CPP 25: Poster Session II

Topics: Complex Fluids and Colloids, Micelles and Vesicles (25.1-25.10); Composites and Functional Polymer Hybrids (25.11-25.18); Emerging Topics in Chemical and Polymer Physics, New Instruments and Methods (25.19-25.20); Hydrogels and Microgels (25.21-25.26); Modeling and Simulation of Soft Matter (25.27-25.35); Nanostructures, Nanostructuring and Nanosized Soft Matter (25.36-25.44); Responsive and Adaptive Systems (25.45-25.49); Wetting, Fluidics and Liquids at Interfaces and Surfaces (25.50-25.58).

Time: Tuesday 14:00–16:00   Location: Poster B1

CPP 25.1 Tue 14:00 Poster B1
Thermodiffusion of Binary Halobenzene-n-Alkane Mixtures — •Bastian Pur, Florian Schock, and Werner Köhler — Universität Bayreuth, 95440 Bayreuth, Germany

The Soret effect (thermophoresis) describes a diffusion flux that is driven by a temperature gradient in a multicomponent mixture. For dilute solutions of polymers with large Kuhn segments there is a remarkable universality for the thermophoretic velocity: it depends only on the viscosity η of the solvent. The thermal diffusion coefficient D_T, also known as the thermophoretic mobility, multiplied by the solvent viscosity leads to a constant value ($\eta D_T \approx$ const.). This universality is asymptotically also found for binary mixtures of methylnaphtalene and toluene in n-alkanes. To pursue these observations we have conducted measurements with halobenzene-n-alkane mixtures. The measured mixtures correspond to the series of halobenzenes fluoro-, chloro- and bromobenze mixed with n-alkanes nC_i (i=6,7,8,10,12,14 and 16). By means of a holographic grating technique we have obtained the Fickian diffusion coefficient D, the Soret coefficient S_T and the thermal diffusion coefficient D_T. These results will be compared to the universal asymptotic limit of ηD_T reported for polymer solutions.

CPP 25.2 Tue 14:00 Poster B1
Measurement of transport processes in multicomponent liquids by multi-color techniques — •Marcel Schraml, Pascal Möckel, Felix Sommer, and Werner Köhler — Department of Physics, University of Bayreuth, 95447 Bayreuth

Diffusive flows in a non-isothermal multicomponent fluid are characterized by complex cross-coupling phenomena between all concentration and temperature gradients. Since the number of unknown coefficients increases quadratically with the number of components, such multicomponent systems quickly become intractable, and today's research focuses mainly on ternary mixtures as multicomponent model systems.

Within the ESA/Roscosmos DCMIX program, measurements are performed both under microgravity conditions aboard the International Space Station ISS and in various laboratories on ground. In order to resolve all components, optical multicolor beam deflection and interferometry experiments are typically employed. The most critical step in the data analysis is the transformation from the multicolor refractive index space to the compositions, for which the so-called contrast factor matrix must be inverted. Since this matrix is frequently ill-conditioned, extremely precise measurements of the partial derivatives of the refractive index with respect to the composition variables and the temperature are required.

In our poster we will present the optical multi-color techniques employed both on ground and in space and discuss consistent multicolor measurements of the optical contrast factors.

CPP 25.3 Tue 14:00 Poster B1
Camphor/Succinonitrile – a model system for metal alloys subjectedto a temperature gradient — •Felix Sommer[1], Marcel Schraml[1], Bastian Pur[1], Werner Köhler[1], Gerhard Zimmermann[2], and Laszlo Sturz[2] — [1]Physikalisches Institut, Universität Bayreuth — [2]Access e.V. Aachen

Hypoeutectic Succinonitrile/Camphor alloys serve as model systems for the solidification of binary metal alloys. The development of the solidification patterns strongly depend on the solute transport at the solid-liquid interface, which is often assumed to be diffusional, even in a thermal gradient. Under such nonequilibrium conditions in a thermal gradient, diffusive flows are characterized by complex cross-coupling phenomena between concentration and temperature gradients. As a consequence, the local composition can significantly shift away from its initial concentration, resulting in unexpected solidification patterns. In order to better understand these mechanisms, we have studied diffusion and thermodiffusion of camphor/succinonitrile binary mixtures around the eutectic composition in the liquid phase. We have been able to determine diffusion, thermodiffusion and Soret coefficients by means of optical beam deflection and photon correlation spectroscopy. For the evaluation of the experiments, precise measurements of the optical contrast factors were performed. Our results prove a significant cross coupling between temperature and composition.

CPP 25.4 Tue 14:00 Poster B1
The Soret effect in ternary mixtures of water + ethanol + triethylene glycol of equal mass fractions: ground and microgravity experiments — •Daniel Sommermann[1], Thomas Triller[1], Marcel Schraml[1], Felix Sommer[1], Werner Köhler[1], Estela Lapeira[2], and Mounir M. Bou-Ali[2] — [1]Physikalisches Institut, Universität Bayreuth, Germany — [2]Mechanical and Manufacturing Department, MGEP Mondragon, Spain

Measurements of the Soret and thermodiffusion coefficients of a symmetric ternary mixture with equal mass fractions of water, ethanol, and tri-ethylene glycol have been performed by two-color optical beam deflection and the thermogravitational column technique in the laboratory and under microgravity conditions in the SODI apparatus aboard the ISS. The results from all three experimental techniques agree within the experimental error bars. The agreement with the microgravity results shows that thermosolutal convection could be well controlled in the 2-OBD experiments by a proper orientation of the temperature gradient. Based on the orientation of the confidence ellipsoid, not all coefficients are equally affected by experimental errors. Although there are appreciable uncertainties for water and ethanol, the Soret and the thermodiffusion coefficients of tri-ethylene glycol could be obtained with a good accuracy. We have found that water behaves thermophobic, whereas both ethanol and tri-ethylene glycol are thermophilic with negative Soret coefficients.[1]

[1] T.Triller et al., Eur. Phys. J. E, submitted 2018

CPP 25.5 Tue 14:00 Poster B1
1D capillary collapse and the role of initial fluctuations in Brownian Dynamics and DDFT — •Anja Schreiber, Johannes Bleibel, and Martin Oettel — Institut für angewandte Physik, Universität Tübingen, Tübingen, Germany

We investigate the so–called capillary collapse of colloidal particles trapped a fluid interface in 1D Brownian Dynamics (BD) simulations. Interfacially trapped, micrometer–sized colloidal particles interact via long–ranged capillary attraction. The interaction is formally analogous to screened Newtonian gravity with the capillary length λ as the tuneable screening length. Within intensive studies of the dynamics in 2D[1], it turned out that radially averaged Dynamical Density Functional Theory (DDFT) only captures the dynamics at initial times and largely deviates from simulation results later on. This discrepancy has been traced to the role of an initially averaged configuration in DDFT[2]. In BD, simulation runs are averaged over initial conditions and noise. The long–ranged potential and initial density fluctuations allow for an early clustering of particles prior to a global, collective collapse similar to a self gravitating fluid. This clustering remains present through most stages of the evolution and renders averaged density profiles, which deviate largely from DDFT. Since the clustering process is much more restricted in 1D, we use 1D simulations in order to shed light on the precise role of initial fluctuations in the averaging process and subsequent dynamics both in BD simulations and DDFT.

[1] Bleibel, Domínguez, Oettel, Dietrich, Soft Matter 10, 4091 (2014).

[2] Bleibel, Domínguez, Oettel, JPCM 28, 244021 (2016).

CPP 25.6 Tue 14:00 Poster B1
Role of pH in Micro-Swimming — •Nadir Möller and Thomas Palberg — Institut für Physik, Johannes Gutenberg-Universtät

Mainz, Staudingerweg 7, 55128 Mainz, Germany

Modular micro-swimmers are self-assembled systems of colloids that are able to directionally traverse in a low Reynolds number environment after assemlby. In our modular micro-swimmer, a settled ion exchange (IEX) sphere exchanges residual Na+ ions for H+ and thus generates a pH-gradient. This gradient in turn induces a diffusion-electric field which drives an electro-osmotic solvent flow along the substrate. The flow assembles dispersed cargo spheres, which, once assembled break the flow symmetry and set the formed complex in motion. While a comprehensive characterisation of swimmer trajectories, speeds and stability as a function of experimental boundary conditions has been performed, and a theoretical model has been developed, the key input of modelling, i.e. the pH gradients, are available only in approximations. To gain insight of the influence the pH has on the particles motions, we utilize a home-built setup for pH-micro-photometry. This method can be employed in a variety of other systems for characterization of microfluidic and chemical attributes of electro-osmotic-driven particles.

