mixture.

CPP 33.20 Tue 14:00 Poster C

**Defect topologies in chiral liquid crystals confined to spherically symmetric cavities** — •ROBERT SKUTNIK, SERGEJ PÜSCHEL-SCHLOTTHAUER, and MARTIN SCHOEN — Stranski-Laboratorium für Physikalische und Theoretische Chemie, Technische Universität Berlin, Sekr. C7, Straße des 17. Juni 135, Berlin 10623, Germany

Liquid crystals exhibit an orientational long range order whereas the positional order remains short ranged. The orientational order of achiral liquid crystals can be described by global quantities. For instance, the molecules align with their symmetry axes along the global director  $\hat{n}$ . In chiral liquid crystals the orientational order becomes local and is given by the local directorfield  $\hat{n}(\mathbf{r})$ . Particularly, chiral Blue Phases attract the interest of the scientific community because their orientational distribution appears to be isotropic on a macroscopic length scale whereas regular orientational order is found locally. These properties provide an application as tunable photonic devices. This raises the question for the manipulation of blue phases by external fields (i. e., electromagnetic fields or confinement). Here, we focus on the case of a Blue Phase II confined to a spherical cavity. In order to investigate properties of confined Blue Phases, we perform Monte Carlo simulations in the grand canonical ensemble. The chiral liquid crystal is modeled by a modified 12-6 Lennard-Jones potential which has been repeatedly used to model all known chiral phases adequately. Depending on the cavity diameter as well as on the local alignment at the interface we observe a zoo of novel topological disclination networks.

CPP 33.21 Tue 14:00 Poster C

**Entanglement in semiflexible polyelectrolyte solutions** — •CARLOS LOPEZ — RWTH Aachen University

We present shear rheology data for solutions of semiflexible polyelectrolyte sodium carboxymethyl cellulose (NaCMC) in salt-free water and aqueous solutions of various electrolytes.

The plateau modulus ( $G_e$ ), estimated from the crossover between the elastic modulus and loss modulus in oscillatory shear, scales as with concentration  $G_e \sim c^{1.7}$ . The entanglement concentration is approximately independent of added salt concentration. The data presented here, along with a review of the literature suggests that electrostatics have only a weak effect on entanglements, despite having a large effect on polymer conformation.

The reptation model correctly predicts the variation of solution viscosities with concentration and molecular weight in high salt solution but fails in salt-free solution, where an exponent  $\simeq \times 3$  larger than the reptation prediction is observed.

These observations presented here clash with scaling arguments which assume that the entanglement tube diameter is proportional to the correlation length and hence dependent on solvent quality.

CPP 33.22 Tue 14:00 Poster C

**Non-Equilibrium States of Sticky Colloidal Particles: Phase Separation and Dynamical Arrest** — •JAN HANSEN, CAROLYN J. MOLL, FLORIAN PLATTEN, and STEFAN U. EGELHAAF — Condensed Matter Physics Laboratory, Heinrich Heine University, Düsseldorf, Germany

Soft materials can form amorphous solids, e.g. gels and glasses, which are relevant for such diverse fields as food engineering, pharmaceutical industry and materials science. To analyze the non-equilibrium states of colloidal particles interacting via short-ranged attractions, we use a perfectly monodisperse suspension of nearly spherical particles, namely globular proteins (lysozyme). The metastable gas-liquid binodal, the attractive glass line and the second virial coefficient  $B_2$  for various solution conditions, i.e. salt concentrations, have been determined by optical microscopy, centrifugation experiments and light scattering. If the temperature axis of the binodals is expressed in terms of  $B_2$ , data obtained under various conditions fall onto a master curve, as suggested by the corresponding states law. For colloids with short-ranged attractions, gelation has previously been related to gas-liquid phase separation and a universal state diagram has been proposed if scaled by  $B_2$ . However, this is in contrast to our findings. Arrest lines for different salt concentrations overlap within experimental errors, whereas they do not overlap if the temperature axis is replaced by  $B_2$ . This indicates that the binodals are not sensitive to the details of the potential, but can be described by one integral parameter, i.e.  $B_2$ , whereas the arrest line appears governed by its attractive part.

