

## CPP 50: Poster Session III

Topics: Complex Fluids and Colloids, Micelles and Vesicles (50.1-50.15); Composites and Functional Polymer Hybrids (50.16); Emerging Topics in Chemical and Polymer Physics, New Instruments and Methods (50.17-50.19); Fundamentals of molecular liquids, ionic liquids and mixtures (50.20-50.23); Modeling and Simulation of Soft Matter (50.24-50.30); Nanostructures, Nanostructuring and Nano-sized Soft Matter (50.31-50.33); Polymer and Molecular Dynamics, Friction and Rheology (50.34-50.37); Polymers under confinement (50.38-50.40); Responsive and Adaptive Systems (50.41-50.47); Wetting, Fluidics and Liquids at Interfaces and Surfaces (50.48-50.52).

Time: Tuesday 14:00–16:00

Location: P1C

CPP 50.1 Tue 14:00 P1C

**Cluster of supracolloidal magnetic polymers in a flow** — ●EKATERINA NOVAK, ELENA PYANZINA, and PEDRO SANCHEZ — Ural Federal University, Ekaterinburg, Russia

The active study of nanoparticles has opened new perspectives in the soft matter physics. Construction of supracolloidal magnetic polymers (polymer-like structures in which magnetic nanoparticles are playing the role of monomers) has recently been made possible. The advantage of such magnetic polymers is that they keep their structure independently from the temperature and that is why they can be potentially used as an alternative to nanoparticles in magnetic fluids to obtain a desired and easily controlled magnetic or rheological response. In suspension of magnetic polymers with ferromagnetic particles and central attraction in the absence of an applied field quasi-spherical clusters are formed. One of that clusters is placed in the microchannel, where its behavior in the shear flow is investigated, varying a wide range of system parameters. We find that with time the cluster gets elongated. The higher is the shear rate the faster the flow can deform the cluster. The deformation happens slower if the dipolar interaction is stronger.

CPP 50.2 Tue 14:00 P1C

**Impact of microstructure on the flow behaviour of micellar systems - a theoretical approach** — ●BENJAMIN VON LOSPICH<sup>1,2</sup>, VALENTINA ALBERINI<sup>1</sup>, MICHAEL GRADZIELSKI<sup>2</sup>, and SABINE H. L. KLAPP<sup>1</sup> — <sup>1</sup>Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstraße 36, D-10623 Berlin — <sup>2</sup>Institut für Chemie, Technische Universität Berlin, Straße des 17. Juni 124, D-10623 Berlin

It has been shown by various experiments that elongated or wormlike micelles exhibit a unique viscoelastic behaviour yielding a non-linear flow [1]. The theoretical descriptions for this phenomenon can be either of tensorial form [2] or they correspond to one-dimensional models including additional degrees of freedom, e.g. a coupling of the mechanical variables and the microstructure [3]. Such a coupling yields a destabilization in the high shear rate branch of the flow curve as well as interesting dynamical states such as oscillatory and/or chaotic states. To improve the performance of this specific model and for a better (quantitative) comparison to experimental results, we explore the possibilities of introducing additional terms to describe the high shear rate behaviour. We also include concentration effects which strongly influence e.g., branching in wormlike micellar systems.

[1] C. Dreiss, *Soft Matter* **3**, 956, (2007)[2] M. Johnson, D. Segalman, *J. Non-Newton. Fluid Mech.* **2**, 255, (1977)[3] B. v. Lospichl, S. H. L. Klapp, *Phys. Rev. E* **98**, 042605, (2018)

CPP 50.3 Tue 14:00 P1C

**The free-energy profile of a copolymer micelle fusing with a homopolymer interface** — ●NIKLAS BLAGOJEVIC und MARCUS MÜLLER — Georg-August Universität, Göttingen, Institut für Theoretische Physik

In a blend containing immiscible A and B homopolymers, the polymers will phase-separate and form domains. If the blend also contains the corresponding AB diblock copolymers, the copolymers will segregate to the interface between the immiscible homopolymers and reduce the interface tension. In order to deliver the copolymers to the interface, micelles that form in one phase have to move to the interface and fuse. The movement of the micelles is protracted, and the fusion of the micelles with the AB interface is characterized by a free-energy barrier. Here, we will focus on the fusion barrier and gain insight into the free-energy landscape, and its dependence on the system parameters, and the molecular asymmetry of the diblock copolymer. Explicitly, we will study the minimum free-energy path (MFEP), i.e. the most probable transition pathway, that connects these two states on the free-

energy landscape and obtain the concomitant free-energy profile along the pathway. To do so, we will use highly parallelizable particle-based SCMF (Single-Chain in Mean Field) simulations in conjunction with Umbrella-sampling and the String-method to calculate the MFEP. For this purpose, we will investigate the accuracy of the Umbrella-sampling as a function of the simulation parameters, such that an optimal sampling takes place.

CPP 50.4 Tue 14:00 P1C

**The role of non-adiabatic forces during the collapse of a 1D capillary system** — ●ANJA SCHREIBER, JOHANNES BLEIBEL, and MARTIN OETTEL — Institut für angewandte Physik, Universität Tübingen, Tübingen, Germany

We study the behavior of a one-dimensional system of colloidal particles trapped at a fluid interface using Brownian Dynamics (BD) simulations. Inter-facially trapped, micrometer-sized colloidal particles interact via long-ranged capillary attraction. The interaction is formally analogous to screened Newtonian gravity with the capillary length  $\lambda$  as the tuneable screening length. For a certain range of parameters, the system exhibits clustering behavior. After a characteristic timescale the system collapses globally and collectively to a close-packed patch, similar to a self-gravitating fluid, and thus reaches the equilibrium state. Within studies of the impact of noise and starting position on the density profile during the clustering process, a significant discrepancy between simulation and Dynamical Density Functional Theory (DDFT) was found. Hence, it was concluded that non-adiabatic forces may contribute considerably to the dynamics. We obtain these non-adiabatic forces from applying an iterative scheme, developed for short-range interactions [1]. In order to investigate possible modifications for the DDFT, this method is adapted and appropriately modified for our long-ranged attractive system.

[1] D. de las Heras, J. Renner, and M. Schmidt, *Phys. Rev. E* **99**, 023306 (2019)

CPP 50.5 Tue 14:00 P1C

**Structural properties of biaxial phases formed by mixtures composed of uniaxial liquid crystal particles** — ●LOUIS LEHMANN<sup>1</sup>, ROBERT SKUTNIK<sup>1</sup>, SERGEJ PÜSCHEL-SCHLOTTHAUER<sup>1</sup>, MARTIN SCHOEN<sup>1,2</sup>, and GEORGE JACKSON<sup>2</sup> — <sup>1</sup>Stranski-Laboratorium für Physikalische und Theoretische Chemie, Technische Universität Berlin — <sup>2</sup>Imperial College London, United Kingdom

In previous work, we investigated the formation of biaxial nematic phases in a model system consisting of a binary mixture of uniaxial molecules. The model potential was set up such that like molecules of each mixture component prefer a parallel alignment whereas two unlike molecules align preferentially in a T-shaped configuration. By tuning the potential parameters, we avoid a decomposition of the mixture which has hampered earlier studies because of its competition with the formation of an ordered biaxial phase. In this work we study the local orientational structure in a binary, decomposed mixture of uniaxial liquid crystals, using the same model as for the mixed phases, but lowering the interaction potential between particles of different kinds.

CPP 50.6 Tue 14:00 P1C

**Molecular theory of a ferromagnetic nematic liquid crystal** — ●IMMANUEL SEBASTIAN GEIER<sup>1</sup>, STEFANIE WANDREI<sup>1</sup>, ROBERT ARNOLD SKUTNIK<sup>1</sup>, and MARTIN SCHOEN<sup>1,2</sup> — <sup>1</sup>Stranski-Laboratorium für Physikalische und Theoretische Chemie, Fakultät für Mathematik und Naturwissenschaften, Technische Universität Berlin, Straße des 17. Juni 115, 10623 Berlin, Germany — <sup>2</sup>Department of Chemical Engineering, Imperial College London, South Kensington Campus, London SW7 2AZ, United Kingdom

We employ a version of classical density functional theory to study the phase behavior of a simple model liquid crystal in an external field. The uniaxially symmetric molecules have a spherically symmetric core with superimposed orientation-dependent attractions. The interaction between the cores consist of a hard-sphere repulsion plus an isotropic square-well attraction. The anisotropic part of the interaction potential allows for the formation of a uniaxially symmetric nematic phase. The orientation of the molecules couples to an external polar field. The external field is capable of rotating the nematic director in the x-z plane. The field is also capable of changing the topology of the phase diagram in that it suppresses the phase coexistence between an isotropic liquid and a nematic phase observed in the absence of the field. We study the transition from an unipolar to a polar nematic phase in terms of the orientation-distribution function (odf), nematic and polar order parameters, and components of the nematic director.