CPP 25.7   Tue 14:00   Poster B1
Competing nucleation and fractionation in hard sphere crystals — •Nicole Schaertl[1], Jennifer Wenzl[1], Thomas Palberg[1], and Eckhard Bartsch[2] — [1]Institute of Physics, Johannes Gutenberg University, Mainz, Germany — [2]Institute of Physical Chemistry, Albert Ludwigs University, Freiburg, Germany

Fluid to crystal first order phase transition of monodisperse hard spheres (HS) upon increasing volume fraction was predicted in the 1950s and later confirmed experimentally on sterically stabilized HS approximants [1]. In particle synthesis, size polydispersity is unavoidable. According to theory, a polydisperse fluid should yield coexisting solid phases upon compression [2]. Despite the general anticipation towards fractionation in HS systems, no direct observation has been reported so far. We decided to focus on PS microgel particles with 6% polydispersity in a good solvent. Sufficiently steep steric repulsion for HS-like behavior is obtained at high degree of crosslinking. Recent studies have shown that this colloidal system is less prone to jamming effects than other common HS approximants [3]. This makes this systems particularly interesting for crystallization studies. Time resolved static light scattering revealed several series of well indexable Bragg reflexes shortly after shear melting and re-solidification. This demonstrates the existence of crystals with same fcc structure but different lattice constants. During ripening stage the number of identifiable fractions slowly reduces from half a dozen to three. [1] Pusey, van Megen, Nature 320, 340 (1986) [2] Fasolo, Sollich, Phys. Rev. Lett. 91, 068301 (2003) [3] Schaertl et al., Soft Matter, 14, 5130 (2018)

CPP 25.8   Tue 14:00   Poster B1
Dynamic susceptibility of a cluster interacting superparamagnetic particles in an oscillating magnetic field — •Vladimir Zverev and Alexandr Ambarov — Ural Federal University, Ekaterinburg, Russia

At the present moment several methods for reconstructing the spatial distribution of magnetic particles are being developed. Most of them are based on measurements of the dynamic susceptibility and an ensemble of magnetic nanoparticles is used as a sensitive element. Multicore magnetic nanoparticles allow an increase the temporal resolution and improves the signal-to-noise ratio. In this work we investigate dynamic response of a single cluster of an ensemble of interacting ferroparticles that are formed multicore magnetic particle. It is assumed that the relaxation of the magnetic moments occurs due to Neel mechanism. Dynamic response of a cluster of single-domain particles in a viscous carrier are determined from the solution of the Fokker-Planck equation. The modified mean-field approach of first-order is used to take into account the dipole-dipole interaction. The time dependence of the magnetization is calculated to determine effective magnetic moment and relaxation time.

CPP 25.9   Tue 14:00   Poster B1
Colloidal particle sizing using various techniques — •Kathrin Eitel and Hans-Joachim Schöpe — Institut für Angewandte Physik, Tübingen

Nanoscience and nanotechnology are playing key roles in different scientific disciplines and its importance increased significantly over the last years. Particle size analysis is of essential importance in research and development as well as in industrial production. Different techniques are used for particle sizing, all given optimal results in a certain particle size range. In dispersions of nano- to micrometer-sized particles, DLS is commonly used. DDM might be a more exact alternative method for particle sizing. In this work, we compared DDM with the established methods such as DLS and SLS working out their advantages and disadvantages.

Keywords: colloids, SLS, DLS, and DDM.

CPP 25.10   Tue 14:00   Poster B1
Pressure-induced phase transition 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 thermal energy storage or medical chemistry. Silica nanoparticles in aqueous solution show a repulsive Coulomb interaction. By adding non-adsorbing polymers (e.g. polyethylene glycol), the total particle-particle interaction can become more attractive. With increasing polymer concentration, the system undergoes a phase transition from the homogenous phase into a liquid-liquid phase separated phase (LLPS). If the system is exposed to high pressure the system switches back into the homogenous phase. In this work, light transmission and small-angle X-ray scattering measurements on systems, containing 1 wt.% silica nanoparticles and various molecular weight and concentration of PEG, were performed to understand of the phase transition on a microscopic level. By combining these techniques, we were able to determine a pressure-dependent phase diagram, and obtained information about typical distances between the nanoparticles in the LLPS phase. The measurements showed that the transition pressure strongly depends on concentration and the size ratio between the polymers and the nanoparticles.

CPP 25.11   Tue 14:00   Poster B1
Polymers for lithium ion batteries - investigating composite electrodes — •Cristian Telescu, Simon J. Schaper, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany.

With the development of new technologies the demand for reliable, cheap and long life batteries with high specific energy and high efficiency is constantly increasing. Therefore, a significant effort is devoted to the improvement of battery performance. The lithium-ion polymer battery is a prospective candidate for powering the new generation of electrical devices and vehicles due to outstanding advantages as low weight, high negative potential and high specific capacity. These features are of critical significance for the automotive and electronics industries. Improving materials, composition, and interfaces is still necessary to exploit the possibilities of polymer based lithium-ion batteries. In this work, a study of polymer composite cathodes with lithium iron phosphate (LFP) and lithium nickel cadmium aluminum oxide (NCA) as active materials is presented and the key performance results are provided.

CPP 25.12   Tue 14:00   Poster B1
Influencing the properties of fullerene-free bulk heterojunction blends for photovoltaic applications — •Amir Kotobi[1], Sebastian Grott[1], Claudia Ott[2], Tom Nilges[2], and Peter Müller-Buschbaum[1] — [1]1TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching — [2]2 TU München, Department Chemie, LS innovative Materialien, Lichtenbergstraße 4, 85748 Garching

Over the past decades, organic electronics have attracted increased focus in the field of research. Especially organic solar cells received a high attention, due to their advantages, such as the tuneability of photo-active properties, the possibility to be produced at low-cost, the flexibility and the light-weight, compared to commonly-used inorganic based solar cells. Recently, the most widely investigated bulk heterojunction donor-acceptor system of P3HT:PCBM was doped with iron oxide nanoparticles, resulting in an increase of efficiency. Based on this approach, we investigate the effect of doping photoactive layers consisting of the low-bandgap polymer PBDB-T and the non-fullerene acceptor ITIC with SnIP nanoparticles We study the influence of different nanoparticle concentrations on current-density voltage characteristics and the absorbance. These optoelectronic properties are related to structure information obtained via advanced scattering techniques in order to optimize the device performance.

CPP 25.13   Tue 14:00   Poster B1
Synthesis of Well-Controlled Titania Hollow Spheres —

•Anna Lechner and Markus Retsch — University of Bayreuth, Bayreuth, Germany

Over the past few decades, the interest in titania based materials increased enormously because of its strong oxidative potential and photocatalytic activity.

The controlled synthesis of monodisperse and well-defined titania particles on the mesoscale still poses a challenge. In particular core-shell architectures and hollow spheres are interesting titania morphologies owing to their hierarchical architecture controlled by a large diameter and thin shell. In contrast to the synthesis of silica hollow spheres, the synthesis of titania hollow spheres is more challenging because of the highly reactive precursors.

This contribution presents the three steps of a controlled and scalable synthesis of titania hollow spheres of various sizes. First, the synthesis of polystyrene particles via dispersion polymerization is explained. Here, several parameters for the adjustment of the particle size are discussed. Furthermore, the synthesis of smooth titania shells of defined thicknesses is presented following a simple precursor condensation strategy. Finally, the template core removal can compromise the integrity of the titania shell. We assess strategies to retain the structural control to yield monodisperse titania hollow spheres.

We will also provide an outlook of the exciting properties of such hierarchically structured porous titania materials with respect to their optical and thermal transport properties.

CPP 25.14   Tue 14:00   Poster B1

Thermo-mechanical behavior of silver-filled thermoplastic polymers — •Amira Baccari and Peter Müller-Buschbaum — TU München, Physik Department, LS Funktionelle Materialien, 85748 Garching, Germany

Filled thermosetting and thermoplastic polymers are used for silver-filled, electrically conductive adhesives in the printed circuit board industry. These are a type of glue containing usually 80% of a conductive material and 20% of a polymer matrix that has the necessary mechanical and thermal properties. The produced electronic devices need to pass several thermo-mechanical tests using dynamic mechanical analysis and thermal mechanical analysis (DMA and TMA) techniques in order to get a good expectancy of the lifetime performance and behavior of the products. Companies concerned with the manufacturing of electronics want to use experiments and simulation for assessing a new adhesive based on a thermoplastic polymer matrix (instead of the usual epoxy-based composite adhesive). Thermo-mechanical material models of polymers are essential for obtaining meaningful results from thermo-mechanical simulation. The electronics packaging community has an acceptable understanding of the thermo-mechanical behavior of thermosetting epoxy polymers, but not yet of silver-filled thermoplastic polymer matrices, which will be focused in this work.

CPP 25.15   Tue 14:00   Poster B1

Polybutadiene in Alumina nanopores — •Lama Tannoury — Institute of Physics, Martin Luther University, Halle (Saale), Germany

Several studies concerning 1,4-polyutadiene (PBD) confined between graphite walls have been performed perviously. They have shown that the polymer melts experience, at close distances to the confining walls, a variation in both monomer and chain density. Furthermore, that layer also experiences a change in dynamics incorporated in the slowing down of and an extra process of relaxation. These studies are essential to the comprehension of composite materials made of polymer matrices and inorganic filler particles such as rubber tires. The latter is a composite material filled with nanoparticles. However, since previous research on PBD melts permeated by nano-sized fillers could not reach relaxation time scales accessible by Molecular Dynamics (MD) simulations, we attempt to study a chemically realistic model of a PBD melt inside alumina and silica pores using the GROMACS package. We aim to enhance our view concerning bulk relaxation processes and any modifications they experience due to confinement.