CPP 33.23 Tue 14:00 Poster C

**Pressure-induced phase separation in silica nanoparticle-polymer solutions** — •MARC MORON, JULIAN SCHULZE, JULIA NASE, MICHAEL PAULUS, and METIN TOLAN — Fakultät Physik/DELTA, TU Dortmund, 44221 Dortmund, Germany

Nanoparticles are in the focus of current research because they are important for many applications like e.g. thermal energy storage or in medical chemistry for gene delivery. Silica nanoparticles in aqueous solution show a repulsive interaction. By adding small non-adsorbing polymers (e.g. polyethylene glycol), the total particle-particle interaction can become attractive. With increasing polymer concentration, the system undergoes a liquid-liquid phase separation. Further increase of the PEG concentration leads to a homogenous solution, which is explained by the repulsive interaction between the polymers. This concentration-dependent phase transition can also be achieved by exposing the system to high pressure. However, a complete understanding of the effect of pressure on the nanoparticle-polymer system is still missing. In this work light transmission and small-angle X-ray scattering (SAXS) measurements are performed, to study systematically the effect of hydrostatic pressure, the molecular weight of PEG and the sample environment on the phase behavior. In that way a complete picture of the system is obtained and the understanding of the phase transition on a microscopic level is increased.

CPP 33.24 Tue 14:00 Poster C

**Collective Orientational Order and Phase Behavior of a Discotic Liquid Crystal under Confinement** — •ARDA YILDIRIM<sup>1</sup>, KATHRIN SENTKER<sup>2</sup>, PATRICK HUBER<sup>2</sup>, and ANDREAS SCHÖNHALS<sup>1</sup> — <sup>1</sup>Bundesanstalt für Materialforschung und -prüfung (BAM), Unter den Eichen 87, 12205 Berlin, Germany — <sup>2</sup>Institut für Materialphysik und -technologie, Technische Universität Hamburg, Eißendorfer Str. 42, 21073 Hamburg, Germany

Discotic liquid crystals (DLCs) are a promising class of soft matter for electronic applications. This is due to their ability to self-organize into columns in a hexagonal columnar mesophase, driven by the overlapping of the  $\pi$  orbitals of their aromatic cores. This leads to a high charge-carrier mobility along the column axis. Previous studies on DLCs showed that their properties, such as phase transition temperatures and enthalpies, are susceptible to nanoconfinement [1,2]. In this study, 2,3,6,7,10,11 hexakis[hexyloxy] triphenylene (HAT6) was confined into parallel aligned cylindrical nanopores of anodic aluminum oxide (AAO) membranes by melt infiltration. Furthermore, the pore surfaces of a series of membranes were chemically modified, resulting in a more hydrophobic pore surface than the unmodified ones. Collective orientational order and phase behavior of HAT6 confined into modified and unmodified nanopores of AAO were investigated by broadband dielectric spectroscopy and differential scanning calorimetry respectively. [1] C. Krause and A. Schönhals, J. Phys. Chem. C, 2013, 117, 19712. [2] C. Krause et al., Colloid Polym. Sci., 2014, 292, 1949.

CPP 33.25 Tue 14:00 Poster C

**Static properties of confined hard-sphere fluids** — •LUKAS SCHRACK and THOMAS FRANOSCH — Institut für Theoretische Physik, Leopold-Franzens-Universität, Technikerstraße 21A, 6020 Innsbruck, Austria

We investigate static properties in a strongly confined hard-sphere liq-

uid between two parallel flat walls. For this purpose, the Ornstein-Zernike integral equation using Percus-Yevick closure relation is solved numerically. The theory requires the density profile perpendicular to the plates as input, which can be obtained from density functional theory. The resulting convolution integral is most efficiently solved by a Fast Hankel transform of zeroth-order with a logarithmically spaced grid yielding to an algebraic equation.

The confinement induces a modulation of the equilibrium density profile with plane waves as the suitable eigenmodes for the planar geometry. We try to solve the inhomogeneous Ornstein-Zernike equation in mode representation and compare our results to the calculated Fourier decomposition of the direct correlation function and the static structure factor obtained from the real-space solution.

CPP 33.26 Tue 14:00 Poster C

**Cusp-Shaped Elastic Creases and Furrows** — ●STEFAN KARPITSCHKA<sup>1,2</sup>, JENS EGGERS<sup>3</sup>, ANUPAM PANDEY<sup>1</sup>, and JACCO H. SNOEIJER<sup>1,4</sup> — <sup>1</sup>Physics of Fluids Group, Faculty of Science and Technology, University of Twente, Enschede, Netherlands — <sup>2</sup>Max Planck Institute for Dynamics and Self-Organization, Göttingen — <sup>3</sup>School of Mathematics, University of Bristol, United Kingdom — <sup>4</sup>Mesoscopic Transport Phenomena, Eindhoven University of Technology, Netherlands