CPP 50.7 Tue 14:00 P1C

**Nanoparticle dynamics in magnetic liquid crystal hybrid materials** — ●JOACHIM LANDERS<sup>1</sup>, DAMIAN GÜNZING<sup>1</sup>, KARIN KOCH<sup>2</sup>, SOMA SALAMON<sup>1</sup>, ANNETTE M. SCHMIDT<sup>2</sup>, and HEIKO WENDE<sup>1</sup> — <sup>1</sup>Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen — <sup>2</sup>Department of Chemistry, Institute of Physical Chemistry, University of Cologne

By adding magnetic nanoparticles to liquid crystals and liquid crystal elastomers, promising hybrid materials can be prepared, inheriting self-organization as well as a strong response to external magnetic fields. We utilize the ability of Mössbauer spectroscopy to provide information on particle dynamics as well as their magnetic alignment to study particle-matrix interaction across liquid crystal phase transitions. Thereby, the effect of self-ordering across the transition to the nematic state on particle dynamics will be analyzed, as well as the possibility of matrix reorientation via a magnetic stimulus. Regarding the possibility to extract direction-resolved particle diffusion coefficients from Doppler line-broadening, preliminary results on aligned anisotropic nanoparticles are discussed, which could represent a valuable approach for the future analysis of these hybrid materials aligned via magnetic or electric fields and other anisotropic soft magnetic composites. Funding by the DFG through SPP 1681 (project WE 2623/7-3 and SCHM1747/10) is gratefully acknowledged.

CPP 50.8 Tue 14:00 P1C

**Magnetic properties of Stocmayer supracolloidal magnetic polymers** — ●VLADIMIR ZVEREV<sup>1</sup>, IVAN NOVIKAU<sup>2</sup>, PEDRO SANCHEZ<sup>1,2</sup>, and EKATERINA NOVAK<sup>1</sup> — <sup>1</sup>URFU, Ekaterinburg, Russia — <sup>2</sup>UNIVIE, Vienna, Austria

This work is devoted to magnetic properties of aggregates formed in suspensions of supracolloidal magnetic polymer-like structures of different topology. We find that due to the formation of compact clusters, the overall initial magnetic susceptibility decreases dramatically for chain-, Y- and X-like topologies. However, this decrease for chain-like supracolloidal magnetic polymers is much stronger than that of other topologies, especially for systems with strong magnetic interactions [1]. If an external field is applied, clusters deform as a result of complex interplay between four forces: external field tends to align each dipole, the dipole-dipole interaction between magnetic particles tend to prevent rotations, permanent crosslinking prevent translation and finally central attraction favours the overall spherical shape of the cluster. Range of parameters when clusters remain stable and do not disintegrate is identified.

[1] E. Novak et al, JMMM 497, 166025 (2020).

CPP 50.9 Tue 14:00 P1C

**Translational and rotational dynamics of anisotropic colloids** — ●LISA ROHDE, MANUEL A. ESCOBEDO-SANCHEZ, JUAN PABLO SEGOVIA-GUTIERREZ, and STEFAN U. EGELHAAF — Condensed Matter Physics Laboratory, Heinrich Heine University, Düsseldorf, Germany

Micron-sized colloids show many physical phenomena, also encountered in more complex environments. In contrast to molecular systems, they are experimentally more accessible due to their larger size and slower dynamics. For example, they can be observed by optical microscopy. This renders them powerful model systems. While spherical particles have been used in many studies, the interest now moves to more complex structures. Here, we present experiments with ‘colloidal molecules’, namely trimers formed by three fused spherical particles[1]. The dynamics of spherical particles has been investigated in dependence of the particle concentration[2]. With increasing con-

centration, the dynamics slows down and eventually dynamical arrest is observed. A non-spherical shape introduces more complex dynamics with translation and rotation. In our experiments, the particles are in quasi-2D confinement resulting in translational motion as well as rotation around (only) one axis. The dynamics of pure trimers as well as the dynamics of trimers in the presence of spherical particles are investigated. The translational and rotational motions are quantitatively studied using microscopy and particle tracking.

[1]Manoharan et al.,Science,301,483-487,2003. [2]Pusey:Liquids,Freezing and Glass Transition,Elsevier p.763-942,1991.

CPP 50.10 Tue 14:00 P1C

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

We tackle the problem of a single charged colloid immersed in an electrolyte solution in the presence of an external applied small temperature gradient. Consequently electrical body forces are no longer counter balanced by pressure gradients, thereby inducing solvent flow and a directed motion of the colloidal particle.

The associated linearized electro-kinetic equations are solved numerically by adapting an adjusted solution scheme, originally invented by O’Brien and White [1] for the electrophoresis problem. Thus the thermal diffusivity is determined from the velocity field of a force-free Stokes flow. In addition a decomposition of the thermophoresis problem in two auxiliary ones simplifies the aim of calculating the thermal mobility considerably as it does not appear explicitly as a boundary condition. In the end we examine its dependence on the surface potential and the Soret coefficients of the different ions in the electrolyte for arbitrary Debye-layer thickness.

[1] R. W. O’Brien and L. R. White, J. Chem. Soc.,Faraday Trans. 2, 1978, 74, 1607.

CPP 50.11 Tue 14:00 P1C

**Diffusion and thermodiffusion of polymers in mixed solvents** — JANNIK KANTELHARDT, ●DANIEL SOMMERMANN, and WERNER KÖHLER — Physikalisches Institut, Universität Bayreuth, Germany

We present first results of experiments on diffusion and thermodiffusion of polymers in mixed solvents. So far, most works on thermodiffusion have dealt with binary or, more recently, ternary mixtures of small molecules. While binary mixtures are readily characterized by one diffusion and one thermodiffusion coefficient, the number of coefficients increases to four plus two for ternaries. Hardly any experiments exist for highly asymmetric ternary systems, like a polymer in a binary solvent. Two-color optical beam deflection (2-OBD) and supporting single-color thermal diffusion forced Rayleigh scattering (TDFRS) experiments show three well separated modes that can be assigned to the thermal diffusivity and the two eigenvalues of the mass diffusion matrix. We are particularly interested in the question, to what extent the dynamics of the large entity, the polymer, is coupled to the solvent-dynamics, both with respect to diffusion and thermodiffusion. A first analysis supports the picture of an effective solvent whose internal dynamics is decoupled from the one of the polymer. The investigations are supplemented by recent microgravity experiments on a similar system within the DCMIX project and by the planned investigation of non-equilibrium fluctuations within the GIANT FLUCTUATIONS program of ESA.

CPP 50.12 Tue 14:00 P1C

**DCMIX-4: experiments on thermodiffusion in fullerene and solvent mixtures on ground and aboard the International Space Station ISS** — ●MARCEL SCHRAML<sup>1</sup>, ANE ERRARTE<sup>2</sup>, MOHAMMED MOUNIR BOU-ALI<sup>2</sup>, and WERNER KÖHLER<sup>1</sup> — <sup>1</sup>Institute of Physics, University of Bayreuth, 95440 Bayreuth, Germany — <sup>2</sup>Mechanical and Manufacturing Department, MGEP Mondragon Goi Eskola Politeknikoa, Mondragon, Spain

Diffusive flows in a non-isothermal multicomponent fluid are characterized by complex cross-coupling phenomena between all concentration and temperature gradients. Beside the well known Fickian diffusion, a mass flux due to a concentration gradient, there is another contribution to the total mass flux, the so-called Soret effect or thermodiffusion. 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 under microgravity conditions aboard the International Space Station ISS to generate a benchmark system for comparison with ground-based laboratory experiments. On the poster we will focus on the currently completed DCMIX-4 campaign which includes a sample of solvents and fullerene. We are going to explain the different measurement techniques on ground and aboard the ISS and present some first results of the experiments.

CPP 50.13 Tue 14:00 P1C

**Particle sorting by Marangoni convection in microfluidic channels** — ●ROMAN REH, LORENZ KIEL, DANIEL ZAPP, and WERNER KÖHLER — Physikalisches Institut, Universität Bayreuth, Germany

Thermosolutal and thermocapillary Marangoni convection at a liquid-gas interface in a T-shaped microchannel structure of approximately  $100 \times 100 \mu\text{m}^2$  cross section creates localized vortices that can be used for particle trapping, steering, and sorting. Experiments have been performed with water-ethanol mixtures as carrier liquid and dispersed micrometer-sized polystyrene beads. Due to collisions with the meniscus, particles are displaced from streamlines that approach the interface closer than one particle radius. These streamlines feed liquid volumes that are entirely cleared of particles. Particle accumulations structures form inside the vortex, from where only small particles can escape by diffusion. Since the critical streamline, which separates the depletion from the accumulation region, depends on the particle radius, the mechanism can be used for particle sorting by superposition of a Poiseuille flow and splitting of the flow downstream from the meniscus. In the simplest case, the initially homogeneous flow is split into two arms, one where the particles are enriched and one where all particles are removed from the liquid. The microchannel structures consist of crosslinked PDMS and the dispersed particles are observed by video microscopy. Flow fields are constructed by means of image correlation techniques and numerical simulations are performed that almost perfectly match the experimental observations.

