

CPP 17: Poster 2

Topics: 2D Materials (17.1-17.3), Composites and Functional Polymer Hybrids (17.4-17.6), Crystallization, Nucleation and Self-Assembly (17.7-17.12), General Session to the Symposium: Interplay of Substrate Adaptivity and Wetting Dynamics from Soft Matter to Biology (17.13-17.15), Hydrogels and Microgels (17.16-17.21), Interfaces and Thin Films (17.22-17.31), Nanostructures, Nanostructuring and Nanosized Soft Matter (17.32-17.35), Polymer and Molecular Dynamics, Friction and Rheology (17.36-17.38), Polymer Networks and Elastomers (17.39-17.41).

Time: Tuesday 11:00–13:00

Location: P2

CPP 17.1 Tue 11:00 P2

Simulation of vapour flow through aperture arrays for quantifying gravimetric mass loss measurements — ●RIKO KORZETZ, LENNART SCHULTE, and ANDRÉ BEYER — Bielefeld University

Gravimetric mass loss measurements are frequently employed to investigate the permeative behaviour of 2D membranes with respect to vapours of different solvents. Due to constraints in these measurements, insufficient circulation causes the build-up of concentration gradients in the vapour phase, which is known as concentration polarization. This leads to a seemingly non-intuitive permeation behaviour, which complicates the evaluation of the measured data.

Here, we present finite-element simulations that were employed to investigate this effect with respect to different types of membrane supporting apertures and aperture arrays. Both open orifices as well as membranes with different permeance values have been modelled to achieve a quantitative understanding of the relevant effects in mass loss measurements.

We found that for open orifices and apertures with highly permeable membranes, the diffusion from the bulk towards the membrane is the rate-limiting step. This results, for example, in a linear dependence between the permeation rate and the edge length of single open orifices. On the other hand, a dependence on the free-standing area occurs in the case of membranes with a sufficiently low permeance. We devised a phenomenological model to describe the permeation rate in dependence of the membrane permeance as well as support geometry, which allows correction of these effects when evaluating such measured data.

CPP 17.2 Tue 11:00 P2

Preparation and characterization of photosensitive nanomembranes — ●VERENA MÜLLER¹, MARIA KÜLLMER¹, FLORIAN KÜLLMER^{1,2}, HANS-DIETER ARNDT², and ANDREY TURCHANIN¹ — ¹Friedrich Schiller University Jena, Institute of Physical Chemistry, Lessingstraße 10, 07743 Jena, Germany — ²Friedrich Schiller University Jena, Institute of Organic Chemistry and Macromolecular Chemistry, Humboldtstraße 10, 07743 Jena

Carbon nanomembranes (CNMs) are two-dimensional (2D) organic materials with a molecular thickness that are synthesized by low-energy electron irradiation of aromatic self-assembled monolayers (SAMs). Using the molecular design, CNMs can be prepared with tunable physical and chemical properties and employed on their own, e.g. as separation membranes or in combination with other 2D materials in hierarchically assembled van-der-Waals heterostructures. Here we present the engineering of photosensitive nanomembranes *via* post-functionalization of ~ 1 nm thick amino-terminated CNMs with azobenzene molecules. We characterize their properties using surface science techniques including X-ray photoelectron spectroscopy (XPS) and compare the obtained characteristics with the azobenzene-based SAMs.

CPP 17.3 Tue 11:00 P2

Selective Diffusion of CO₂ and H₂O through Carbon Nanomembranes in Aqueous Solution as Studied with Radioactive Tracers — RAPHAEL DALPKE¹, ANNA DREYER², RIKO KORZETZ¹, ●LENNART SCHULTE¹, ANDRÉ BEYER¹, and KARL JOSEF DIEZ² — ¹Faculty of Physics, Bielefeld University — ²Faculty of Biology, Bielefeld University

A well-known approach of improving membrane separation processes is the attempt to utilize 2D materials. In particular, carbon nanomembranes (CNMs) are promising candidates due to their extremely high areal pore density. Specifically, CNMs made from terphenylthiol (TPT) exhibit a very high water permeance while blocking ions as well as many gases and vapours. Here, we present permeation measurements of TPT-CNMs utilizing radioactive tracer molecules to charac-

terize diffusion of [³H]H₂O, [¹⁴C]NaHCO₃, and [³²P]H₃PO₄ in aqueous solution. For full consideration of concentration polarization and outgassing effects a mathematical model was developed and verified using finite-element simulations. The experiment shows that water and carbonate can pass through the CNM while phosphate ions are completely blocked. Considering ion conductivity measurements, the obtained diffusion coefficients indicate that the permeation across the membrane primarily occurs by transport of neutral species.