The surfaces of growing biological tissues, swelling gels, and compressed rubbers do not remain smooth, but frequently exhibit highly localized inward folds. In biology, such elastic structures are called sulci, which are prime morphological features of human brains and growing tumors. Yet in spite of their ubiquity and importance, a quantitative theoretical description of the morphology of localized indentations is still missing. We reveal the morphology of this surface folding in a novel experimental setup, which permits us to deform the surface of a soft gel in a controlled fashion [Phys. Rev. Lett. 119, 198001 (2017)]. The interface first forms an increasingly sharp furrow. Above a critical deformation, the furrow bifurcates to an inward folded crease of vanishing tip size. We show experimentally and numerically that both creases and furrows exhibit a universal cusp shape, whose width scales like  $y^{3/2}$  at a distance  $y$  from the tip. We provide a similarity theory that captures the singular profiles before and after the self-folding bifurcation, and derive the length of the fold from finite deformation elasticity.

CPP 33.27 Tue 14:00 Poster C

**Spheroidal and conical shapes of ferrofluid-filled capsules in magnetic fields** — ●CHRISTIAN WISCHNEWSKI and JAN KIERFELD — Department of Physics, Technische Universität Dortmund, 44221 Dortmund, Germany

We investigate the deformation of soft spherical elastic capsules filled with a ferrofluid in external uniform magnetic fields at fixed volume by a combination of numerical and analytical approaches. We develop a numerical iterative solution strategy based on nonlinear elastic shape equations to calculate the stretched capsule shape numerically and a coupled finite element and boundary element method to solve the corresponding magnetostatic problem, and employ different analytical approximations. The observed deformation behavior is qualitatively similar to the deformation of ferrofluid droplets in uniform magnetic fields. Homogeneous magnetic fields elongate the capsule, and a discontinuous shape transition from a spheroidal shape to a conical shape takes place at a critical field strength. We investigate how capsule elasticity modifies this hysteretic shape transition and show that conical capsule shapes are possible but involve diverging stretch factors at the tips, which gives rise to rupture for real capsule materials. At small fields capsules remain spheroidal, and we characterize the deformation of spheroidal capsules both analytically and numerically. Our results can be helpful in order to quantitatively determine capsule or ferrofluid material properties from magnetic deformation experiments. All results also apply to elastic capsules filled with a dielectric liquid in an external uniform electric field.

CPP 33.28 Tue 14:00 Poster C

**Beyond the standard line tension: Size-dependent contact angles of water nanodroplets** — ●MATEJ KANDUC — Soft Matter and Functional Materials, Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, D-14109 Berlin, Germany

The dependence of the contact angle on the size of a nanoscopic droplet residing on a flat substrate is traditionally ascribed solely to line tension. Other contributions, stemming from the droplet geometry dependence of the surface tension and line tension, are typically ignored. We

performed molecular dynamics simulations of water droplets of cylindrical morphology on surfaces of a wide range of polarities. In the cylindrical geometry, where the line tension is not operative directly, we found significant contact angle dependence on the droplet size [1]. The effect is most pronounced on hydrophilic surfaces, with the contact angle increase of up to  $10^\circ$  with a decreasing droplet size. On hydrophobic surfaces, the trend is reversed and considerably weaker. Our analysis suggests that these effects can be attributed to the Tolman correction due to the curved water-vapor interface and to a generalized line tension that possesses a contact angle dependence. The latter is operative also in the cylindrical geometry and yields a comparable contribution to the contact angle as the line tension itself in case of spherical droplets.

[1] M. Kanduc, J. Chem. Phys. 147, 174701 (2017)

CPP 33.29 Tue 14:00 Poster C

**Solvation effects and self-organization of a multi-azobenzene photochromic system in aqueous and DMSO/water solutions** — ●MARKUS KOCH<sup>1</sup>, ANASTASIA B. DANILOVA<sup>2</sup>, ALEKSANDR S. PAVLOV<sup>2</sup>, and OLGA GUSKOVA<sup>1</sup> — <sup>1</sup>Institute Theory of Polymers, IPF Dresden, Germany — <sup>2</sup>Department of Physical Chemistry, Faculty of Chemistry and Technology, Tver State University, Russia

The star-shaped molecules with benzene-1,3,5-tricarboxamide center (playing a role of gelator) and three photo-sensitive azobenzene arms were found to self-assemble into supramolecular columnar phases in solution [1]. Upon UV-light stimulus, when azobenzenes are isomerized from a planar trans- to a bent cis-state, these aggregates undergo order/disorder transition, which was largely attributed to the changes in molecular geometry. In this work, the concentrated solutions of multi-azobenzene photochromic system [2] in water and DMSO/water mixture are studied at Ångström resolution using all-atom MD simulations aiming at further understanding of the self-assembly and disassembly triggered by light. Comparing the solvation properties of the stars in water and DMSO/water mixtures, we conclude about possible impact of DMSO molecules on the structural properties of the star. Our results represent a useful conceptual starting point to deeper understanding of the experimentally observed morphological transitions triggered by light and upon exposure of columnar phases to pure DMSO.