CPP 25.16   Tue 14:00   Poster B1

Magnetic Nanoparticle / Polymer Brush Composites: The Effect of pH and Concentration on Particle Adsorption — •Philipp Ritzert, Dikran Boyaciyan, and Regine v Klitzing — Soft Matter at Interfaces, Institut für Festkörperphysik, TU Darmstadt

Polymer chains, which are end-grafted chemically to a substrate are referred as polymer brushes and have attracted a growing interest in the field of surface coating over the last few decades due to their high mechanical and chemical stability. Based on the functional group of the monomer unit, it may exhibit sensitivity to external stimuli, such as temperature, pH or solvent (1). Polymer brushes can bind different kinds of material with a high selectivity, depending on the available functional groups. Recent studies demonstrated the incorporation of nanoparticles into different kinds of polymer brushes (1; 2; 3). In the case of gold nanoparticles (AuNPs), the uptake induced novel optical properties, due to the Surface Plasmon Resonance of the AuNPs (3).

The present work demonstrated the successful immobilization of magnetic nanoparticles (MNPs) on Poly(N-isopropylacrylamide) (PNIPAM) brushes. The pH-sensitive citrate capping of the MNPs stabilizes the MNPs in the neutral to basic pH regime and simultaneously binds to the PNIPAM brush via H-bonding. The goal of this work is to characterize the adsorption of MNP on PNIPAM brushes by changing the pH value and concentration of the MNP suspension.

1. S. Christau, et al. Macromolecules. 2017, 50, pp. 7333-7343.
2. D. Boyaciyan, et al. SoftMatter. 2018, 14, pp. 4029-4039.
3. S. Christau, et al. Polymers. 2014, 6, pp. 1877-1896.

CPP 25.17   Tue 14:00   Poster B1

Thermoelectric Characterization of Polymer Composite Thin Films — •Marie Siegert[1], Alexander Steeger[2], and Jens Pflaum[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Bavarian Center for Applied Energy Research (ZAE Bayern), 97074 Würzburg

In recent years, organic thin films have become of interest for thermoelectric applications as a low-cost, sustainable alternative to inorganic semiconductors. To achieve a high thermoelectric figure of merit $zT = \sigma S^2 T / \kappa$, which is a measure for the efficiency of converting waste heat into electricity, the thermal conductivity κ of the thin film needs to be minimized, while maximizing its electrical conductivity σ. Polymer thin films, which can be prepared by solution processing at large scales, exhibit sufficiently low thermal conductivities, but lack high electrical conductivity as a result of their inherent disorder. In contrast, crystalline organic metals, requesting high efforts on their preparation, show superior charge carrier transport characterized by a metallic conductivity behavior over a wide temperature range [1]. Here we report on the combination of the two material approaches by preparing composite thin films of the well studied polymer PEDOT:PSS blended with crystallites of the low-dimensional molecular metal TTT_2I_3. First results on the electrical and thermal properties of these polymer-molecular metal composites will be presented and evaluated with respect to their application potential in thin film based thermoelectric generators.

[1] F. Huewe, A. Steeger, et al., Adv. Mat. 29 (2017) 1605682

CPP 25.18   Tue 14:00   Poster B1

Characterization of interfaces in coextruded polypropylene-based multilayer structures via confocal Raman spectroscopy — •Claudia Leimhofer[1], Sabine Hild[1], and Elias Mayrhofer[2] — [1]Institute of Polymer Science, Johannes Kepler University, Linz, Austria — [2]Institute of Polymer Extrusion and Compounding, Johannes Kepler University, Linz, Austria

Co-extrusion of polymers is a powerful tool to produce multilayer composites that combine properties which cannot be achieved by pure substances alone. The strength of the total composite is determined by the adhesion between the adjacent layers. The polyolefines used in industrial applications often are non-polar and show low surface free energy which impairs the overall adhesion. Different adhesion mechanisms for polymers were proposed in the literature. One widely accepted model is based on interdiffusion of the materials and the formation of an interface layer. The aim of the study is to characterize the interdiffusion layers of a co-extruded polypropylene-based composite by confocal Raman spectroscopy. With Raman spectroscopy, the chemical composition of the substances in the bulk layers as well as at the interface can be determined. In the characterized seven-layered systems, a polyethylene- and vinyl alcohol-based barrier layer is combined with a maleic acid grafted polypropylene adhesive, pure polypropylene and a regrind material. The different layers can be clearly differentiated, and the presence of interface layers with spectral properties deviating from the pure substances can be observed.

CPP 25.19   Tue 14:00   Poster B1

Protein dynamics of a thermophile photosystem — •Dominik Schwaiger[1], Maksym Golub[2], Ina Seuffert[3], Athina Zouni[3], Wiebke Lohstroh[4], Peter Müller-Buschbaum[1], and Jörg Pieper[2] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]Institute of Physics, University of Tartu,

Tartu, Estonia — [3]Institute of Biology, Humboldt-Universität zu Berlin, Berlin, Germany — [4]Heinz Maier-Leibnitz Zentrum (MLZ), TU München, Garching, Germany

Photosynthesis is the key mechanism in utilization of solar radiation for living organisms and thus provides the base for most food chains and all fossil fuels. The functionality of photosynthetic proteins is - in part- critically influenced by dynamics on a timescale of pico- to milliseconds and on sub-nanometer length scale. The neutron time of flight spectrometer TOFTOF at MLZ-Garching is well suited to study such dynamics, and we currently develop a laser pump setup for TOFTOF allowing us to trigger photoreactions and subsequently probe the dynamics of specific functional states with neutrons. In a first step towards time-resolved measurements, static quasielastic neutron scattering (QENS) experiments were performed on photosystem II (PSII) complexes of the thermophile bacterium thermococcus elongatus, whose protein dynamics is expected to play a pivotal role in thermal adaptation. Using QENS, we have directly investigated PS II protein dynamics on the picosecond timescale in a range from 200 K to 340 K. The results suggest a shift of the onset of protein dynamics towards higher temperatures in thermophile PSII.

CPP 25.20   Tue 14:00   Poster B1

NMR investigations of microfluidics using stripline geometry — •Raoul Nitzsche, Benjamin Kresse, Alexei F. Privalov, and Michael Vogel — TU Darmstadt, Institut für Festkörperphysik, Hochschulstr. 6, 64289, Darmstadt, Germany

NMR spectroscopy with microfluidic devices puts high requirements on the probeheads sensitivity. Due to small sample volumes in the μl range, common high frequency (HF) coils of typically 5 to 10 mm cannot be completely filled. A solution to this problem is the stripline, a component commonly used in HF-technique. A flat wire instead of a coil produces the RF pulse in the NMR experiment and detects the signal. This design allows a high filling factor and a homogeneous RF field for signal enhancement and, thus, also a high time resolution. It enables a lab-on-a-chip implementation which is a simple and effective design to examine small amounts of liquids. The stripline is successfully implemented in NMR spectroscopy using microchannels by the Kentgens group [1]. Our test experiments revealed an increased signal-to-noise ratio and a good spectral resolution, as required to distinguish different molecular species with sufficient time resolution. Our goal is to follow the mixing process of two liquids by recording images in a static field gradient spectrometer. For this purpose, we implemented a Y-shaped microfluidic device in a stripline to control the mixing. This design enables the possibility to monitor chemical reactions in a standard cryomagnet.

[1] P.J.M. van Bentum et al., J. Mag. Res., 189 (2007) 104-113

CPP 25.21   Tue 14:00   Poster B1

Mussel-inspired hydrogels with adhesive potential and mechanical robustness — •Sandra Forg and Regine von Klitzing — Technische Universität Darmstadt, Alarich-Weiss-Straße 10, D-64287 Darmstadt

Polymer hydrogels offer unique properties. Especially their responsiveness to external stimuli including pH and temperature provides a huge potential for various technological applications. Combining this stimuli-responsiveness with adhesive attributes would be of use for tissue engineering or medical purposes. Therefore, hydrogels inspired by marine organisms such as mussels have recently become highly attractive. Mussels can strongly adhere to other substrates even in wet conditions, which is mainly determined by the protein 3,4-dihydroxyphenyl-L-alanine (DOPA). This DOPA-group can easily be incorporated into the hydrogel structure. However, most of these hydrogels are mechanically weak and / or possess a low elastic modulus, which remarkably limits their use in in vivo environments.

In this work, temperature-responsive poly(N-isopropylacrylamide) (PNIPAM) microgels are synthesized. They are modified with DOPA to obtain adhesive properties. Their charge is varied by copolymerisation with the anionic monomer acrylic acid (AA). Moreover, their size and cross-linker content can be tuned. Their properties are studied by DLS and Zetasizer measurements. Afterwards, thin films of these DOPA-modified microgels are produced by spin-coating. They are analysed by static and dynamic indentation measurements to get an insight into the mechanical and rheological properties of thin films.