CPP 50.14 Tue 14:00 P1C

**Photosensitive Surfactants at Hydrophilic and Hydrophobic Surfaces** — ●MAREN UMLANDT, DAVID FELDMANN, and SVETLANA SANTER — University of Potsdam, Potsdam, Germany

Here we report the adsorption kinetics of photosensitive azobenzene containing surfactants on different substrates under illumination with UV and green light. The work is motivated by the newly discovered phenomena of light driven diffusioosmosis (LDDO) where flow is generated at the solid/liquid interface [1]. Colloidal particles trapped at solid/liquid interface move passively within this LDDO flow, and can be arranged in different pattern, removed selectively or gathered on demand. The main ingredient of this process is photosensitive azobenzene containing surfactant which undergoes photo-isomerization reaction from trans- to cis- state with corresponding changes in physical properties such as dipole moment, shape and size. In trans-state the molecule is hydrophobic, while in cis-state hydrophilic. Here we perform analysis of the surfactant adsorption on a hydrophilic and a hydrophobic surfaces using Zeta potential and quartz crystal microbalance (QCM-D) measurements. We analyse the adsorption isotherms in terms of four and five step models. It has been shown that the adsorption of trans- and cis-isomers differs significantly on each type of surfaces.

1. D. Feldmann, S. S. Maduar, N. Lomadze, O. Vinogradova and S. Santer, *Scientific Reports*, 6, 36443 (2016).

CPP 50.15 Tue 14:00 P1C

**Synthesis and characterization of charged and sterically stabilized optically transparent aqueous suspensions** — ●KATHRIN EITEL and HANS-JOACHIM SCHÖPE — Universität Tübingen, Germany

We report the synthesis and characterization of monodisperse, highly charged and sterically stabilized colloidal particles with low index of refraction ( $n=1.38$ ). The core shell particles consist of 1H-1H Heptafluorobutyl-methacrylate (core) and polyethylenecol-methacrylate (shell). We characterize the particles using various methods to determine the particle size and the size polydispersity, the core and shell dimensions, the optical properties, the diffusion coefficients, the effective particle charge and structure formation. The fluorination of the core allows an optical index match using DMSO as a co-solvent. The interparticle interaction potential can in principle be tuned by the content of excess ions and by the addition of free polymer over an extremely wide range. These fluorinated particle core shell particles

are excellently suited as model system to study structure, dynamics and rheology as function of the interaction potential in and out of thermodynamic equilibrium using optical methods.

CPP 50.16 Tue 14:00 P1C

**Adsorption of Magnetic Nanoparticles onto PNIPAM Brushes and Structure of Composite Materials** — ●PHILIPP RITZERT<sup>1</sup>, DIKRAN BOYACIYAN<sup>1</sup>, LUCA SILVI<sup>2</sup>, OLAF SOLFWEDEL<sup>1</sup>, LARISSA BRAUN<sup>1</sup>, and REGINE V. KLITZING<sup>1</sup> — <sup>1</sup>TU Darmstadt, Department of Physics, Hochschulstrasse 8, D-64289 Darmstadt — <sup>2</sup>Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, D-14109, Berlin

End-grafted polymer chains, covalently bound to a substrate are commonly referred to as polymer brushes. In recent decades, great attention was paid to their investigation as thin surface coating, due to their versatile applicability, as well as, high mechanical and chemical stability. The usage of various monomer units enables sensitivity to external stimuli (e.g. temperature, pH value) [1]. Furthermore, polymer brushes can bind different kinds of material with a high selectivity, depending on the available functional groups. Recent studies demonstrate *in-situ* synthesis of magnetic nanoparticles in polymer brushes resulting in sensitivity to external magnetic fields [2].

In this work, the adsorption behaviour of citric acid-capped, magnetic nanoparticles (MNPs) onto Poly(N-isopropylacrylamide) brushes is investigated. Thereby, pH value and MNP concentration during the attachment are varied. Moreover, the structure of the resulting composite materials is investigated by neutron reflectometry.

[1] S. Christau et al. *Macromolecules*, 2017, 50, pp. 7333-7343

[2] W. Choi et al. *Advanced Materials*, 2008, 20, pp. 4504-4508

CPP 50.17 Tue 14:00 P1C

**Unveiling the recombination processes of free carriers in high-efficient organic solar cells by steady-state photoinduced absorption and photocurrent spectroscopy** — ●LE PHUONG<sup>1,2</sup>, SEYED MEHRDAD HOSSEINI<sup>1</sup>, CHANG WOO KOH<sup>3</sup>, HAN YOUNG WOO<sup>3</sup>, and SAFA SHOAEI<sup>1</sup> — <sup>1</sup>Institute of Physics and Astronomy, University of Potsdam, Karl-Liebknecht-Straße 24-25, Potsdam-Golm 14476, Germany — <sup>2</sup>Institute of Materials Science, Vietnam Academy of Science and Technology, 18 Hoang Quoc Viet, Hanoi, Vietnam — <sup>3</sup>Department of Chemistry, College of Science, Korea University, 145 Anam-ro, Seongbuk-gu, Seoul 136-713, Republic of Korea

Coupling steady state photoinduced absorption (PIA) and photocurrent (PC) spectroscopy, we investigate the recombination dynamics of long-lived carriers in high-efficient PPDT2FBT/PC70BM bulk heterojunction (BHJ) solar cells. By comparing the PIA and PC data measured under open-circuit and short-circuit conditions, the absorption cross sections of free carriers can be evaluated. In addition, the excitation-fluence- and modulation-frequency-dependent PIA measurements enable to reveal the recombination mechanism of free carriers in the BHJ solar cells. Our results show that the PIAPC spectroscopy provides an alternative and versatile technique to understand the recombination and extraction processes of free carriers in BHJ solar cells [1].

[1]. L. Q. Phuong et al., *J. Phys. Chem. C* 123, 27417 (2019).

CPP 50.18 Tue 14:00 P1C

**Mechanochemical synthesis and topology transformation in polymorphic Zr-MOF qubit candidates** — ●BAHAR KARADENIZ, KRUNOSLAV UŽAREVIĆ, DIJANA ŽILIC, and SENADA MURATOVIĆ — Division of Physical Chemistry, R. Bošković Institute, Zagreb, Croatia

Among the large family of metal organic frameworks (MOFs), highly stable Zr-based MOFs are one of the most interesting members with various application areas owing to their stability, high porosity, high density of metal centers included in the cluster nodes, and varied types of topologies. Herein we present rapid, clean, high yield mechanochemical synthesis of pure phase cubic MOF-525 and hexagonal PCN-223 polymorphs built on tetrapotic porphyrin linker by liquid-assisted grinding technique.[1] In-situ powder X-ray diffraction monitoring performed at the DESY synchrotron source reveals that particular ball-milling conditions can induce the transformation from cubic to hexagonal phase, denoting MOF-525 to be a kinetic phase in this polymorphic system. Electron spin resonance (ESR) data of these polymorphic MOFs showed significant differences due to the different spatial arrangement and efficient separation of the metal centres (Cu(II), Mn(II) and Fe(III)) in the porphyrin rings, denoting them also as candidates for advanced spintronics applications.

[1] B. Karadeniz, K. Užarević et al. *Journal of American Chemical*

Society (2019).

The authors acknowledge support from the European Social Fund and the Croatian Science Foundation (PZS-2019-02-4129) and the DAAD-MZO bilateral project.

CPP 50.19 Tue 14:00 P1C

**Improved virtual orbitals for charge transfer excitations in time dependent DFT** — ●ROLF WÜRDEMANN<sup>1</sup> and MICHAEL WALTER<sup>2,3</sup> — <sup>1</sup>reiburger Materialforschungszentrum, Freiburg, Germany — <sup>2</sup>Freiburger Zentrum für interaktive Werkstoffe und bioinspirierte Technologien, Freiburg, Germany — <sup>3</sup>Institut für Werkstoffmechanik, Freiburg, Germany

Charge transfer excitations (CTE) are of high importance in photovoltaics, organic electronics and molecular and organic magnetism. Range separated functionals (RSF) can be used to correctly determine the energetics of CTEs within linear response time dependent density functional theory (TDDFT).

TDDFT becomes numerically very demanding on grids if hybrid or RSF are used due to the inclusion of exact exchange derived from Hartree-Fock theory.

We present the implementation of RSF on real space grids and discuss a way to circumvent the problem mentioned above by utilizing Huzinagas improved virtual orbitals (IVOs) that form an improved basis for this type of calculations. The CTE energetics may be even obtained by means of DFT ground-state calculations using IVOs[1].

[1] R. Würdemann, M. Walter, J. Chem. Theory Comput. 2018, 14, 7, 3667-3676

CPP 50.20 Tue 14:00 P1C

**Surfaces of ionic liquid mixtures studied by temperature-dependent ARXPS** — ●ULRIKE PAAP, BETTINA HELLER, FLORIAN MAIER, and HANS-PETER STEINRÜCK — Lehrstuhl für Physikalische Chemie II, FAU Erlangen-Nürnberg, Egerlandstraße 3, 91058 Erlangen, Germany

Ionic liquids (ILs) are characterized by a low melting point, low vapor pressure and low surface tension. Many ILs carrying fluorinated moieties exhibit high gas solubility together with chemical and thermal stability. Such properties are beneficial for a potential substitution of fluorinated organic compounds in many areas such as gas absorbents, refrigerants, lubricants and surfactants.