This work was supported by DFG (Project No GU 1510/3-1).

[1] S. Lee et al. Langmuir 2013, 29, 5869.

[2] M. Koch et al. J. Phys. Chem. B 2017, 121, 8854.

CPP 33.30 Tue 14:00 Poster C

**Responsive Copolymer-Graphene Oxide Hybrid Microspheres with Improved Drug Release Kinetic** — ●IZABELA FIRKOWSKA-BODEN<sup>1</sup>, FUPING DONG<sup>1,2</sup>, MATTHIAS M. L. ARRAS<sup>1,3</sup>, and KLAUS. D. JANDT<sup>1,4</sup> — <sup>1</sup>Chair of Materials Science, Otto Schott Institute of Materials Research, Faculty of Physics and Astronomy, Friedrich-Schiller-University Jena, Löbdergraben 32, 07743 Jena, Germany — <sup>2</sup>Department of Polymer Materials and Engineering, College of Materials and Metallurgy, Guizhou University, Guiyang, 550025, China — <sup>3</sup>Oak Ridge National Lab, Biology and Soft Matter Division, Oak Ridge, TN 37831, USA — <sup>4</sup>Jena Center for Soft Matter (ICSM), Friedrich-Schiller-University Jena, Philosophenweg 7, 07743 Jena, Germany

Polymeric hollow spheres with sizes ranging from the nanometer to the micrometer scale are particularly functional materials owing to their potential application as drug delivery system. In order to control the encapsulation and releasing of drug molecules from the interiors under physiological conditions, smart hollow spheres, which are sensitive to temperature have been reported. In this study we aimed to integrate both high loading efficiency and controlled drug release into a hybrid composite material composed of thermoresponsive copolymer hollow microspheres poly(N-isopropylacrylamide-co-styrene) (PNIPAAm-co-PS) and outer graphene oxide layer. The diffusion-driven drug release is controlled by the electrostatically deposited layer of GO nanosheets, which effectively suppresses the initial burst release and enables sustained drug release in in vitro testing.

CPP 33.31 Tue 14:00 Poster C

**Mechano-Responsive Polymer Structures for Sensing Forces** — ●JENS W. NEUBAUER<sup>1</sup>, NICOLAS HAUCK<sup>1</sup>, JULIAN THIELE<sup>1</sup>, and ANDREAS FERY<sup>1,2</sup> — <sup>1</sup>Leibniz-Institut für Polymerforschung Dresden e.V., Germany — <sup>2</sup>Chair of Physical Chemistry of Polymeric Materials, Technische Universität Dresden, Germany

We design mechano-responsive polymer structures for spatially resolved force sensing. Local deformations of the polymer cause localized

changes in the fluorescence of labelled dyes. Hence, the deformations can be correlated with the mechanical properties of the polymer structure.

Recently, we applied a mechano-responsive polyelectrolyte brush to resolve the stress distributions in the contact area of gecko-inspired microstructures. The polyelectrolyte brush carried permanent cationic charges which could quench the fluorescence of the labelled dye. Accordingly, compressive and tensile stresses could be read out from locally decreased and increased fluorescence intensity, respectively. In earlier work, the sensitivity upon compression was determined to 10 kPa with a spatial resolution better than human skin (1  $\mu\text{m}$ ).

As the polymer brush layers are limited in geometry, we aim for extending the responsiveness to three-dimensional polymer networks. For this purpose, we utilize droplet microfluidics.

Neubauer, J. W. *et al.* *ACS Appl. Mater. Interfaces* **8** (2016) 17870.

Bünsow, J. *et al.* *Angew. Chem. Int. Ed.* **50** (2011) 9629.

Heida, T. *et al.* *Macromol. Chem. Phys.* **218** (2017) 1600418.