CPP 25.22   Tue 14:00   Poster B1

Investigation of Non-Equilibrium Actuation Dynamics of Microgel Disks — •Niklas O. Junker[1], Jonas Staudenmeir[1], Mar-

cel van Dongen[2], Sebastian Meyer[1], Dmitry N. Chigrin[1,2], Ahmed Mourran[2], Martin Möller[2], and Gero von Plessen[1] — [1]Institute of Physics (IA), RWTH Aachen, Germany — [2]DWI - Leibniz Institute for Interactive Materials, Aachen, Germany

Microgels are cross-linked polymer networks of micrometer or submicrometer dimensions. Suspended in a solvent, they can undergo large and fast volume changes in response to variations of external parameters (temperature, pH, etc.). In the present work, microgel disks made of poly(N-isopropylacrylamide) (PNIPAm) homogeneously loaded with gold nanorods have been investigated in water. Nonequilibrium actuation dynamics triggered by rapid heating and cooling is studied. The microgels are found to swell with decreasing temperature much faster than they shrink with increasing temperature. This behavior is systematically studied for different heating rates (up to $150°C$/min for conventional heating and up to approximately $1°C$/ms for photothermal heating, in which the gold nanorods are used as fast and efficient photoabsorbers and local heaters). Experimental and simulation results are compared for both cases.

CPP 25.23   Tue 14:00   Poster B1

Co-nonsolvency induced self-organization of thermo-responsive block copolymers in thin films — •Christina Geiger[1], Cristiane Henschel[2], André Laschewsky[2], Christine M. Papadakis[3], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]Universität Potsdam, Institut für Chemie, Angewandte Polymerchemie, 14476 Potsdam — [3]TU München, Physik-Department, Physik weicher Materie, 85748 Garching

PMMA-b-PNIPAM and PMMA-b-PNIPMAM in aqueous solution undergo a reversible shell collapse transition at the lower critical solution temperature (LCST), which can be moderated by gradually introducing organic solvents. In thin film configuration, this co-nonsolvency behavior makes them promising materials for vapor-sensitive nanosensors and actuators. We prepare and examine thin films exhibiting various block ratios and subsequently perform swelling experiments in mixed vapor atmospheres. Morphological changes, as well as the kinetics of individual solvent and cosolvent diffusion into the films, concentration gradients and the development of thickness and refractive index are investigated with a focus on white light interferometry and *in-situ* TOF neutron reflectometry experiments.

CPP 25.24   Tue 14:00   Poster B1

Metallo-polymers and -gels based on photosensitive ruthenium(II) complexes and polyethylene glycol — •Leonhard Buchriegler[1], Sabrina Theis[2], Ian Teasdale[3], Sabine Hild[1], and Uwe Monkowius[4] — [1]Institute of Polymer Science, Johannes Kepler University Linz, Austria — [2]Institute of Inorganic Chemistry, Johannes Kepler University Linz, Austria — [3]Institute of Polymer Chemistry, Johannes Kepler University Linz, Austria — [4]Linz School of Education, Johannes Kepler University Linz, Austria

The interest in photo-cleavable polymers has increased significantly due to their broad range of potential applications. The complex $[Ru(II)(bpy)_2(4-AMP)_2]^{2+}$ (bpy = 2,2'-bipyridine, 4-AMP = 4-(aminomethyl)pyridine) can be used to generate light-sensitive polyurea supramolecular organogels. This complex has a high photocleavage quantum yield and high storage stability in solution in the dark as well as in neat form. In this contribution, we present a light-sensitive organogel which is composed of the Ru-complex and an 8-arm polyethylene glycol (PEG). The gel is prepared via reaction between amine functions of the Ru-complex and the terminal modified polyethylene glycol forming a crosslinked polyurethane with both 4-(aminomethyl)pyridine ligands connecting two PEG-arms. Irreversible de-gelation occurs within minutes upon irradiation with visible light ($\lambda > 395$ nm), i.e. the Ru-bound pyridine is replaced by a solvent molecule, here acetonitrile. The synthesis and photocleavage-process were investigated by ^{1}H-NMR spectroscopy, mass spectrometry and UV/Vis-spectroscopy.

CPP 25.25   Tue 14:00   Poster B1

Microgel of different topologies: computational study of their properties — •Elena Minina[1,2], Pedro Sanchez[1,2], Christos Likos[1], and Sofia Kantorovich[1,2] — [1]University of Vienna, Vienna, Austria — [2]Ural Federal University, Ekaterinburg, Russia

Nano/microgels are colloidal spherical particles consisting of polymer network. These particles show a fascinating swelling response to external stimuli and therefore are very promising materials in food industry

and medicine including drug delivery applications. Due to advances in microgel synthesis, resulting polymer network of nano/microgels can be of different topologies: homogeneous and core-shell topologies. We developed computational coarse-grained models for studying nano/microgels of both topologies. The models are aimed at reproducing microgels synthesized inside a droplet. The main feature of these models is that the resulting polymer network has a random mesh size and its topology depends on the size of the confining sphere where the crosslinking process takes place. We study the structural and swelling properties of the modeled nano/microgels under different solvent conditions. We also include electrostatic interactions to reveal how their influence on the microgel properties.

CPP 25.26   Tue 14:00   Poster B1

Suspensions of magnetic microgels — •Ivan Novikau[1], Elena Minina[1,2], and Sofia Kantorovich[1,2] — [1]University of Vienna — [2]Ural Federal University

Microgels have gained a lot of attention due to their ability to swell and shrink as a response to their external environment [1]. The presence of magnetic particles inside the microgels offers an additional mechanism to control their properties by means of applied magnetic fields.

Study of a single microgel with magnetic particles showed that the magnetic susceptibility of these object strongly depends on the rigidity of the matrix and on the content of magnetic particles [2].

Here, is investigate a suspension of magnetic microgels by means of molecular dynamics computer simulations in order to elucidate possible microgel self-assembly scenarios. Each microgel is initially modeled as bead-spring polymer chains randomly cross-linked into a polymer network. Magnetic particles are randomly incorporated into this network.

Both dilute and relatively dense suspensions of microgels are considered with dipolar interactions in order to observe the self-assembly and figure out which factors are crucial for this process in the zero field case.

[1] A. Fernandez-Nieves, H. M. Wyss, J. Mattsson, and D. A. Weitz. Microgel Suspensions: Fundamentals and Applications. 2011.
[2] E.S. Minina, P.A. Sanchez, C.N. Likos and S.S. Kantorovich, JMMM 459, 226 (2018).

CPP 25.27   Tue 14:00   Poster B1

Computational study of multi-step catalysis in fibrous membranes — •Gabriel Sitaru and Stephan Gekle — University of Bayreuth, Germany

Multi-step catalytic reactions using incompatible catalysts in a one-pot are notoriously difficult to realize in technical settings. In this work, we investigate the potential of fibrous membranes as catalyst carriers by analysing the interplay of three different time scales: advection, diffusion and reaction.

The time-dependent concentration profiles throughout the reactor are computed using a Lattice-Boltzmann based solver for both the advection-diffusion and the Navier-Stokes equations. Using this model it is possible to study various parameters such as flow velocity or different geometries in order to maximize the reaction efficiency.

CPP 25.28   Tue 14:00   Poster B1

Prediction of polymeric nano-structures via machine learning — •Lucia Wesenberg and Ludwig Schneider — Institute for Theoretical Physics, University Göttingen, Germany

The significant length and times scales of the self-assembly of copolymers pose a challenge to particle-based polymer simulation. One possible speed-up strategy consists of using the chemical potential of a non-equilibrium morphology to predict the time evolution. The calculation of the chemical potential by particle-based simulation, however, can take up a vast amount of time, and here we explore the use of machine learning to predict the chemical potential. Machine learning has gained importance due to the introduction of deep neural networks. These enable an efficient implementation of non-linear relations.

Here, we employ this technique to calculate the chemical potential of copolymers in the lamellar phase. Data from different models enable us to tackle the particular interactions separately. First, with data from the Swift-Hohenberg model, we implement the short-range interactions in the neuronal network. Then, we amend the architecture of the network to cover long-range interactions. These are trained using data obtained from the Otha-Kawasaki model. Additionally, a network structure independent of the size of the input data is desirable.

CPP 25.29   Tue 14:00   Poster B1

Machine learning to predict three-body contributions in coarse-graining — •René Scheid, Christoph Scherer, Denis Andrienko, and Tristan Bereau — Max Planck Institute for Polymer Research, Mainz, Germany

Coarse-graining (CG) is a method to systematically reduce the degrees of freedom of a given system. Projecting the fine-grained system into a space with lower degrees of freedom leads to higher order interaction terms which are not considered in most CG models. We employ Kernel-based Machine learning (ML) to predict CG contributions based on decomposed CG energies and forces of atomistic simulations. The ML scheme is implemented in the VOTCA-CSG toolkit. First, we show that the ML scheme can recover two-body CG force fields generated by standard force-matching. This demonstrates that the approach is suitable to complement and expand standard force-matched models. Furthermore, we examine the expansion to three-body contributions. Decomposing the CG atomistic interactions into two- and three-body terms, the residual three-body potentials could be used to improve existing two-body models. The approach is illustrated on a Lennard-Jones liquid as test system, liquid water, and liquid methanol.