In this work, we studied various mixed IL systems in the liquid state at different temperatures with angle-resolved X-ray photoelectron spectroscopy (ARXPS). Thereby, we investigated the surface composition of the topmost nanometers of these mixtures. All ILs studied consist of the same hexafluorophosphate anion ( $[\text{PF}_6]^-$ ) and feature a selection of different fluorinated and non-fluorinated imidazolium cations. Our results allow for a deeper understanding of enrichment and molecular orientation processes at the outermost surface of these mixed IL systems.

U.P., B.H., F.M. and H.P.S. thank the European Research Council (ERC) for financial support of this research in the context of an Advanced Investigator Grant to H.P.S. (693398-ILID).

CPP 50.21 Tue 14:00 P1C

**Chasing Aqueous Biphasic Systems from Simple Salts by Exploring the LiTFSI/LiCl/H<sub>2</sub>O Phase Diagram** — ●CHANBUM PARK<sup>1</sup> and JOACHIM DZUBIELLA<sup>1,2</sup> — <sup>1</sup>Research Group for Simulations of Energy Materials, Hahn-Meitner-Platz 1, D-14109, Berlin, Germany — <sup>2</sup>Applied Theoretical Physics-Computational Physics, Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Hermann-Herder-Str. 3, D-79104, Freiburg, Germany

Aqueous biphasic systems (ABSs), in which two aqueous phases with different compositions coexist as separate liquids, were first reported more than a century ago with polymer solutions. Recent observations of ABS forming from concentrated mixtures of inorganic salts and ionic liquids raise the fundamental question of how "different" the components of such mixtures should be for a liquid-liquid phase separation to occur. Here we show that even two monovalent salts sharing a common cation (lithium) but with different anions, namely, LiCl and lithium bis(trifluoromethanesulfonyl)imide (LiTFSI), may result in the formation of ABSs over a wide range of compositions at room temperature. Using a combination of experimental techniques and molecular simulations, we analyze the coexistence diagram and the mechanism driving the phase separation, arising from the different anion sizes.[1] The understanding and control of ABS may provide new avenues for aqueous-based battery systems.

[1] Dubouis, N.; Park, C.; Deschamps, M.; Abdelghani-Idrissi, S.;

Kanduč, M.; Colin, A.; Salanne, M.; Dzubiella, J.; Grimaud, A.; Rotenberg, B. ACS Cent. Sci. 2019, 5, 4, 640-643.

CPP 50.22 Tue 14:00 P1C

**Electrolyte solvents for high voltage lithium ion batteries: ion correlation and specific anion effects in adiponitrile** — ●ANAND NARAYANAN KRISHNAMOORTHY<sup>1,2</sup>, KRISTINA OLDIGES<sup>2</sup>, MARTIN WINTER<sup>2,3</sup>, ANDREAS HEUER<sup>4</sup>, ISIDORA CEKIC-LASKOVIC<sup>2</sup>, CHRISTIAN HOLM<sup>1</sup>, and JENS SMIA TEK<sup>1,2</sup> — <sup>1</sup>Institute for Computational Physics - University of Stuttgart — <sup>2</sup>Helmholtz Institute Muenster — <sup>3</sup>MEET - Battery research Muenster — <sup>4</sup>Institute for Physical Chemistry - University of Muenster

We studied dynamic and structural properties of two lithium conducting salts in the aprotic organic solvent adiponitrile by a combination of atomistic molecular dynamics (MD) simulations, quantum chemical calculations, and experimental findings. The outcomes of our simulations reveal significant differences between both lithium salts, namely lithium tetrafluoroborate (LiBF<sub>4</sub>) and lithium bis(trifluoromethanesulfonyl)imide (LiTFSI) at various concentrations, which can be mainly attributed to the solvation behavior of the individual anions. The increased tendency of ion complex formation for LiBF<sub>4</sub> is reflected by lower values regarding the measured and computed effective ionic conductivities when compared to LiTFSI. All findings highlight the crucial importance of specific anion effects in combination with molecular details of solvation, and advocate the use of adiponitrile as a beneficial solvent in modern lithium ion battery technology with high voltage electrodes.

CPP 50.23 Tue 14:00 P1C

**Experimental Thermodynamics of NiPAM in Water** — ●JAKUB POLAK, DANIEL ONDO, and JAN HEYDA — University of Chemistry and Technology, Prague, Czechia

Unlike for thermoresponsive polymer PNiPAM, the knowledge of thermodynamic properties of aqueous N-isopropylacryl amide (NiPAM) is far from being complete.

In this contribution, the macroscopic thermodynamic properties of aqueous NiPAM are measured and the workflow towards Kirkwood-Buff integrals is presented. Namely, we report the experimental determination of partial molar volumes, osmotic coefficients, and excess partial molar enthalpies of NiPAM in water. These thermodynamic functions are subject to the Kirkwood-Buff inversion procedure. The concentration and temperature dependence of Kirkwood-Buff integrals is discussed and compared to other amides.

CPP 50.24 Tue 14:00 P1C

**Competing chain extension between exchange and irreversible reactions** — ●MICHAEL LANG and FRANK BÖHME — Leibniz-Institut für Polymerforschung Dresden Hohe Straße 6, 01069 Dresden

A co-polycondensation reaction is discussed analytically and by Monte-Carlo simulations where two reactive units compete for reactions with an alternating third reactive unit, whereby irreversible reactions replace bonds which are able to undergo exchange reactions. The resulting number average molar mass,  $M_n$ , exhibits only one distinct peak at the stoichiometric condition of both competitors with the alternating partner. The weight average molar mass,  $M_w$ , reaches an additional second peak at the stoichiometric condition between the dominating competitor and the alternating partner. Both peaks of  $M_w$  surround a range of compositions where a rather high and approximately constant  $M_w$  is obtained. The degree of polymerization of the dominating and alternating reaction partners is rather insensitive towards composition fluctuations if the reaction mixture remains within this composition window. This promotes high molecular weight species and more homogeneous weight distributions at incomplete mixing conditions. An ideal reference case (identical reaction rates for all reactions) is solved analytically to describe these reactions. The position of the stable composition window and the average molar masses inside this window can be tuned by choosing appropriate precursor molecules, reaction mixtures, or post-tuning steps at later times.

CPP 50.25 Tue 14:00 P1C

**Generic hysteresis model for palpation in the elasto-capillary regime** — ●PAUL ZECH, ANDREAS OTTO, MARTIN DEHNERT, and ROBERT MAGERLE — Fakultät für Naturwissenschaften, TU Chemnitz

We develop a multisensory interface that allows humans to perceive

and to explore interactively the mechanical response of soft materials and tissues on the nanometer scale. To this end, we use an atomic force microscope for measuring force–distance curves which inform about the material’s viscoelastic properties as well as its deformation behavior and capillary forces. Humans explore a material in much more variable ways than an instrumented indentation experiment. Therefore, existing models do not describe an arbitrary user–material interaction. We present a generic hysteresis model that predicts the force (output) of a haptic device for a given indentation trajectory (input). The model uses built-in memory in form of a hysteretic play operator and allows the user to perceive dissipative as well as elastic nanomechanical properties equally well.

CPP 50.26 Tue 14:00 P1C

**The physics of the adaptive resolution approach to open systems** — ●ABBAS GHOLAMI, FELIX HÖFLING, RUPERT KLEIN, and LUIGI DELLE SITE — Department of Mathematics and Computer Science, Freie Universität Berlin

The Adaptive Resolution Simulation (AdResS) scheme in its recent formulation couples an open region of interest to a reservoir of non-interacting particles [1]. Building on the statistical mechanics of the grand-canonical ensemble, we relate the chemical potential of the simulated atomistic liquid to the ingredients of the AdResS setup. Numerical tests for Lennard-Jones liquids were carried out to corroborate the formal derivation. The obtained expression differs in structure from that for AdResS with smoothly interpolated forces [2] and permits an interpretation in the framework of stochastic thermodynamics and the Jarzynski equality.

[1] L. Delle Site, C. Krekeler, J. Whittaker, A. Agarwal, R. Klein, and F. Höfling, *Adv. Theory Simul.* **2**, 1900014 (2019).

[2] A. Agarwal, H. Wang, C. Schütte, and L. Delle Site, *J. Chem. Phys.* **141**, 034102 (2014).