CPP 33.32 Tue 14:00 Poster C

**Polymer structure formation in ITPC foils studied by SAXS** — ●ANN-KATHRIN GREFE, BJÖRN KUTTICH, and BERND STÜHN — Institut für Festkörperphysik, Technische Universität Darmstadt

Nanopores obtained by etching of heavy ion irradiated polycarbonate foils present ideal systems for studying polymer structure formation under confinement. Their perfect cylindrical geometry, strict orientation perpendicular to the surface and random lateral distribution allow for an straightforward investigation via small angle x-ray scattering [1].

Polycarbonate foils with pore radii ranging from 17 nm to 59 nm are prepared and characterized via SAXS. The dependency of the pore radius and its polydispersity on the etching time are examined. Subsequent coating of the pores with 10 nm of SiO<sub>2</sub> via atomic layer deposition is shown to result in a well-defined and homogenous surface which does not alter the cylindrical form of the pores.

Two different polymer systems are introduced into the pores via melt infiltration: For a bulk cylinder forming PS-b-PI diblock copolymer in situ SAXS measurements confirm that a nearly complete filling of the pores with polymer can be achieved and a full profile fit can be used to directly monitor the filling kinetics. However, the scattering curves show no indications for a structure formation of the polymer inside the pores. For a PEG homopolymer with a semi-crystalline lamellar structure in bulk the filling process is too fast to be resolved via SAXS. But here changes in the scattering curves of pores with a diameter over 100 nm hint at a structure formation due to partial crystallization.

[1] M. Engel *et al.*, *Appl Phys A* **97**, 99-108 (2009)

CPP 33.33 Tue 14:00 Poster C

**Molecular AC electrokinetics using interdigitated electrodes** — ●EVA-MARIA LAUX<sup>1</sup>, CHRISTIAN WENGER<sup>2</sup>, FRANK F. BIER<sup>1</sup>, and RALPH HÖLZEL<sup>1</sup> — <sup>1</sup>Fraunhofer IZI-BB, Potsdam, Germany — <sup>2</sup>IHP GmbH - Leibniz Institute for Innovative Microelectronics, Frankfurt (Oder), Germany

Electrokinetic effects are universally applicable to particles regardless of their charge and - in principle - of their size. However, as a consequence of the interference of thermal motion, a successful manipulation of particles in the nanometer range calls for increasingly high electric field gradients. These can be produced by further miniaturized electrode structures, Here we use interdigitated nanoelectrodes made of tungsten, embedded in silicon dioxide, fabricated on a silicon substrate. Whilst the electrode width and gap width are 750 nm and 450 nm, respectively, the thickness amounts to 100 nm and the curvature of the electrode edges - which is the decisive parameter for dielectrophoretic action - is below 50 nm.

Using these electrodes, we attracted fluorescent proteins (eGFP) to the electrodes and achieved immobilization as well as alignment of the protein molecules. With its cylindrical shape with 2.4 nm diameter and 4.2 nm height, eGFP belongs to the smallest objects manipulated by AC electrokinetics up to date. We are pushing this limit further by handling, as an example, the fluorescence dye rhodamine 6G, which has a diameter of approx. 1 nm. The dye molecules are indeed attracted towards the electrode structures and accumulated in the electrode gaps as revealed by fluorescence microscopy.

CPP 33.34 Tue 14:00 Poster C

**AC field assisted deposition of antibodies for virus detection** — ●SANDRA STANKE<sup>1,2</sup>, CHRISTIAN WENGER<sup>3</sup>, FRANK BIER<sup>1,2</sup>, and RALPH HOELZEL<sup>1</sup> — <sup>1</sup>Fraunhofer Institute for Cell Therapy and

Immunology, Branch Bioanalysis and Bioprocesses IZI-BB, Potsdam, Germany — <sup>2</sup>University of Potsdam, Germany — <sup>3</sup>IHP GmbH, Leibniz Institute for Innovative Microelectronics, Frankfurt/Oder, Germany

Alternating current (AC) electrokinetics is a set of different effects that can be used for the manipulation of nano-particles in a non-uniform electric field. Here, we present an AC-electrokinetic driven sensor for the manipulation and movement of biological nanoparticles. This sensor consists of four individual arrays, each built up of more than 6000 nano-electrodes with a diameter of 500 nm each. Individually controlled functionalization of the sub-arrays is performed by AC electrokinetic forces: dielectrophoresis and AC electroosmosis. Consequently, molecules like antibodies can be attracted to the electrode surface. This allows the local concentration of the analyte at the sensor surface. Since these arrays can be addressed individually, each array can be functionalized with a different antibody. Thus, it is possible to detect, characterize and subtype different strains of the influenza virus. Additionally, each electrode is part of an on-chip resonant circuit, whose frequency changes with surface coverage of the electrode and, hence, serves as a measure of the amount of viruses bound to the antibody. The universal chip design does not limit the application to influenza viruses but also to different viruses, bacteria and parasites.