CPP 25.30   Tue 14:00   Poster B1

Application of data mining techniques in soft matter systems — •Arghya Dutta[1], Luca M. Ghiringhelli[2], Jilles Vreeken[3], and Tristan Bereau[1] — [1]Max Planck Institute for Polymer Research, 55128 Mainz, Germany — [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft, 14195 Berlin-Dahlem, Germany — [3]Max Planck Institute for Informatics and Saarland University, Saarland Informatics Campus, Saarbrucken, Germany

Data mining is the method for finding patterns in datasets using techniques borrowed from machine learning and statistics. It is particularly useful when the patterns we are looking for become too intricate to be amenable to a simple physical modelling. I will present results from our ongoing study which show how data mining, particularly text mining and subgroup discovery, can help us in finding patterns, and thus making predictions, in both experimental and computational studies of complex soft matter systems.

CPP 25.31   Tue 14:00   Poster B1

Phase Stability Simulation of Copper Chalcogenide Nanoparticles From First Principles — •Alkit Beqiraj, Ahed Abbousie, Andreas Taubert, and Thomnas Körzdörfer — Uni Potsdam, Am Neuen Palais 10, 14469 Potsdam

Being p-type semiconductors, CuS based nanoparticles demonstrate a large variety of potential applications in optoelectronic devices or energy technology. F.i. CuS nanoparticles can be used as an efficient hole collection layer in an organic solar cell. The CuSx nanoparticles can be synthesized at room temperature using an ionic liquid precursor. This synthesis, however, is very challenging, since even minor variation of the synthesis conditions can change the bias of the reaction, leading to the unexpected precipitation and phase transformation of different oxidative species of copper sulfides. Especially one polymorph of covellite (CuS), i.e., the semiconductor digenit (Cu1.8S), is of particular interest, as it is a frequently encountered byproduct of the synthesis. In order to understand the phase transformation, the chemical parameters, and the nature of the synthesis we carried out DFT calculations. To predict phase stability, vibrational contributions to the free energy were calculated within the harmonic supercell approach. From these calculations, we predict ab initio thermodynamic alloy phase diagrams. From these results, it is possible to analyze which parameters influence the phase evolution of digenit and covellite. Overall, our theoretical results are in a good agreement with the experimental observations and, thus, can be used to intentionally manipulate the experimental conditions in favor of the desired polymorph.

CPP 25.32   Tue 14:00   Poster B1

DFT calculations of K-edge X-ray adsorption spectra for organic molecules — •Rolf Würdemann[1], Julia Melke[1], Anna Fischer[1], and Michael Walter[2] — [1]Freiburger Materialforschungszentrum, Freiburg, Germany — [2]Freiburger Zentrum für interaktive Werkstoffe und bioinspirierte Technologien, Freiburg, Germany

X-ray adsorption spectroscopy (XAS) is an element specific local probe used for the analysis of materials. To compare and interpret these spectra ab initio calculations of XAS spectra can be performed for molecules in given geometries. This can be used to distinguish between different isomers and gain a deeper understanding of the bonding sit-

uation.

A common way to calculate XAS spectra by DFT is the utilization of a transition state potential (DFT-TP). In this approach an energetic offset correcting the approximate nature of the used functional has to be applied. To calculate this offset, one has to match the energetic value of the first calculated excitation to experiment. A similar problem in matching energy scales is also known from X-ray photolectron spectroscopy (XPS). Walter et al.[WMP16] have shown, that the offset needed in XPS is nearly constant in respect to the element under consideration and its value can be obtained empirically from experimental data.

In our contribution we extend the approach from Walter et al. to the calculation of XAS spectra and compare our results to experiment.
[WMP16] M. Walter et al., Phys. Rev. B 94 (4), 041112, 2016

CPP 25.33 Tue 14:00 Poster B1

Clarifying the role of 3-body correlations for determining optimal coarse-grained pair potentials — •Svenja Woerner, Kurt Kremer, Tristan Bereau, and Joseph F. Rudzinski — Max Planck Institute for Polymer Research, Mainz, Germany

Structure-based coarse-graining methods often determine optimal pair potentials for reproducing a given set of radial distribution functions. These procedures treat many-body correlations that arise in the condensed phase in various ways. Direct Boltzmann inversion, for example, assumes there are no correlations present in the system, resulting in potentials that tend to overcompensate for the missing correlations. Force matching, on the other hand, uses 3-body correlations from an underlying atomistic model to determine the optimal potentials. This can also result in inadequate potentials, since the coarse-grained model is often incapable of precisely reproducing the atomistic correlations. In this work, we apply the generalized-Yvon-Born-Green integral equation framework to explore the interplay between 2- and 3-body contributions to the pair mean force in coarse-grained models of liquids. As a model system, we consider a one-site per molecule representation for liquid water with isotropic pair interactions. Prominent tetrahedral packing generates 3-body correlations that cannot be reproduced by the coarse-grained model. Our analysis suggests an approach for directly modifying the atomistic 3-body correlations to more accurately reflect the correlations generated by the coarse-grained models.

CPP 25.34 Tue 14:00 Poster B1

Quantifying the reduction of chemical compound space due to coarse-graining — •Kiran Kanekal, Kurt Kremer, and Tristan Bereau — Max Planck Institute for Polymer Research, Mainz, Germany

Increasing the efficiency of materials design and discovery remains a significant challenge, especially given the prohibitively large size of chemical compound space. In addition to reducing computational expense, use of a chemically transferable coarse-grained model enables different molecular fragments to map to the same bead type. This further increases sampling efficiency, effectively reducing the size of chemical compound space. For example, we previously showed that over 400,000 molecules could be mapped to 119 Martini representations, demonstrating a drastic reduction of chemical compound space. Here, we demonstrate that the Martini model is not optimal for chemical transferability, and we propose new criteria for the rational design of coarse-grained models that allows for the optimization of their chemical transferability. We validate this hypothesis by parameterizing three Martini-like force fields, in which the number of bead types ranges from five to sixteen for the different force fields. We demonstrate that a level of performance and accuracy comparable to Martini can be obtained by using a force field with fewer bead types, thus making this force field more efficient at reducing the chemical compound space. Furthermore, constructing this force field with chemical transferability as a foundation allows us to know a priori the most likely chemistries that correspond to a specific bead type.

CPP 25.35 Tue 14:00 Poster B1

Hoobas: A python-based flexible molecular builder — •Martin Girard[1], Annaliese Ehlen[2], Anisha Shakya[2,3], Tristan Bereau[1], and Monica Olvera de la Cruz[2] — [1]Max Planck Institute for Polymer Physics, Mainz, Germany — [2]Department of Material Science and Engineering, Northwestern University, Evanston, IL, USA — [3]Center for Soft and Living Matter, Institude for Basic Science, Ulsan, South Korea

Molecular dynamics has emerged as a powerful and efficient tool to study soft matter. As the computing power available increases, so

does the complexity of studied systems. In order to perform a simulation, initial positions and topologies must be built. A few tools already exist, but are generally very specific in terms of systems they can build. Here, we introduce Hoobas, a molecular building tool able to handle very general systems and nearly arbitrary polydispersity using a prototype-builder design pattern. As examples, we show building of DNA-coated colloidal crystals, lipid membranes and random hyperbranched polymer melts. The objects provided are easily extensible to other topologies.

CPP 25.36 Tue 14:00 Poster B1

Boehmite Microcrystal Growth and its Interaction with Polymers at the Interface. — •Mateusz Dudziak, Dorothee Silbernagl, and Heinz Sturm — Bundesanstalt für Materialforschung und prüfung (BAM), Berlin, Germany

Nanocomposites are extremely versatile due to their physicochemical properties, which differ significantly from bulk homopolymers. One of the inorganic nanomaterials, which is increasingly used as a filler in polymer matrices is boehmite, due to its flame-retardant properties. Here, it is utilized as a nanofiller in polycarbonate and polyamide, expecting to improve their mechanical properties. For industrial use boehmite is obtained by the solvothermal method, resulting in a layered nanomaterial, whereas naturally it occurs as single crystals with the size of <50*m. In this work we are obtaining and isolating boehmite monocrystals by a bottom-up method, in which a reaction between aluminum salts and hydroxides takes place in a polymer gel. Obtaining boehmite as microcrystals is necessary for its analysis and characterization, as well as to investigate its interaction with polymer matrices at the polymer/particle interface. Here, the obtained particles are characterized by small- and wide-angle X-ray scattering and further in polymer matrices with differential scanning calorimetry and intermodulation atomic force microscopy (ImAFM), probing local stiffness.