CPP 50.27 Tue 14:00 P1C

**Open systems approach to molecular dynamics simulations of liquids out of equilibrium** — ●ROYA EBRAHIMI VIAND, LUIGI DELLE SITE, RUPERT KLEIN, and FELIX HÖFLING — Department of Mathematics and Computer Science, Freie Universität Berlin

We discuss the simulation of Lennard-Jones liquids subject to thermal and/or density gradients. In particular, we employ Adaptive Resolution Simulations (AdResS) in their recent form [1] to realise open boundaries and grand-canonical reservoirs. The model is validated by comparing it with full non-equilibrium simulations of atomistic resolution. The combination of out-of-equilibrium systems with open boundaries prompts for the development of a theoretical framework that treats the boundary conditions in a physically consistent manner. In this perspective, our study represents a numerical implementation of the conceptual approach put forward by Bergman and Lebowitz [2] for such situations.

[1] L. Delle Site *et al.*, *Adv. Theory Simul.* **2**, 1900014 (2019).

[2] P. G. Bergman and J. L. Lebowitz, *Phys. Rev.* **99**, 578 (1955).

CPP 50.28 Tue 14:00 P1C

**Ground- and excited-state properties of tetraphenyl compounds from first-principles calculations** — ●KEVIN EBERHEIM, DUES CHRISTOF, and SANNA SIMONE — Institut für Theoretische Physik and Center for Materials Research, Justus-Liebig-Universität Gießen, 35392 Gießen, Germany

Tetraphenyl compounds with formula  $X(C_6H_5)_4$  ( $X$  being a tetravalent atom of the 14<sup>th</sup> group such as C, Si, Ge, Sn, Pb), crystallize either in a tetragonal crystalline structure or in an amorphous phase [1]. Depending on their habitus, the compounds are characterized by very different optical properties. The molecular crystals are known for their second harmonic generation (SHG) properties, while the amorphous phase is a white light emitter. Tetraphenyl molecules feature indeed the delocalized  $\pi$ -orbitals, which have been proposed as a prerequisite for the white-light generation [2]. In an attempt to understand the mechanisms related to the white light emission, we model the structural, electronic and vibrational properties of different  $X(C_6H_5)_4$  structures within density functional theory. The calculated structural parameters closely reproduce the measured values, however vdW corrections are crucial for a correct description of the structural properties. This confirms that dispersion forces are responsible for the intermolecular bonds in the compound. Different implementations of the vdW forces lead to very similar results. Calculated vibrational properties are in agreement with measured Raman spectra. [1] A Kitaigorodsky, *Molecular Crystals and Molecules*, Acad. Press (1973). [2] Nils W. Rosemann *et*

al., *J. Am. Chem. Soc.* **138**, 16224 (2016), *Science* **352**, 1301 (2016).

CPP 50.29 Tue 14:00 P1C

**Optical properties of adamantane based molecular clusters** — ●CHRISTOF DUES<sup>1,2</sup>, KEVIN EBERHEIM<sup>1,2</sup>, and SIMONE SANNA<sup>1,2</sup> — <sup>1</sup>Institut für Theoretische Physik, Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 16, 35392 Gießen, Germany — <sup>2</sup>Zentrum für Materialforschung (ZfM/LaMa), Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 16, 35392 Gießen, Germany

A new class of molecular materials based on adamantane-type organotetrel chalcogenide clusters has recently attracted the attention of the scientific community due to its outstanding optical properties [1]. Depending on the composition (organic substituents and tetrel atoms in the cluster core), these materials show either white-light generation or strong non-linear response upon IR radiation [2]. In order to determine the prerequisites for white light generation, different related clusters have been synthesized, which possess an additional ligand based on a coinage-metal atom [3]. To explore the optical response, we perform first-principles calculations within the density functional theory. Linear optical properties such as absorption and transmission are calculated based on the electronic structure for both single molecules and molecular crystals. Furthermore, the frequency dependent non-linear optical response is estimated calculating the second harmonic coefficients  $\chi_{SHG}^{(2)}$  and the photoluminescence is modeled by constrained total energy calculations.

[1] N. W. Rosemann *et al.*, *Science* **352**, 1301 (2016).

[2] N. W. Rosemann *et al.*, *J. Am. Chem. Soc.* **138**, 16224 (2016).

[3] E. Dornsiepen *et al.*, *Adv. Optical Mater.* **7**, 1801793 (2019).

CPP 50.30 Tue 14:00 P1C

**Noise-induced symmetry breaking of self-regulators: An asymmetric phase transition towards homochirality** — ●RAFNA RAFEEK<sup>1</sup> and DEBASISH MONDAL<sup>2</sup> — <sup>1</sup>Department of Chemistry, Indian Institute of Science Education And Research Tirupati, Tirupati, India 517507 — <sup>2</sup>Department of Chemistry, Indian Institute of Technology Tirupati, Tirupati, India 517506

Studies on the origin of spontaneous chiral symmetry breaking have become a ‘Holy Grail’ in recent research developments related to the origin of life. The paradigm of Frank (1953) and its subsequent variants indicate that a self-regulatory process may result in such single handedness in different reaction conditions. We consider a collection of Brownian particles, which can stay in any of the three possible isomeric states: one achiral and two enantiomers. Isomers are undergoing self-regulatory reaction along with chiral inhibition and achiral decay processes. The time evolution of the isomeric states is guided by those of its neighbors as well as the temperature of the system. We find that the relative dominance of self-regulation, chiral inhibition and achiral decay processes results in asymmetric transition between four different population phases, namely three-isomer coexistence, enantiomeric coexistence, chiral-achiral coexistence and homochiral phase. We also report that a fast stochastic self-regulation and an optimally slow chiral inhibition reaction along with a threshold population of interacting neighbors suffice the requisite for transition towards a completely symmetry broken state i.e., homochirality.

CPP 50.31 Tue 14:00 P1C

**The Removal of NPs After Accident - How to Avoid Skin Penetration?** — ●JONAS SCHUBERT<sup>1,2</sup> and MAX SCHNEFF<sup>1,2</sup> — <sup>1</sup>Functional Colloidal Materials, Leibniz Institute of Polymer Research Dresden, 01069 Dresden, Germany — <sup>2</sup>Physical Chemistry of Polymer Materials, Technische Universität Dresden, D-01062 Dresden, Germany

In this contribution we present a novel gel that is able to remove NPs from the skin. This is getting more and more important as NPs are frequently used in research as well as in industry. After skin contact some of the NPs are able to penetrate the skin and are then potentially harmful for the human health.[1] Normal soap is insufficient for the removal of NPs. Compared to that, our gel removes the majority of the NPs from the skin.

[1] Nafisi, S.; Maibach, H. I., Chapter 3 - Skin penetration of nanoparticles. In *Emerging Nanotechnologies in Immunology*, Shegokar, R.; Souto, E. B., Eds. Elsevier: Boston, 2018; pp 47-88.

CPP 50.32 Tue 14:00 P1C

**CdZnSe/ZnS quantum dots - gold nanoparticle nanostructured complexes and the influence of the ligand length on their optical properties** — ●TATIANA KORMILINA<sup>1,3</sup>, IRINA

AREFINA<sup>1</sup>, EVGENIYA STEPANIDENKO<sup>1</sup>, DANIL KURSHANOV<sup>1</sup>, ALIAKSEI DUBAVIK<sup>1</sup>, and ELENA USHAKOVA<sup>1,2</sup> — <sup>1</sup>Center of Information Optical Technologies, ITMO University, Saint Petersburg, Russia — <sup>2</sup>Department of Materials Science and Engineering, City University of Hong Kong, Hong Kong SAR, PR China — <sup>3</sup>Friedrich-Alexander Universität Erlangen-Nürnberg, Erlangen, Germany

Hybrid systems formed from semiconductor nanocrystals and noble metal nanoparticles are widely utilized in development of multicomponent materials for the photonic applications, biological imaging, and solar cell technologies, where these materials can be used as colloidal solutions or solid thin films. Of great importance are not only the nanomaterials themselves, but also the nanostructure of their linkage. In this work we show how optical properties of a semiconductor quantum dot - noble metal nanoparticle complex can depend on the chain length of the binding molecule. We developed a formation procedure for the colloidal complexes based on alloyed CdZnSe/ZnS quantum dots and gold nanoparticles where various mercaptocarboxylic acids are used as the binding molecules. The QD photoluminescence enhancement (up to 3.1) can be achieved by the control of the interparticle distance in colloidal solutions. The influence of the linking molecules on the optical parameters of the nanoparticle complexes is analyzed and compared through the steady-state and time-resolved spectral measurements.

CPP 50.33 Tue 14:00 P1C

**Fluorescence Quenching of Copper Indium Sulfide/Zinc sulfide Quantum Dot-Dye Assembly** — ●ABEY ISSAC<sup>1</sup>, SUMESH SOFIN R.G<sup>1</sup>, and OSAMA K. ABOU-ZIED<sup>2</sup> — <sup>1</sup>Department of Physics, College of Science, Sultan Qaboos University, Muscat 123, OMAN — <sup>2</sup>Department of Chemistry, College of Science, Sultan Qaboos University, Muscat 123, OMAN

Deep understanding of electronic transitions in semiconductor quantum dots (QDs) are crucial for the realization of QD-based applications. Though enormous works have been reported on cadmium based QDs such as CdSe or CdS at ensemble and single particle level, current research interest is devoted to cadmium free QDs due to the carcinogenic activity of cadmium. In this work, we study the fluorescence quenching of Copper Indium Sulfide/Zinc sulfide core/shell QDs (CIS/ZnS) in QD-dye complexes. Time resolved spectroscopy techniques such as fluorescence decay (ns) and fluorescence up conversion (sub ps) are employed in this work. Different quenching pathways are identified in this QD-Dye assembly.