CPP 33.35 Tue 14:00 Poster C

**Evolution of atomic structure and nanoparticle formation during spray deposition of metal organic decomposition inks**

— ●BJÖRN FRICKE<sup>1</sup>, WIEBKE OHM<sup>1</sup>, CALVIN BRETT<sup>1,2</sup>, MATTHIAS SCHWARTZKOPF<sup>1</sup>, ANDRÉ ROTHKIRCH<sup>1</sup>, TIM LAARMANN<sup>1,3</sup>, and STEPHAN V. ROTH<sup>1,4</sup> — <sup>1</sup>Deutsches Elektronen-Synchrotron Hamburg, Notkestraße 85, 22607 Hamburg — <sup>2</sup>KTH Royal Institute of Technology, Department of Mechanics, Teknikringen 8, SE-100 44 Stockholm, Sweden — <sup>3</sup>The Hamburg Centre for Ultrafast Imaging CUI, Luruper Chaussee 149, Hamburg 22761, Germany — <sup>4</sup>KTH Royal Institute of Technology, Department of Fibre and Polymer Technology, Teknikringen 56-58, SE-100 44 Stockholm, Sweden

We present a spray deposition process for fabrication of nanostructured silver layers which is advantageous in comparison to other methods. Silver nitrate solution was used as precursor for the nanostructures, which is beneficial, because of its solubility and the low toxicity. We investigated the growth of deposited silver nitrate nanoparticles as well as the influence of an annealing process, by optical and atomic force microscopy and UV-VIS spectroscopy. In addition, in situ GISAXS and GIWAXS were used to identify morphological and chemical changes during the spraying/heating process: The nanoparticle growth was investigated as a function of the spray duration. During the heat-induced transformation, the nanoparticles show coalescence, resulting in a larger percentage of surface coverage in comparison to the as deposited films. Additionally, the temperature dependent conversion from silver nitrate to silver is shown.

CPP 33.36 Tue 14:00 Poster C

**Application of the Microfluid Segment Technology for the Preparation of Noble Metal Nanoparticles** — ●ANDREA KNAUER and J. MICHAEL KÖHLER — Technische Universität Ilmenau, FG Physikalische Chemie/Mikroreaktionstechnik, Prof.-Schmidt-Str. 26, 98693 Ilmenau, Deutschland

The microfluid segment technology allows the realization of fast mixing processes and thus a very narrow residence time distribution. This enables optimum preconditions for a fast nanoparticle nucleation and opens up the possibility to generate nanoparticles with highly homogeneous shapes and compositions, narrow particle diameter distributions, and thus pronounced sharp absorption bands in optical spectroscopy. Therefore, a microfluid segment based technique was used for the generation of noble metal nanoparticles. Within this work, microfluidically processed Au/Ag core/shell nanoparticles, triangular silver nanoprisms, silver nanoprisms with a gold shell, or gold nanoframes, and single crystalline gold nanocubes are presented as model systems. By choosing the appropriate reactant ratios, the nanoparticles sizes and thus their optical properties can be tuned with a fine resolution. Depending on size, shape and composition, the spectral position of the absorption maximum can be shifted between 390 and 1000 nm.

CPP 33.37 Tue 14:00 Poster C

**How do amino acids behave in intercalation compounds?** — ●ROBBY BÜCHNER<sup>1</sup>, ANNETTE PIETZSCH<sup>1</sup>, and ISTVÁN PÁLINCÓ<sup>2</sup> — <sup>1</sup>Helmholtz-Zentrum Berlin für Materialien und Energie, Germany — <sup>2</sup>University of Szeged, Hungary

The first soft X-ray spectra of a Layered Double Hydroxide (LDH) and intercalated amino acids are presented. LDHs are clay minerals with the ability to store arbitrary anionic guest species between their positively charged layers. This property enables numerous applications ranging from environmental remediation, to controlled drug delivery and even gene transfer. In order to systematically develop and improve these applications, a profound understanding of the host-guest interactions is essential. Therefore, near-edge X-ray absorption fine structure (NEXAFS) and resonant inelastic X-ray scattering (RIXS) measurements were carried out. They confirmed the widely assumed Coulomb attraction between the LDH host and the guest ions. Additionally, an at least partially covalent bond between the host layers and the amino acids can be stated.