CPP 25.37 Tue 14:00 Poster B1

A different kind of True Random Number Generator - Stoachastic Assembly of Ag/Au Single Particle Lines — •Daniel Schletz[1], Martin Mayer[1,2], Anja Maria Steiner[1,2], and Andreas Fery[1,2,3] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., Germany — [2]Cluster of Excellence Center for Advancing Electronics Dresden, Germany — [3]Department of Physical Chemistry of Polymeric Materials TU Dresden, Germany

Standard hardware random number generators often use quantum mechanical phenomena or thermal noise to produce bit streams of random, but often biased, origin. In contrast, colloidal self-assembly of billions of particles on $1\,cm^2$ can assure bias-free, heterogeneous particle sequences to be employed as bits in a hardware random number generator.

Utilizing template-assisted colloidal self-assembly of two different particle types (Au spheres and Ag spheres), heterogeneous single particle lines are assembled and subsequently analyzed *via* electron microscopy. Statistical evaluation shows that Ag and Au do not assemble in any way preferential to any particle type, generating random distributions only dependent on employed Ag/Au particle share.

CPP 25.38 Tue 14:00 Poster B1

Synthesis of protein-coated gold nanoparticles and investigations on their uptake by diatoms — •Marisa Hoffmann[1,2], Nathalie Pytlik[1], Roland P. M. Höller[2], Christian Kuttner[2], Andreas Fery[2,3], and Eike Brunner[1] — [1]Department of Bioanalytical Chemistry, TU Dresden, Germany — [2]Leibniz-Institut für Polymerforschung Dresden e.V., Germany — [3]Department of Physical Chemistry of Polymeric Materials, TU Dresden, Germany

Because of the inertness and the surface plasmon resonance (SPR) of gold nanoparticles (AuNPs) and the biocompatibility of natural proteins, the combination of both provides a promising system for *in vivo* surface enhanced Raman spectroscopy (SERS) applications. AuNPs were synthesized by the citrate reduction method and the kinetically controlled seeded growth of citrate-stabilized AuNPs (Bastús 2011). Ligand exchange of the citrate by bovine serum albumin (BSA) was then performed. Gold/gold 3D core/satellite nanoclusters were synthesized by protein assisted self-assembly in solution (Höller 2016). After incubating cells of the diatom species *stephanopyxis turris* with the mentioned protein-coated AuNPs and gold nanoclusters, respectively, *in vivo* 3D Raman imaging was carried out. As, for a detectable SERS enhancement, plasmonic nanostructures in the vicinity of the analyte are necessary, the localization of AuNPs can be determined by the po-

sition of the SERS signals. That way it was possible to successfully investigate the uptake of AuNPs and gold nanoclusters by the diatom cells. This opens up the way for a new method in prospective *in vivo* research of algal metabolism.

CPP 25.39   Tue 14:00   Poster B1

Dynamic Fluorescence Properties of Graphene Quantum Dots — •CHRISTIAN WIMMENAUER[1], RALF KÜNEMUTH[2], STEFAN FASBENDER[1], CLAUS A M SEIDEL[2], and THOMAS HEINZEL[1] — [1]Institute of Experimantal Condensed Matter Physics, Heinrich-Heine-University Düsseldorf — [2]Institute of Physical Chemistry, Heinrich-Heine-University Düsseldorf

Graphene quantum dots (GQDs) are a promising candidate for various biomedical applications ranging from drug delivery to single particle tracking, due to their small size and low toxicity. To characterize GQDs concerning their viability as a fluorescence marker time correlated single photon counting and fluorescence correlation spectroscopy are employed. The fluorescence lifetime, the time scales of different dark states and the diffusive properties are determined. Dark states are discussed for coupled and uncoupled GQDs at different pH values. The measured properties allow for an assessment of the usability in biomedical applications, such as single particle tracking or super resolution microscopy.

CPP 25.40   Tue 14:00   Poster B1

Energy Spectra of Triangular Multilayer Graphene Quantum Dots — •JULIENNE SCHELLER, CHRISTIAN WIMMENAUER, and THOMAS HEINZEL — Institute of Experimantal Condensed Matter Physics, Heinrich-Heine-University Düsseldorf

Triangular Multilayer Graphene Quantum Dots (GQDs) are modelled using a tight binding approach. The energy gaps are calculated as a function of disk radius, number of disk layers and edge type. Armchair edge type and zigzag edge type GQDs are investigated for up to 7 layers and in the limit of infinitely many layers. To further discuss the differences between both edge types the density of states and the ground state wavefunctions are calculated.

CPP 25.41   Tue 14:00   Poster B1

Momentum Space Calculations of Nano Scaled Semiconductor Materials — •MARCEL DOHRMANN, CHRISTIAN STRELOW, and ALF MEWS — Institute of Physical Chemistry, University Hamburg, Grindelalle 117, 20146 Hamburg, Germany

Excitons energy calculations are done by solving Schrödinger's equations of kinetic terms, including the effective mass of electrons and holes, and potential terms. In position space, three-dimensional self-consistent calculations with hole and electron functions are used to understand different nano sized semiconductors like CdSe/CdS dot-rods.[1] Using fourier transformations the kinetic and potential Hamiltonians in position space can be adapted to momentum space. A potential landscape in momentum space is an approach to calculate energy levels of electrons and holes in different composites. We see forward to study interaction between heavy and light holes in semiconductor nanomaterials.

[1] S.-H. Lohmann, C. Strelow, A. Mews, T. Kipp, ACS Nano 2017, DOI 10.1021/acsnano.7b05303.

CPP 25.42   Tue 14:00   Poster B1

A Combined SAXS-SANS instrument at ILL — •EZZELDIN METWALLI, KLAUS GÖTZ, CHRISTIAN BÄR, and TOBIAS UNRUH — Institute for Crystallography and Structural Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

In the last few decades, small angle X-ray and neutron scattering (SAXS/SANS) methods have been used extensively for investigating nano-scale structured materials. Combining both SAXS and SANS techniques in a single experiment will open a new route for a novel nano-analytical method. Simultaneous SAXS and SANS measurements will provide structural information from the same sample volume allowing unique different contrast conditions. Moreover, exploiting X-ray and neutron radiation for time-resolved studies will simultaneously provide nano-scale structural information at two different contrast situations, ensuring the exactness of the probed samples compared with independent experimental approach. Here, we introduce an advanced portable SAXS system that is dimensionally suitable to be installed on D22 instrument at ILL. The new portable SAXS system is based on Copper/Molybdenum switchable microfocus rotating anode X-ray generator and a Dectris detector with a changeanble sample-to-detector distance of up to 1.5 m in a vacuum tube. The unprecedented combined experimental approach using simultaneous SAXS/SANS methods will open the way for investigating a truly wide range of innovative materials such as smart self-assembling nanomaterials, multifunctional materials, and organic/inorganic hybrid nanomaterials.

CPP 25.43   Tue 14:00   Poster B1

Self-assembly in magnetic filament systems: impact of internal factors — ELENA PYANZINA, TATYANA BELYAEVA, MARINA KASHPUROVA, and •EKATERINA NOVAK — Ural Federal University

The fundamental understanding of the self-assembly properties of colloidal systems is one of the key topics in current research on novel microstructured soft materials and technologies. In this work we investigate self-assembly of magnetic filaments of different topology with different additional interaction and particles polydispersity. We performed molecular dynamics simulations using a Langevin thermostat. Cluster analysis based on graph theory is used to analyze the obtained data. At the moment we are analyzing the results, but we can already say that the introduction of additional attraction and particles polydispersity significantly expands the structural diversity of the self-assembly of magnetic filaments, and the effect of magnetic dipole-dipole interaction remains substantial. All these results will pave the way for the development of analytical models and identify the most interesting building block candidates for the design of new magnetoresponsive materials.

CPP 25.44   Tue 14:00   Poster B1

Equilibrium behavior of surface-grafted supracolloidal ferromagnetic filaments — •PEDRO A. SÁNCHEZ[1,2], JOAN J. CERDÀ[3], TOMÁS SINTES[4], and SOFIA S. KANTOROVICH[1,2] — [1]Computational Physics, University of Vienna, Vienna, Austria — [2]Ural Federal University, Ekaterinburg, Russia — [3]IAC3, Universitat de les Illes Balears, Palma de Mallorca, Spain — [4]Instituto de Física Interdisciplinar y Sistemas Complejos, UIB-CSIC, Palma de Mallorca, Spain

Supracolloidal magnetic filaments, that are semiflexible chains of magnetic micro- or nanoparticles permanently crosslinked by polymers, are used for the creation of magnetically driven microfluidic propellers and pumpers, micromechanical sensors and contrast imaging agents. These systems have been also proposed as building blocks of thin films that can change their structure and rheological properties as a response to external magnetic fields. Most of such applications involve the interaction of free or end grafted filaments with inert or attracting surfaces.

Here we study, by means of computer simulations, the equilibrium structures of individual magnetic filaments made of ferromagnetic particles when placed near to interacting flat surfaces. We focus on the structural changes that take place on cooling depending on the strength of the interaction with the surface and the applied field, comparing the cases of free and grafted filaments.