CPP 50.34 Tue 14:00 P1C

**Stress components in adhesive joints of micromechanical structures** — ●RIKA UNKELBACH<sup>1,2</sup>, JAN KUYPERS<sup>1</sup>, and CHRISTINE PAPADAKIS<sup>2</sup> — <sup>1</sup>Blickfeld GmbH, 80339 München, Germany — <sup>2</sup>TU München, Physik-Department, Physik weicher Materie, 85748 Garching, Germany

The use of adhesives as a joining technique in structural applications is widespread and on the rise. For simple geometries such as lap shear joints, stress components can be analytically predicted and are well understood. However, the stress distribution for unusual joints or loading conditions is more complex and requires a more detailed analysis.

We present an approach to identify the stress components that eventually will lead to a failure of the joint in a specific micromechanical structure under torsional loading that has motivated this research. The influence of peeling and shear stress components in regards to the joint stability is discussed based on experimental data and results obtained from finite element analysis (FEA).

CPP 50.35 Tue 14:00 P1C

**Insights in Structure and Dynamics of PEO-LiTFSI Electrolytes near Graphene Electrodes from Molecular Dynamics Simulations** — ●ANDREAS THUM<sup>1</sup>, DIDDO DIDDENS<sup>2</sup>, and ANDREAS HEUER<sup>1</sup> — <sup>1</sup>Institut für Physikalische Chemie, Westfälische Wilhelms-Universität Münster, Corrensstraße 28/30, 48149 Münster, Germany — <sup>2</sup>Helmholtz-Institut Münster (IEK-12), Forschungszentrum Jülich GmbH, Corrensstraße 46, 48149 Münster, Germany

All-solid-state lithium-ion batteries gain increasing attention as potentially safe and cheap second generation batteries. Polymer electrolytes are – besides other materials like inorganic ceramics – a promising replacement for the currently used flammable liquid organic electrolytes. However, the electrode-electrolyte interphase (EEL) of polymer electrolytes is even more complex than that of liquid electrolytes. Since the EEL is considered to affect the cycling performance and cell safety seriously, it is crucial to get a better understanding of its formation

process, its structure and the lithium ion transport therein. Here we present atomistic molecular dynamics simulations of poly(ethylene oxide) (PEO) doped with lithium bis(trifluoromethanesulfonyl)imide (LiTFSI) near charged and uncharged graphene electrodes. We explore the structure and dynamics of the polymer electrolyte which are governed by anisotropic effects and strong local electric fields in the vicinity of the electrodes.

CPP 50.36 Tue 14:00 P1C

**Tunable-slip boundary for the soft coarse-grained model of polymer fluid** — ●PRITAM KUMAR JANA, LUDWIG SCHNEIDER, VERONICA CHAPPA, and MARCUS MÜLLER — Institut für Theoretische Physik, Universität Göttingen, Germany

The rheological properties of composites derived from fillers in a polymer matrix depend on particle size, filler loading, and dispersion, as well as the interfacial interaction between the fillers and polymer matrix. For the coarse-grained modeling of such systems, it is crucial to pay attention to the fluid flows past the solid filler surface because classical no-slip hydrodynamic boundary condition does not hold on the micro- and nanoscopic length scale. Instead, the flow is characterized by a microscopically small but finite slip length. To tailor the hydrodynamic boundary condition, we have implemented a strategy by forming dynamic bonds between the solid filler surface and polymer beads, using a grand-canonical Monte Carlo approach. Polymers are modeled as highly coarse-grained segments with soft potentials, including reduced extensibility for strong elongations. Entanglements between polymers are represented by slip-springs [1]. We perform molecular dynamics simulations in conjunction with a dissipative particle dynamics (DPD) thermostat. We successfully demonstrate that the equilibrium properties, e.g., density profile close to the wall, are independent of the number of dynamic bonds and explore the relation between the density of dynamic bonds and hydrodynamic boundary condition.

References 1. Chappa et al., Physical Review Letters 109 148302 (2012)

CPP 50.37 Tue 14:00 P1C

**Microrheology of Newtonian fluid** — ●PANKAJ PANDEY<sup>1</sup>, PATRICK GALENSCHOWSKI<sup>2</sup>, CHRISTIAN WAGNER<sup>3</sup>, and THOMAS JOHN<sup>4</sup> — <sup>1</sup>Saarland University Campus, building E2 6 Saarbrücken Germany — <sup>2</sup>Saarland University Campus, building E2 6 Saarbrücken Germany — <sup>3</sup>Saarland University Campus, building E2 6 Saarbrücken Germany — <sup>4</sup>Saarland University Campus, building E2 6 Saarbrücken Germany

We have studied polystyrene particle in Newtonian (deionized water and Sucrose solution) fluid by dark field microscopy (DFM). Trajectory of the particle is analyzed in terms of the mean squared displacement (MSD). We have recorded very long trajectories comprising 10000 number of frames with 10 frames per second at room temperature. This enabled a statistical analysis of the resulting MSD curves as a function of the time. We find that the relative error of the diffusion coefficient can be minimized by taking long trajectory lengths into account by fitting the time dependent MSD curves with power law. Finally, we found these results are very good qualitative and quantitative agreement between experiment and theory.

CPP 50.38 Tue 14:00 P1C

**Polymer adsorption in a micro channel** — ●TOBIAS A. KAMP-MANN, BJÖRN LINDHAUER, and JAN KIERFELD — TU Dortmund University, Germany

Two entangled semiflexible polymers such as actin or DNA filaments confined to a channel exhibit at least three distinct scaling regimes of entropic repulsion. If the persistence length  $L_p$  exceeds the channel width  $d$  the entropic repulsion is  $\sim L_p^{-1/3}$  and governed by deflections from the channel walls. If the polymer is more flexible such that the persistence length is smaller than the channel width, the entropic repulsion is governed by polymer blobs forming in confinement and scales  $\sim L_p^{-1}$ . In the presence of attractive interactions we find a single transition into a bundled phase upon increasing the potential strength. An intermediate entangled phase, where polymers are drawn into parallel alignment without bundling is absent. We conclude that parallel alignment and bundling of two confined polymers happen in a single transition. The results shed light on the self-assembly process of filament bundles in confinement.

CPP 50.39 Tue 14:00 P1C

**Rheology of Oligo- and Polymers in Oxidic Nanoporous Ma-**

**terials: Gravimetric and Optofluidic Experiments** — ●GUIDO DITTRICH and PATRICK HUBER — Institute of Materials Physics and Technology, Hamburg University of Technology (TUHH), Eißendorfer Str. 42, D-21073 Hamburg-Harburg, Germany

The rheology in nanometer sized pores is a research field with many open questions especially for complex molecules. Oxidic nanoporous materials offer a stiff scaffold with high specific surface area and confining geometries. Therefore, surface tension and capillarity are dominant and affect along with interface interactions and pure spatial restrictions the flow properties. From a scientific point of view oligo- and polymers add to the complexity by a rheology that depends on the chain length and chemistry. We investigate the transport dynamics of styrene-based oligo- and polymer melts in anodic aluminum oxide (AAO) and compare them with those in controlled porous glasses (CPG). These materials exhibit a cylindrical, hexagonally arranged and a sponge-like pore morphology, respectively. Due to the different morphologies AAO is investigated with an opto-interferometric [1] and CPG with a gravimetric technique [2].

[1] Cencha, Luisa G., et al.: "Nondestructive high-throughput screening of nanopore geometry in porous membranes by imbibition." *Applied Physics Letters* 115 (2019) 113701.

[2] Gruener, Simon, and Patrick Huber: "Imbibition in mesoporous silica: rheological concepts and experiments on water and a liquid crystal." *Journal of Physics: Condensed Matter* 23 (2011) 184109.