CPP 33.38 Tue 14:00 Poster C

**Gold Nanoparticle Growth on Homopolymer Thin Films** — ●SUSANN FRENZKE<sup>1</sup>, MATTHIAS SCHWARTZKOPF<sup>2</sup>, PALLAVI PANDIT<sup>2</sup>, WIEBKE OHM<sup>2</sup>, MARC GENSCH<sup>2</sup>, BJOERN FRICKE<sup>2</sup>, CALVIN BRETT<sup>2,3</sup>, and STEPHAN V. ROTH<sup>2,4</sup> — <sup>1</sup>FernUniversität in Hagen, Universitätsstr. 1, D-58097 Hagen — <sup>2</sup>DESY, Notkestr. 85, D-22607 Hamburg — <sup>3</sup>KTH Royal Institute of Technology, Department of Mechanics, Teknikringen 8, SE-10044 Stockholm — <sup>4</sup>KTH Royal Institute of Technology, Department of Fibre and Polymer Technology, Teknikringen 56-58, SE-10044 Stockholm

Nanostructured noble metal films on polymer layers are of fundamental importance in the field of organic electronics. Moreover, such material combinations have gained importance for stabilizing thin polymer films. We combine sputter deposition with grazing incidence X-ray scattering (GIXS) to investigate in situ [1,2] the growth kinetics of Gold (Au) on polystyrene (PS). We therefore analyze quantitatively the Au nanoparticle layer growth such films and correlate the change in optical properties of the Au/PS system with the thickness of the gold-capped PS layer. Optical measurement methods such as UV-Vis spectroscopy or imaging ellipsometry were employed.

[1] Schwartzkopf, Roth, *Nanomaterials* 6, 239 (2016).

[2] Schwartzkopf et al., *ACS Appl. Mater. Interfaces* 7, 13547 (2015).

CPP 33.39 Tue 14:00 Poster C

**Tailoring thermal properties of biodegradable polyester based nanoparticles for drug delivery** — ●CHRISTIAN HELBIG<sup>1</sup>, DAMIANO BANDELLI<sup>2,3</sup>, CHRISTINE WEBER<sup>2,3</sup>, ULRICH S. SCHUBERT<sup>2,3</sup>, and KLAUS D. JANDT<sup>1,3</sup> — <sup>1</sup>Chair of Materials Science, Otto-Schott-Institute of Materials Research, Friedrich Schiller University Jena, Germany — <sup>2</sup>Laboratory of Organic and Macromolecular Chemistry (IOMC), Friedrich Schiller University Jena, Germany — <sup>3</sup>Jena Center for Soft Matter (JCSM), Friedrich Schiller University Jena, Germany

According to literature reports, the thermal properties of biodegradable polyesters influence their degradation and hence the release kinetics of actives from corresponding nanoparticles (NP). However, factors such as the hydrophilic / hydrophobic balance (HHB) and the drug loading impact release kinetics as well. We therefore tailor-made polyester based NPs with different thermal properties but constant HHB and size, as confirmed by means of dynamic light scattering and scanning electron microscopy. The NP are composed of a) poly( $\epsilon$ -caprolactone), b) block and c) gradient copolymers of  $\delta$ -valerolactone and  $\delta$ -decalactone. Differential scanning calorimetry measurements revealed semicrystalline materials with a significantly lowered melting temperature and degree of crystallinity of P(VL-grad-DL). Atomic force microscopy revealed that the NP stiffness correlates with the degree of crystallinity of the used polymer. This work is part of the Collaborative Research Center 1278 "Polytarget: Polymer-based nanoparticle libraries for targeted anti-inflammatory strategies" which is funded by the DFG.

CPP 33.40 Tue 14:00 Poster C

**Directed self-assembly supported by laser interference lithography of plasmonic particles for high optical quality application.** — ●VAIBHAV GUPTA<sup>1</sup>, PATRICK T. PROBST<sup>1</sup>, ANDREAS

FERY<sup>1,2</sup>, and TOBIAS A. F. KÖNIG<sup>1,2</sup> — <sup>1</sup>Leibniz-Institut für Polymerforschung, e.V., Hohe Str. 6, 01069 Dresden, Germany — <sup>2</sup>Cluster of Excellence Centre for Advancing Electronics Dresden, Mommsen Str. 4, D-01062 Dresden, Germany

Selective arrangement of nanoparticles with predetermined nanometer-scale accuracy is crucial to exploit the collective properties of the resulting assemblies, in particular for photonic and electro-optical nano devices. Here, we fabricate topographically patterned templates comprised of laser interference lithography and soft molding to achieve control over position and interparticle distance of the plasmonic building block. We are able to produce 2D square lattice of gold nanoparticles on a centimeter-scale substrate with cost-effective and up-scalable method. Finally, we prove our results using finite-difference time domain simulation and discuss the tunability of the generated surface lattice resonance (SLR), which is correlated to fill factor 0.8.