CPP 17.4 Tue 11:00 P2

Dipolar Molecular Rotors in Surface-Anchored Metal Organic Frameworks — ●XIANGHUI ZHANG¹, SEBASTIAN HAMER², RITESH HALDAR³, DANIEL REUTER⁴, FLORIAN PANEFF¹, DIRK VOLKMER⁴, PETER LUNKENHEIMER⁴, ANDRÉ BEYER¹, IAN HOWARD³, and RAINER HERGES² — ¹Faculty of Physics, Bielefeld University, 33615 Bielefeld — ²Otto-Diels-Institute for Organic Chemistry, Christian-Albrechts-University of Kiel, 24098 Kiel — ³Karlsruhe Institute of Technology (KIT), 76344 Karlsruhe — ⁴Institute of Physics, Augsburg University, 86135 Augsburg, Germany

Molecular rotors arranged in the surface-anchored metal-organic frameworks (SURMOF) were investigated. The rotating part of each linker molecule consists of a fluorine-substituted phenyl group connected with acetylene linkages to the Cu clusters. Dielectric spectroscopy was used to investigate the rotation dynamics of molecular rotors in a parallel capacitor assembly. We determined an activation energy of 10 kJ/mol for one SURMOF type consisting of 3-[4-(2-carboxyethynyl)-2,3-difluoro-phenyl]prop-2-ynoic acid (C12H4F2O4) as dipolar linkers and 1,4-diazabicyclo(2.2.2)octane (DABCO) as pillars, at temperatures above 170 K. A smaller barrier of about 2 kJ/mol was found for the corresponding SURMOFs without any pillars. The analog made from the non-polar linker was used as a control system and showed no dielectric relaxation processes down to 20 K. The observed activation energy barriers are consistent with *ab initio* DFT modelling and classical dipole-dipole interaction calculations.

CPP 17.5 Tue 11:00 P2

Design, fabrication and nano-scale characterization of novel SEI layers — ●ZHUIJUN XU¹, YANJUN CHENG², YONGGAO XIA², and PETER MÜLLER-BUSCHBAUM^{1,3} — ¹TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — ²Ningbo Institute of Materials Technology and Engineering, Chinese Academy of Sciences, 315201, Ningbo, China — ³MLZ, TU München, 85748 Garching, Germany

Rechargeable lithium metal batteries have been recognized as one of the most promising energy storage devices due to their superior energy density. However, serious safety concerns and poor cyclability are challenges originating from an uncontrolled lithium dendrite growth and an unstable solid electrolyte interface (SEI) layer. One strategy to suppress dendrite growth is a surface modification with amphiphilic block copolymers, such as PDMS-b-PAA, which bear some clear advantages including absorbing mechanical stress, conducting lithium ion and controlling the lithium dendrite growth process. With *ex-situ* scattering techniques or *in-situ* scattering studies, the structures of the surface modified lithium metal anodes and structure formation processes are studied. In particular, by applying GISAXS, the horizontal structures and vertical structures of the polymer films on the lithium metal surfaces are investigated.

CPP 17.6 Tue 11:00 P2

In situ GISAXS printing of inorganic-organic hybrid nanostructures based on biopolymer templating — ●LINUS F. HUBER¹, STEPHAN V. ROTH³, KUN SUN¹, MANUEL A. REUS¹, and PETER MÜLLER-BUSCHBAUM^{1,2} — ¹TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — ²MLZ,

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Inorganic-organic hybrid nanostructures are interesting for the energy conversion through the thermoelectric effect. Thermoelectric generators based on abundant, environmentally friendly and affordable materials have historically had low efficiencies. The electrical conductivity, the Seebeck coefficient and the thermal conductivity need to be individually improved, to significantly enhance the thermoelectric figure of merit. Nanostructuring can improve these parameters and maximize the performance of thermoelectric materials. Beta-lactoglobulin is a bovine whey protein that is used as a template during sol-gel synthesis. Different titania thin film morphologies can be achieved by changing the pH-value and the beta-lactoglobuline concentration. To investigate the different titania morphologies, in situ GISAXS, GIWAXS and SEM are used. In situ GISAXS printing enables a time resolved investigation of the structure formation, domain sizes and domain distances. UV-Vis and PI are used to analyze differences in the optical properties of the thin films. These structural and optical changes are then correlated with measurements of the Seebeck coefficient and the electrical conductivity.

CPP 17.7 Tue 11:00 P2

Two-step nucleation in confined geometry on a lattice gas model — ●JACOB HOLDER, RALF SCHMID, and PETER NIELABA — Physics Department University of Konstanz, Konstanz, Germany

We deploy a degenerated Ising model to describe nucleation and crystallization from solution in a confined two-component system. The free energy is calculated using Metadynamics simulation. With nudged elastic band simulation we calculate the minimum energy path and give properties of the crystallization path. From the parameters and setup we find necessary conditions for the occurrence of two-step nucleation in our system.

CPP 17.8 Tue 11:00 P2

Nucleation patterns in polymer crystallization analyzed by machine learning — ●ATMIKA BHARDWAJ^{1,2}, MARCO WERNER¹, and JENS-UWE SOMMER^{1,2} — ¹Leibniz-Institut für Polymerforschung Dresden e. V., Hohe Str. 6, Germany 01069 — ²Technische Universität Dresden (TUD)

Today, many efforts seek to link machine learning (ML) algorithms to the concepts of theoretical physics. Our work focuses on developing ML tools to derive meaningful interpretations from the data generated through molecular dynamics simulations. We aim to find and quantify the nucleation patterns in polymer crystallization. The transition dynamics occurring under-cooled polymer melt is a local environmental phenomenon rather than a property of individual particles (or monomers), and depends on subtle conformation patterns such as entanglements between the chains. Our first objective is to define a set of fingerprint parameters to capture the crucial information in the local conformation and a monomer's environment and to quantify the degree of crystallinity. We use self-supervised auto-encoders to contain those local fingerprints. The second objective is to recognize the precursors or nucleation sites that stimulate crystal growth before the occurrence of such growth. We are currently working on both convolutional neural networks and recurrent neural networks to investigate the spatial and temporal patterns of the precursors.