CPP 25.45   Tue 14:00   Poster B1

Light-induced deformation of azo-polymer droplets - challenges in modelling the influence of light — •MARKUS KOCH[1], MARINA SAPHIANNIKOVA[1], SVETLANA SANTER[2], and OLGA GUSKOVA[1] — [1]Institute Theory of Polymers, IPF Dresden, Germany — [2]Institute of Physics and Astronomy, University of Potsdam, Germany

In recent years azobenzene-containing materials have been gaining a lof of scientific interest due to the possibility to change their properties by using light as an external stimulus [1]. These effects are based on the trans-cis photoisomerization of azobenzene and its interplay with the surrounding system. To gain a deeper understanding of the deformation of azo-materials we study an azo-polymer droplet on a silica surface exposed to UV-vis light. Here, the azo side groups of the polymer chains reorient perpendicular to the E-field of light due to cyclic photoisomerization [2]. Using MD simulations we study the influence of linearly polarized light on the droplet applying two different approaches. In the first case we simulate the repeated angle-dependent trans-cis photoizomerization of azobenzenes explicitly by temporally changing the torsion angle around the azo bond [3]. In the second case we utilize an effective orientation potential [2], which reorients the azobenzenes without modelling the photoisomerization events.

[1] Yadavalli, N.S. et al. Appl. Phys. Lett. 105, 051601 (2014)
[2] Toshchevikov, V. et al. J. Phys. Chem. B, 113(15), 5032 (2009)
[3] Heinz, H. et al. Chem. Mater. 20, 6444 (2008)

CPP 25.46   Tue 14:00   Poster B1

Structure and Switching of Azobenzene Layers Physisorbed on Mica and Glass — •Amrita Pal[1], Olga Guskova[1], Alexey Kopyshev[2], and Svetlana Santer[2] — [1]Institute Theory of Polymers, IPF Dresden, Germany — [2]Institute of Physics and Astronomy, University of Potsdam

We study the photoswitchable amphiphilic molecules [1] with charged trimethyl ammonium head group and the hydrophobic tail consisting of alkyl and azobenzene (azo) segments. Being physisorbed on mica or glass surfaces, these molecules build the self-assembled monolayers. The reversible photoswitching of thickness of the layers is investigated in both AFM experiments and DFT/MD simulations. The in-situ AFM experiments show that the photoisomerization of the azo molecules under irradiation with light of different wavelength results in significant change of morphology, i.e. thickness and topography of azo multilayers. In DFT, the triple zeta basis set and generalized gradient approach, hybrid and range separated hybrid functionals are used to obtain the isomeric properties at the molecular level. Also, a periodic DFT calculation is performed for a single molecule adsorbed onto a small mica cluster to compare the results of quantum and classical simulations. The DFT calculations of the azo isomers in vacuum and in adsorbed state reveal the influence of the surface on their electronic properties. The MD simulation of denser layers consisting of many azo molecules uncovers their detailed structures and allows a direct comparison with AFM data. We acknowledge support from DFG, GU 1510/5-1. [1] Montagna, M. et al. Langmuir 34(1), 311 (2018)

CPP 25.47   Tue 14:00   Poster B1
Water dynamics in a concentrated poly(N-isopropylacrylamide) solution at high pressure — •Bart-Jan Niebuur[1], Wiebke Lohstroh[2], Marie-Sousai Appavou[3], Alfons Schulte[4], and Christine M. Papadakis[1] — [1]TU München, Physik Department, Garching, Germany Physik weicher Materie, — [2]Heinz Maier-Leibnitz Zentrum (MLZ), TU München, Garching, Germany — [3]FZ Jülich, JCNS at MLZ, Garching, Germany — [4]University of Central Florida, Department of Physics and College of Optics and Photonics, Orlando, U.S.A.

Hydration water is of fundamental importance for the phase transitions of macromolecules in aqueous solution. A complete picture of the dynamics of hydration water is therefore key for identifying the processes involved. Using quasi-elastic neutron scattering, we study the hydration behavior of a concentrated solution of the thermoresponsive polymer poly(N-isopropylacrylamide) during heating through its cloud point (CP). Varying pressure alters its hydration state [1]. At low pressure, the fraction of hydration water decreases sharply at the CP. The diffusion of the remaining fraction gets increasingly hindered, which points to a rearrangement of the hydration water. In the one-phase state at high pressure, the hydration water diffuses more rapidly than at low pressure, which indicates enhanced hydrophobic hydration. At the CP, the fraction of hydration water decreases by a similar amount as at low pressure, but the transition spans over ∼10 K. At high pressure, the hydrophobic groups stay hydrated in the two-phase state. [1] B.-J. Niebuur, C. M. Papadakis et al., *ACS Macro Lett.* 2017, **6**, 1180

CPP 25.48   Tue 14:00   Poster B1
Mesoglobules in PNIPAM solutions: Influence of pressure — Bart-Jan Niebuur[1], •Geethu P. Meledam[1], Vitaliy Pipich[2], Marie-Sousai Appavou[2], Alfons Schulte[3], and Christine M. Papadakis[1] — [1]TU München, Physik-Department, Garching, Germany — [2]FZ Jülich, JCNS at MLZ, Garching, Germany — [3]University of Central Florida, Orlando, U.S.A.

Poly(N-isopropylacrylamide) (PNIPAM) in aqueous solution forms mesoglobules upon heating through the cloud point, which are small and contain only little water. In contrast, at high pressure, much larger clusters are formed, which contain more water than at atmospheric pressure [1]. We use very small angle neutron scattering at temperatures above the cloud point to elucidate the transition between low and high pressures. We find a sharp transition between small mesoglobules and large clusters with the transition pressure depending on temperature. We attribute the pressure-dependent behavior on mesoscopic length scales to the pressure-dependent hydration of PNIPAM.
1. B.-J. Niebuur et al., ACS Macro Lett. 6, 1180 (2017)

CPP 25.49   Tue 14:00   Poster B1
Preferential binding of salts to pNiPAM and its monomer — •Jakub Polák, Adam Kovalčík, Pavel Vrbka, Daniel Ondo, Vladimír Palivec, and Jan Heyda — Department of Physical Chemistry, University of Chemistry and Technology, Prague, Czech

Republic

Over past decade investigation of salt specific effects on biomolecules attracted a lot of experimental, computational and theoretical attention. However, the direct quantitative thermodynamic characterization is still poor. In this contribution we measure a preferential binding coefficient of salts to a well established model biomolecule, poly-N-isopropyl-acrylamide (pNiPAM). The pNiPAM-salt interaction is determined in equilibrium dialysis experiments. The results are supplemented by vapor pressure osmometry experiments of NiPAM, in which salt-monomer interactions at dilute conditions were determined. Finally, in combination with density measurements and upon application of theory of solution the thermodynamically relevant basic ingredients, Kirkwood-Buff integrals, were determined.

CPP 25.50   Tue 14:00   Poster B1
Simulating the hydrodynamics of droplets on photo-switchable substrates — •Josua Grawitter and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, Berlin, Germany

Photo-switchable substrates provide a unique mechanism to manipulate liquid droplets precisely by creating and adapting a heterogeneous wettability landscape. Because droplets respond to changes in the wettability, this is a means to keep them in non-equilibrium and thereby induce new states of dynamic wetting.

We present a boundary element method to determine the Stokes flow inside the droplet with a curved free surface and a flat interface at the substrate, where we apply the Navier boundary condition to permit motion of the contact line. In general, boundary element methods solve integral equations by inverting the discretized integrals of the unknown field variable such as fluid velocity.

In our approach we parametrize the free surface of the droplet by a linear combination of smooth basis functions and, using an automatic differentiation algorithm, we calculate its local metric and curvature. This provides high resolution data for an iterative domain-splitting integration scheme capable of treating singular integrands, which are typical for the boundary element method. Following rigorous validation, we will investigate how droplets respond to specific spatio-temporal wettability patterns that either move or deform the droplet. For example, we will generate directed motion by traveling patterns and vary their properties to maximize droplet speed.

CPP 25.51   Tue 14:00   Poster B1
Stable 2D conductive and transparent metal/metal(hydr)oxide multilayers prepared by manipulated wetting — •Sebastian Runde, Heiko Ahrens, Harm Wulff, and Christiane A. Helm — Institute of Physics, Universität Greifswald, Felix-Hausdorff-Str. 6, 17489 Greifswald

We present a new deposition method allowing ultrathin, conductive and transparent metal-containing layers to be prepared at ambient conditions with cm^2 areas on glass substrates. Multilayers are formed by repetition of the deposition procedure, induced break-up after forced wetting. Different liquid metals and their alloys, Bismuth, Gallium, Indium and Tin were used and compared. These metals all have a low melting temperature, a high wettability and form instantaneously a passivating oxide skin. X-ray measurements show that multilayer thickness increases linearly with the number of deposition cycles, yielding a reproducible single layer thickness between 3 and 6 nm. The largest layer number achieved was 13 (54 nm thick). The sheet resistance and the optical absorbance decrease monotonically with the number of deposited layers.