CPP 50.40 Tue 14:00 P1C

**Low-resolution NMR investigations of polymer immobilization in nanocomposites** — ●MOZHDEH ABBASI<sup>1</sup>, SOL MI OH<sup>2</sup>, ALEXANDER ECKERT<sup>3</sup>, SO YOUN KIM<sup>2</sup>, ANDREAS WALTHER<sup>3</sup>, and KAY SAALWÄCHTER<sup>1</sup> — <sup>1</sup>Inst. f. Physik - NMR, Martin-Luther-Univ. Halle-Wittenberg, Halle (Saale), Germany — <sup>2</sup>School of Energy and Chemical Engineering, UNIST, Ulsan, Republic of Korea — <sup>3</sup>Inst.f. Makromolekulare Chemie, Albert-Ludwigs-Univ. Freiburg, Germany

We used low-resolution <sup>1</sup>H NMR spectroscopy to study the molecular dynamics of poly (ethylene oxide), mixed with spherical silica nanoparticles [1] as well as self-assembled clay sheets (NHT) forming nacre-mimetics [2] as model materials. The decomposition of time-domain signals (FIDs) reveals three different phases of PEO with different dynamics, based on different transverse relaxation behavior [3] which are related to the strength of the dipolar coupling between proton spin pairs. Therefore, fast initial decay on the time scale of microseconds corresponds to a rigid phase with strong dipolar couplings, attributed to the intercalated part of PEO within the clay sheets or adsorbed chains on the silica surface. The intermediate phase with residual dipolar couplings and a mobile phase with faster segmental motions and a rather long T<sub>2</sub> corresponds to free polymer chains. This study addresses the different molecular dynamics of PEO chains subject to different constraints in the two different nanocomposite structures. [1] S. Y. Kim et. al., *Macromolecules* 2012, 45, 4225. [2] P. Das et al., *Nat. Commun.* 2015, 6, 1. [3] K. Schäler et. al., *Macromolecules* 2013, 46, 7818.

CPP 50.41 Tue 14:00 P1C

**Isodesmic or cooperative? The self-assembly scenario of azobenzene stars unraveled in computer simulations** — ●VLADYSLAV SAVCHENKO<sup>1</sup>, MARKUS KOCH<sup>1</sup>, ALEKSANDER S. PAVLOV<sup>2</sup>, MARINA SAPHIANNIKOVA<sup>1</sup>, and OLGA GUSKOVA<sup>1</sup> — <sup>1</sup>IPF Dresden — <sup>2</sup>Department of Physical Chemistry, Faculty of Chemistry and Technology, Tver State University, Tver, Russia

Employing a number of computer simulation techniques, we quantify the intermolecular interactions between three-armed azobenzene stars with benzene-1,3,5-tricarboxamide core [1]. Our results suggest that during the formation of ordered phases [2, 3], these molecules prefer to build columns in which stars are held together via weak interactions whose strength grows with increasing the size of the aggregate. This phenomenon called cooperative self-assembly is proven for azobenzene stars in aqueous solution by calculating the binding energies, hydrogen bond lengths and macrodipoles. The simulations clearly attribute the cooperativity of the self-assembly to the development of a macrodipole, in other words, to the redistribution of the electronic density along the column. This, in turn, enhances the strength of the hydrogen bonds, and subsequently the intermolecular coupling in the stacks [4].

This work is funded by the DFG projects GU1510/3-1 and GU1510/5-1.

[1] M. Koch, et al. *J. Phys. Chem. B* 2017, 121, 8854. [2] S. Lee, et al. *Langmuir* 2013, 29, 5869. [3] M. Koch, et al. *Langmuir* 2019, 35, 14659. [4] V. Savchenko, et al. *Molecules* 2019, 24, 4387.

CPP 50.42 Tue 14:00 P1C

**Do Columns of Azobenzene Stars Disassemble under Light Illumination?** — MARKUS KOCH, MARINA SAPHIANNIKOVA, and ●OLGA GUSKOVA — Leibniz Institute of Polymer Research Dresden

The clustering properties of star-shaped molecules comprising three photochromic azobenzene-containing arms [1] are investigated with a specific focus on the influence of light on these structures. Previous experimental works report the self-assembly of azobenzene stars in aqueous solution into long columnar clusters that are detectable using optical microscopy. These clusters appear to vanish under UV irradiation, which is known to induce trans-to-cis photoisomerization of the azobenzene groups. We have performed MD simulations, density functional theory and density functional tight-binding calculations to determine conformational properties and binding energies of these clusters [2, 3]. Our simulation data suggest that the binding strength of the clusters is large enough to prevent a breaking along their main axis. We conclude that very likely other mechanisms lead to the apparent disappearance of the clusters.

This research was funded by the German Research Foundation (DFG), grant numbers GU1510/3-1, SA1657/13-1 and GU1510/5-1.

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

[2] M. Koch et al. *Langmuir*, 2019, 35, 14659.

[3] V. Savchenko et al. *Molecules*, 2019, 24, 4387.

CPP 50.43 Tue 14:00 P1C

**Spiropyran Sulfonates for Photo and pH Responsive Air-Water Interfaces and Aqueous Foam** — ●MARCO SCHNURBUS<sup>1</sup>, MALGORZATA KABAT<sup>2</sup>, EWELINA JAREK<sup>2</sup>, MARCEL KRZAN<sup>2</sup>, PIOTR WARSZYNSKI<sup>2</sup>, and BJÖRN BRAUNSCHWEIG<sup>1</sup> — <sup>1</sup>Institute of Physical Chemistry, WWU Münster — <sup>2</sup>IKiFP PAN, Krakow

The photochromic reaction of a spiropyran sulfonate surfactant was used to render interfacial and foaming properties active to light stimuli. We have applied sum-frequency generation (SFG) spectroscopy which has provided information on the surface excess and the interfacial charging state as a function of light irradiation and solution pH. Under blue light irradiation, the surfactant forms a closed ring, spiro form (SP), whereas under dark conditions the ring opens and the merocyanine (MC) form is generated. The MC surfactants O-H group can be deprotonated as a function of pH, which is used to tune the molecules net charge at the interface. SFG spectroscopy shows that with increasing pH the intensity of O-H stretching band from interfacial water molecules increases, which we associate to an increase in surface net charge. At a pH of 5.3, irradiation with blue light leads to a reversible decrease of O-H intensities, whereas the C-H intensities were unchanged compared to the corresponding intensities under dark conditions. Measurements of the foam stabilities showed a higher foam stability under dark light conditions. At pH 2.7 this behavior is reversed as far as the surface tension and charging as well as the foam stability are concerned. The light-triggered changes at both pH values can be used to control foams and interfaces on a molecular level.

CPP 50.44 Tue 14:00 P1C

**Cononsolvency-induced collapse transitions in thin PMMA-b-PNIPAM and PMMA-b-PNIPMAM films** — ●JULIJA REITENBACH<sup>1</sup>, CHRISTINA GEIGER<sup>1</sup>, CRISTIANE HENSCHER<sup>2</sup>, ANDRÉ LASCHEWSKY<sup>2</sup>, CHRISTINE M. PAPADAKIS<sup>3</sup>, and PETER MÜLLER-BUSCHBAUM<sup>1</sup> — <sup>1</sup>TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — <sup>2</sup>Fraunhofer-Institut für Angewandte Polymerforschung, 14476 Potsdam-Golm, Germany — <sup>3</sup>TU München, Physik-Department, Physik weicher Materie, 85748 Garching

Thin films of the thermoresponsive diblock copolymers PMMA-b-PNIPAM and PMMA-b-PNIPMAM both exhibit cononsolvency-induced collapse transitions when organic cosolvents are introduced into the surrounding atmosphere. The chemical structures of NIPAM (N-isopropylacrylamide) and NIPMAM (N-isopropylmethacrylamide) differ by a methyl functional group, which is able to influence the film collapse kinetics on a macroscopic scale. We reveal the solvent/cosolvent exchange taking place at the polymer functional groups with FTIR and attribute key changes in the local chemical environment to the macroscopic film collapse stages.

CPP 50.45 Tue 14:00 P1C

**Mussel-inspired pNIPAM-microgels with adhesive potential** — ●SANDRA FORG<sup>1</sup>, XUHONG GUO<sup>2</sup>, and REGINE VON KLITZING<sup>1</sup> — <sup>1</sup>Technische Universität Darmstadt, Institut für Festkörperphysik, Darmstadt, Germany — <sup>2</sup>ECUST, School of Chemical Engineering,

Shanghai, China

The temperature-sensitivity of pNIPAM based hydrogels provides a huge potential for biologically motivated applications due to their phase transition close to the temperature of the human body (32°C). Combining this responsiveness with adhesive attributes would be of use for tissue engineering or medical purposes. Therefore hydrogels inspired by living marine organisms such as mussels have recently become highly attractive. Mussels can strongly adhere to other substrates even under harsh under water conditions, which is mainly determined by the protein 3,4-dihydroxyphenyl-L-alanine (DOPA). This DOPA-group can be incorporated into the hydrogel structure by the addition of a polymerizable group. However, most of these hydrogels are mechanically weak and / or possess a low elastic modulus, which remarkably limits their use in vivo environments.

In this work, pNIPAM microgels are synthesized by free-radical precipitation polymerization. They are modified with DOPA to obtain adhesive properties. To get a closer insight into the polymerization process, time samples are taken during the synthesis. The monomer concentration of those time samples is analysed with mass spectrometry. By this knowledge, future synthesis can be controlled. The properties of these microgels are studied by DLS and Zetasizer measurements.