CPP 33.41 Tue 14:00 Poster C

**Effect of C60 on the Morphology of Strongly Segregated ABC Miktoarm Terpolymers** — ●MATTHIAS M.L. ARRAS<sup>1</sup>, HYEYOUNG KIM<sup>2</sup>, MONOJOY GOSWAMI<sup>1</sup>, HONG KUNLUN<sup>1</sup>, BOBBY G. SUMPTER<sup>1</sup>, THOMAS P. RUSSELL<sup>2,3</sup>, and GREGORY S. SMITH<sup>1</sup> — <sup>1</sup>Oak Ridge National Lab, Oak Ridge, USA — <sup>2</sup>University of Massachusetts Amherst, USA — <sup>3</sup>Lawrence Berkeley National Lab, Berkeley, USA

We investigated the effect of C60 nanoparticles on a series of poly(styrene), poly(isoprene), poly(2-vinylpyridine) (PS-PI-P2VP) miktoarms by small angle scattering. To this end, we synthesized PS-PI-P2VP with symmetric PS and PI blocks and varied the degree of polymerization for P2VP. We denote the ratio between the volume fraction of P2VP and PS (or PI) as  $\alpha$ . C60 addition leads to a reduction in the repeat period due, more than likely, to chain relaxation of the arms of the miktoarm terpolymer, in the hierarchical lamellar microdomain morphology (HLM) which forms for  $\alpha > 2$ . In contrast, in a sample with a tessellated morphology (TM) at short P2VP chains ( $\alpha < 1$ ), we find the opposite behavior, and the repeat period expands dramatically. We explain these distinct differences with the stability of the HLM (observed for  $2 > \alpha > 4$ ) which is robust and insensitive to configurational changes. In contrast, at all-symmetric conditions  $\alpha = 1$  and below  $\alpha < 1$  many TMs in close proximity are reported which means the morphology is susceptible to changes.

This research used resources at the Spallation Neutron Source, a DOE Office of Science User Facility operated by ORNL. HK & TR were supported by AFOSR (16RT1602) and ARO (W911NF-17-1-0003).

CPP 33.42 Tue 14:00 Poster C

**Miktoarm Star Terpolymer PS-PI-P2VP Investigated by Small Angle Neutron Scattering** — ●MATTHIAS M.L. ARRAS<sup>1</sup>, HYEYOUNG KIM<sup>2</sup>, JYOTI P. MAHALIK<sup>1</sup>, WEIYU WANG<sup>1</sup>, HONG KUNLUN<sup>1</sup>, BOBBY G. SUMPTER<sup>1</sup>, THOMAS P. RUSSELL<sup>2,3</sup>, and GREGORY S. SMITH<sup>1</sup> — <sup>1</sup>Oak Ridge National Lab, Oak Ridge, USA — <sup>2</sup>University of Massachusetts Amherst, USA — <sup>3</sup>Lawrence Berkeley National Lab, Berkeley, USA

We are reporting on the structure of a strongly segregated asymmetric ABC miktoarm terpolymer, PS-*arm*-PI-*arm*-P2VP (SIV), which as determined by small angle neutron or X-ray scattering and transmission electron microscopy. We synthesized fully protonated and partially deuterated SIV miktoarm stars of similar composition where the majority component P2VP is approximately four times the molar mass of the PI or PS block. The results were compared to self-consistent field theory calculations which predicted two possible energy-minimized structures. The most consistent of the two structures was an hierarchical lamellae structure, consisting of lamellae in lamellae. This talk will highlight, that with increasing complexity in polymer architecture, one characterization technique will not necessarily be sufficient for the determination of the structure. A brief discussion of the prospects for resonant soft X-ray scattering in these systems will also be given.

This research used resources at the Spallation Neutron Source, a DOE Office of Science User Facility operated by ORNL. HK & TR were supported by AFOSR (16RT1602) and ARO (W911NF-17-1-0003).