CPP 25.52   Tue 14:00   Poster B1
Buckling patterns and their elastic response on the surface of polyelectrolyte multilayer films with short PSS chains — •Amir Azinfar[1], Sven Neuber[1], Jiří Vaněček[2], Marie Vancová[2,3], Jan Sterba[2,3], Vítězslav Straňák[3], and Christiane A. Helm[1] — [1]Institute of Physics, University of Greifswald, 17489 Greifswald, Germany — [2]Biology Centre, Czech Academy of Sciences, 37005 Ceske Budejovice, Czech Republic — [3]Faculty of Science, University of South Bohemia, B 37005 Ceske Budejovice, Czech Republic

We investigate the surface morphology of polyelectrolyte multilayers (PEMs) after drying. A buckling pattern is observed. PEMs are made from poly(diallyldimethylammonium (PDADMA) and poly(styrene sulfonate) (PSS) in 0.1 M NaCl with non-linear and linear growth regimes. When more PSS/PDADMA layer pairs are deposited, for PSS-terminated films the wavelength of the buckling pattern increased

from 185 nm to 225 nm. For PDADMA-terminated films the wavelength was always greater. The buckling pattern is correlated with the elastic modulus of the film, which decreased with increasing film thickness. Annealing in high salt concentrations (0.5 -1.0 mol/l NaCl) decreased the surface roughness and increased the wavelength of the buckling pattern. However, for films containing mobile PSS, annealing caused a damped oscillation of the buckling pattern.

CPP 25.53 Tue 14:00 Poster B1

Wetting and imbibition experiments with aqueous electrolyte solutions and polymers on nanostructured and porous materials — •Guido Dittrich and Patrick Huber — Institute of Materials Physics and Technology, Hamburg University of Technology (TUHH), Eißendorfer Str. 42, D-21073 Hamburg-Harburg, Germany

Nanostructured as well as porous materials offer high specific surface areas per projected area and volume respectively. That makes them interesting for fundamental research since the discovery of super hydrophobicity and super permeation. We are investigating the imbibition kinetics of polystyrene into porous scaffold materials comparing different pore systems. The imbibition kinetics are measured with a gravimetric and an interferometric setup. Analysis of aqueous electrolyte solution droplets may lead to fast tests to get insights regarding surface roughness, successful chemical impregnation and interface fractions. Commercially available p-doped silicon wafers can be nanostructured by electrochemical etching. We seek to overcome their tendency to increase their native oxide layer during electrowetting experiments by chemical modification of the surfaces end groups. Dynamic wetting on carbon nanotube (CNT) arrays glued together by epoxy is driven by capillarity. After the synthesis the CNTs are opened by different techniques. Drop shape analysis is used to supplement scanning electron microscopy to verify open pores.

CPP 25.54 Tue 14:00 Poster B1

Hard sphere electrolyte solution at charged wall — •Maximilian Mussotter[1], Markus Bier[2], and S. Dietrich[1] — [1]Max-Planck Institut für Intelligente Systeme und Universität Stuttgart, 70569 Stuttgart, Germany — [2]University of Applied Sciences Würzburg-Schweinfurt, 97421 Schweinfurt, Germany

Although widely used, upon advancing from electrically neutral fluids and uncharged subtrates, the assumption of homogeneous wall-fluid interactions is questionable beyond molecular length scales when studying fluids comprising electrically charged constituents and charged walls. Therefore, the intention of this work was to gain further insight in the effects occurring at non-uniformly charged substrates. The system is studied by means of classical density functional theory, within the framework of fundamental measure theory using the WBI-functional. The goal of this work was to introduce a basic machinery to study the effects of nonhomogeneously charged surfaces.

CPP 25.55 Tue 14:00 Poster B1

Microscopic investigation of polymer flow in porous media — •Pegah Shakeri[1,2], Michael Jung[1,2], Martin Brinkmann[1], Stephan Herminghaus[2], and Ralf Seemann[1,2] — [1]Universität des Saarlandes, Saarbrücken, Germany — [2]Max Planck-Institute for Dynamics and Self-Organization, Göttingen, Germany

The displacement of a fluid from a permeable medium by injecting a second immiscible fluid is central in many industrial processes like oil recovery. The general assumption is that the polymer modifies the viscosity of the injected fluid; thus improves the volumetric sweep efficiency (the amount of displaced oil) by enhancing mobility ratio and controlling viscous fingering in macro scale. However, recent observations suggest that additionally microscopic effects are important; thus microscopic investigation of a polymer flow in a quasi-2D microfluidic device was conducted to gain clear insight into the pore scale mechanism of oil displacement by a polymer solution in permeable media. Deviation from laminar flow, fluctuating oil-polymer solution interfaces, lower residual saturation in comparison to a flood of water or aqueous glycerol solution (having the same zero shear viscosity as the polymer solutions) were observed. The observed instabilities in the bulk flow,which seem to originate from viscoelasticity of the polymer solution, destabilize the oil-polymer interface and are consequently capable of improving the microscopic displacement.

CPP 25.56 Tue 14:00 Poster B1

Monitoring Pressure Fluctuations in Artificial Porous Me-

dia. — •Michael Jung[1,2], Martin Brinkmann[1], Stephan Herminghaus[2], and Ralf Seemann[1,2] — [1]Universität des Saarlandes, Saarbrücken, Germany — [2]Max Planck-Institute for Dynamics and Self-Organization, Göttingen, Germany

We aim to understand the microscopic mechanisms of individual capillary instabilities which govern slow displacement processes in permeable porous media. Therefore we investigate the influence of the pore space geometry and wettability on the landscape of pressure variations during slow displacement of fluid from an arrangement of glass beads by a second, immiscible fluid. For an experimental verification of the capillary pressure variations, we measure the pressure of a bursting meniscus in a single throat formed by three beads. Different wettability of the glass beads is realized by wet-silanization techniques as OTS (octadecyltrichlorosilane) or APTES (3-aminopropyltriethoxysilane)-coating which result in a water-air contact angle on glass beads of 110° and 60°, respectively. Heterogeneous wettability is achieved by throats assembled from beads with different coatings. The experiments shall be compared with numerical calculations of the capillary pressure in such a heterogeneous throat for various combination of contact angles. Understanding the characteristic pressure variations of single throats, we will extend our setup to small bead-packs consisting of a few layers of glass beads with heterogeneous wettability.

CPP 25.57 Tue 14:00 Poster B1

A fast quartz crystal microbalance (QCM) with millisecond time resolution operating on multiple overtones at the same time — •Arne Langhoff, Frederick Meyer, Astrid Peschel, Judith Petri, and Diethelm Johannsmann — Institut für Physikalische Chemie, TU Clausthal, Germany

Second-generation QCMs (which include the QCM-D) rely on readings of the resonance frequency as well as bandwidth on multiple overtones. The added information gives access to the sample's softness and other properties. Currently, most QCMs need about a second per frequency reading and they access different overtones sequentially. Using a multi-frequency lockin amplifier (MLA, supplied by Intermodulation Products AB, Stockholm), this limitation can be overcome. The MLA excites the resonator at 40 frequencies simultaneously. The channels are distributed over four "combs" (10 frequencies each), where each comb covers one overtone. The time resolution can be close to the inverse resonance bandwidth, which - for high-fundamental-frequency (HFF) resonators - is well below one millisecond. The technique is particularly powerful when applied to repetitive processes because accumulation can then lower the noise in frequency shift of 5-MHz resonators well into the mHz range. Applications chosen for demonstration are the impact of droplets onto the QCM surface (the kinetics of which is in ms range) and electrochemical measurements (in which case accumulation and averaging can be exploited). In the latter case, the fast dynamics after voltage reversal is monitored. The response is governed by changes of viscosity in the double layer.

CPP 25.58 Tue 14:00 Poster B1

Water freezing and frosting on lubricant impregnated surfaces — •Lukas Hauer[1,2] and William Wong[1] — [1]Max Planck Institute for Polymer Research — [2]Institute of Fluid Mechanics and Aerodynamics, Technische Universität Darmstadt

In the scope of the present work, frost formation and drop freezing in/on lubricant-infused surfaces ("under-oil" dynamics) are experimentally investigated. Glass substrates structured with SU-8 micropillar arrays are chosen as model surfaces. To examine frost formation, a sample is placed on a Linkam peltier stage which is enclosed in a chamber with humidity control to induce condensation-frosting. To examine freezing, the sample (and deposited drop) is placed in an alternate chamber with temperature control, which is cooled using liquid nitrogen. Frost formation and drop freezing will be observed using an inverted laser scanning confocal microscope. This spatially and temporally resolved technique allows accurate observation of these dynamic processes close to the substrate surface. By adding a dye to the lubricant, the water-lubricant interfaces can be discriminated, allowing us to monitor lubricant mobility during freezing/frosting. During frost formation, a migration of the lubricant to the top of the ice has been observed. Due to the dendritic morphology of frost, capillary effects are believed to be the driving forces of this phenomenon. Such effects could lead to lubricant drainage and failure of surface functionality. A fundamental understanding of the lubricant migration will help to design more ice-durable slippery surfaces.