CPP 50.46 Tue 14:00 P1C

**The thermoresponsive diblock copolymer PMMA-b-PNIPAM in aqueous solution: Influence of copolymer composition on micelle formation** — ●NADIR AZIZ<sup>1</sup>, CHIA-HSIN KO<sup>1</sup>, CRISTIANE HENSCHL<sup>2</sup>, PETER MÜLLER-BUSCHBAUM<sup>1</sup>, ANDRÉ LASCHEWSKY<sup>2,3</sup>, and CHRISTINE M. PAPADAKIS<sup>1</sup> — <sup>1</sup>Physics Department, Technical University of Munich, Garching, Germany — <sup>2</sup>Institut für Chemie, University of Potsdam, Potsdam-Golm, Germany — <sup>3</sup>Fraunhofer Institute for Applied Polymer Research IAP, Potsdam-Golm, Germany

Amphiphilic diblock copolymers having a hydrophobic poly(methyl methacrylate) (PMMA) block and a thermoresponsive poly(N-isopropylacrylamide) (PNIPAM) block form core-shell micelles in aqueous solution. The PNIPAM shell collapses at the cloud point of this block, and the micelles form large aggregates. We investigate the role of the block copolymer composition on the critical micellization concentration, the micellar size and shape as well as the collapse behavior at the cloud point. At this, we use fluorescence correlation spectroscopy and dynamic light scattering.

CPP 50.47 Tue 14:00 P1C

**Minority Chains with Wall-Adsorbing End Groups Admixed to Polymer Brushes** — ●MARKUS KOCH<sup>1</sup>, DIRK ROMEIS<sup>1</sup>, and JENS-UWE SOMMER<sup>1,2</sup> — <sup>1</sup>Institute Theory of Polymers, IPF Dresden, Germany — <sup>2</sup>Institute Theory of Physics, TU Dresden, Germany

Polymer brushes are one of the most promising systems for the creation of surfaces with stimulus-responsive properties. It is highly desirable for applications to expose or hide specific chemical groups within the brush depending on changing system conditions. To this end, we investigate monodisperse polymer brushes, to which a small fraction of end-modified minority chains is admixed. The minority chains can be of a different length as compared to the brush chains and their terminal groups adsorb to the grafting surface at sufficient attraction energies. We study these systems combining Scheutjens-Fleer self-consistent field calculations [1], MD simulations and analytical theory. Firstly, the conformational changes of the admixed chains are explored, which depend on minority chain lengths as well as the attractivity between their end groups and the grafting wall. Furthermore, we analyze the free energy profiles of the end-group adsorption, from which transition energies are obtained. Lastly, we demonstrate that the adsorption barriers are predicted reasonably well by our theoretical approach and that they are strongly reduced under poor solvent conditions.

[1] Fleer, G. J., Cohen Stuart, M. A., Scheutjens, J. M., Cosgrove, T., Vincent, B., *Polymers at Interfaces*. London, Chapman and Hall, 1993.

CPP 50.48 Tue 14:00 P1C

**Drying of shallow sessile droplets** — ●SWATI KAUSHIK, STEFAN KARPITSCHKA, and OLIVER BÄUMCHEN — Max Planck Institute for Dynamics and Self-Organization (MPIDS), Am Fassberg 17, 37077 Göttingen, Germany

The evaporation of sessile droplets on solid surfaces is an everyday phenomenon. The quantitative description of the evaporation dynamics is not only of interest from a fundamental perspective, but also highly

relevant for practical applications such as coating technologies and inkjet printing. Here, we investigate the evaporation dynamics of shallow sessile droplets of pure n-Tetradecane on functionalized Si-wafers. We use an optical interference microscopy technique to construct the droplet profile over the course of drying process along with the dynamic measurement of the contact angle  $\theta$ . The contact radius and droplet volume are also quantified taking into account the spherical cap approximation. This technique allows for measuring contact angles with a precision of 0.1°. The droplet dynamics are studied for different substrate temperatures and surface functionalization during the early stages of evaporation where the drop stays pinned to the substrate. We find a good agreement of the experimental results with theoretical models for diffusion-based evaporation. In addition, it is found that the depinning time varies with the initial contact angle and substrate temperature. We also report an interesting linear dependency of the rate at which the contact angle changes,  $d\theta/dt$ , on the inverse of the initial contact area in the limit of small contact angles.

CPP 50.49 Tue 14:00 P1C

**Photo-Switchable Arylazopyrazole Phosphonic Acid SAMs on Al<sub>2</sub>O<sub>3</sub>** — ●CHRISTIAN HONNIGFORT and BJÖRN BRAUNSCHEWIG — Institute of Physical Chemistry and Center for Soft Nanoscience SoN, University of Münster, Germany

The great interest in smart surfaces that can change their wetting behaviour on demand arises from their potential applications for self-cleaning surfaces, tunable lenses or microfluidics. Using light as a stimulus to change the wetting behaviour allows the spatio-temporal confinement of the external stimulus. One way to exploit this is the decoration of surfaces with photo-responsive SAMs, e.g. phosphonic acids on Al<sub>2</sub>O<sub>3</sub> surfaces. Here we used arylazopyrazole-functionalized phosphonic acids to induce the formation of photoresponsive SAMs on Al<sub>2</sub>O<sub>3</sub>. We show that the wetting behaviour can be changed reversibly with  $\Delta\Theta = 8^\circ$ . The quantitative description of these wetting dynamics is still challenging. While contact angle measurements can quantify the changes in the macroscopic wetting behaviour the application of inherently interface specific sum-frequency generation spectroscopy can provide information on the wetting dynamics on a molecular level for instance by observing C-H and O-H stretching vibrations under different light irradiations. It allows to quantify the degree of ordering within the monolayer and to gain information on the interfacial water structure.

CPP 50.50 Tue 14:00 P1C

**Simple model for drops on elastic substrates** — ●CHRISTOPHER HENKEL<sup>1</sup>, JOHANNES KEMPER<sup>1</sup>, JACCO SNOEIJER<sup>2</sup>, and UWE THIELE<sup>1</sup> — <sup>1</sup>Institut für Theoretische Physik, Münster, Germany — <sup>2</sup>Fac. of Science and Technology, Twente, Netherlands

The investigation of the wetting behaviour on viscoelastic or elastic substrates is of great interest. We present a simple model for steady liquid drops on fully compressible elastic substrates, and show that a double transition appears under variation of the substrate softness, similar to the one described in [1]. We further investigate how the transition depends on wettability and how it is amended by the Shuttleworth effect, i.e., the dependency of the interfacial tensions on local strain. Finally, we employ a gradient dynamics model in the long-wave limit and show first results of direct time simulations.

[1] Lubbers, L. A., Wejjs, J. H., Botto, L., Das, S., Andreotti, B., and Snoeijer, J. H. (2014). Drops on soft solids: free energy and double transition of contact angles. *Journal of fluid mechanics*, 747.

CPP 50.51 Tue 14:00 P1C

**Characterization of nano-particles with regard to hydrophobicity, size and emulsion-stabilizing capabilities** — ●KAI LUCA SPANHEIMER<sup>1</sup>, SEBASTIAN STOCK<sup>1</sup>, ANNIKA SCHLANDER<sup>2</sup>, MARCUS GALLET<sup>2</sup>, and REGINE VON KLITZING<sup>1</sup> — <sup>1</sup>TU Darmstadt, Condensed Matter Physics — <sup>2</sup>TU Darmstadt, Makromolekulare Chemie

For particle stabilized foams and emulsions the hydrophobicity of the used particles is an important parameter. For instance in case of Pickering emulsions (PE) the main effect of the particle hydrophobicity is the emulsion type (oil in water or water in oil). In an attempt to find a procedure determining the hydrophobicity of colloidal particles different types of silica-spheres were modified to achieve specific surface properties. Using silanization differently charged and hydrophobic groups were bound the surface. Contact angle measurements via sessile-drop are used to determine the surface energy of water on the coated wafer, which is a measure for the hydrophobicity of the surface. In the wetting case the contact angle depends on the roughness of the



surface. Therefore, atomic-force-microscopy studies of the particle-layer were performed to determine the roughness and to ensure the comparability. It could be shown that the resulting emulsion type for prepared Pickering emulsions corresponds to the prediction (Bancroft rule) based on the measured particle-hydrophobicity.

CPP 50.52 Tue 14:00 P1C

**Properties of droplets on (prestructured) switchable surfaces**  
— •LEON TOPP and ANDREAS HEUER — Westfälische Wilhelms-Universität, Institut für Physikalische Chemie, 48149 Münster, Germany

It is possible to switch the wettability of surfaces which consist for ex-

ample of azobenzenes by external stimuli like light of a defined wavelength. When a droplet is placed on such a substrate and it is switched this leads to a relaxation of the droplet to the new surface properties and as a consequence to a change of the contact angle and shape.

To investigate this process theoretically we performed Molecular Dynamic Simulations of droplets placed on a fcc lattice consisting of Lennard-Jones particles. By changing the interaction strength between the liquid particles and the surface we can control the wetting properties and have the possibility to switch them. Thus, we considered different switching frequencies and study how the contact angle and the shape of the droplet evolves. Also we prestructured the surface and examine the influence of switching on droplets placed on such substrates.