CPP 17.9 Tue 11:00 P2

Laser control over crystallization and morphology of tetracene thin films — ●STEFAN KOWARIK¹, ANDIKA ASYUDA², LINUS PITHAN³, and ANDREAS OPITZ⁴ — ¹Physical Chemistry, University of Graz, Austria — ²Institute for Physical Chemistry, Universität Heidelberg, Germany — ³Institut für Angewandte Physik, Universität Tübingen, Germany — ⁴Institut für Physik, Humboldt-Universität zu Berlin, Germany

Nucleation and crystallization in thin-film growth are notoriously difficult to steer, but optical control offers exciting new possibilities for selecting specific polymorphic forms [1] or aligning the crystallite orientation in thin films [2]. Here we report an increase in crystallite size in vacuum-deposited tetracene thin films under illumination with a wavelength tuned to a specific absorption band of tetracene crystals. The morphological changes are induced with linearly and circularly polarized light and the larger crystallite size is accompanied by higher photoluminescence of tetracene. We propose a mechanism based on optical heating of specifically oriented crystals during growth, which leads to enhanced surface migration processes in these crystals and

consequently larger crystals via Oswald ripening effects. The light-induced temperature effects are distinct from substrate heating both for linearly and circularly polarized light. Laser illumination, therefore, is a novel control parameter of growth and enables high crystallinity even for low substrate temperature deposition.

[1] L. Pithan, et al., *Crystal Growth & Design* 15.3 (2015): 1319-1324. [2] L. Pithan, et al., *Advanced Materials* 29.6 (2017): 1604382.

CPP 17.10 Tue 11:00 P2

Synthesis of Hard-Carbon Microspheres with Binary Size Distribution via Hydrothermal Carbonization of Trehalose —

●MARTIN WORTMANN¹, WALDEMAR KEIL², MICHAEL WESTPHAL¹, ELISE DIESTELHORST³, JAN BIEDINGER¹, BENNET BROCKHAGEN³, GÜNTER REISS¹, CLAUDIA SCHMIDT², KLAUS SATTTLER⁴, and NATALIE FRESE¹ — ¹Bielefeld University, Bielefeld, Germany — ²Paderborn University, Paderborn, Germany — ³Bielefeld University of Applied Sciences, Bielefeld, Germany — ⁴University of Hawaii, Honolulu, USA
Hard Carbon microspheres (HCS) were synthesized via hydrothermal carbonization (HTC) of trehalose and subsequent pyrolytic post-carbonization at 1000°C. It was found that HTC of trehalose, in contrast to other saccharides, results in a distinctly binary sphere diameter distribution with monodisperse small spheres and polydisperse large spheres. Pore formation, as visualized by charge-compensated helium ion microscopy, results in a strong increase in BET surface area. The chemical composition and crystallinity were examined before and after pyrolysis using a variety of spectroscopic methods. Strong compositional similarities were found to other saccharide-derived hydrochars, with a cross-linked furan-based polymer-structure before, and nano-crystalline carbon structure after pyrolysis. The binary size-distribution and large BET surface area make trehalose-derived HCS a highly promising material for applications in energy storage or catalysis.

CPP 17.11 Tue 11:00 P2

Physics of supersaturated, agitated sucrose solutions: Crystal nucleation and growth — ●HANNAH M. HARTGE and THOMAS A. VILGIS — Max Planck Institute for Polymer Research, Mainz, Germany

Supersaturated sucrose solutions that have been sufficiently cooled without nucleation constitute a meta-stable system in which agitation promotes fast crystallization. Applications of this physically interesting process can be found for example in the production of fondant in confectionery. While just water and sucrose are present, the system goes through complex thermodynamic processes during crystallization, which are highly dependent on composition, temperature, and agitation.

In this work, we investigate how temperature and concentration affect nucleation, crystal growth and final particle size distribution of highly supersaturated sucrose solutions under agitation. To do so, the torque was measured during kneading of the samples at controlled temperature, followed by light microscopy and corresponding image analysis. When crystallization times were compared to classical nucleation theory, variations were found to be related to temperature and supersaturation in the same way as indicated by induction time models of statistical physics. Additionally, size distributions of the resulting crystal phases showed a strong dependence on temperature during agitation, sucrose content and according initial supersaturation.

CPP 17.12 Tue 11:00 P2

Following the directed self-assembly of crystallizable block co oligomers via in situ AFM — ●ALEXANDER MEINHARDT and THOMAS F. KELLER — Centre for X-ray and Nano Science (CXNS), Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany

Bottom up nanofabrication utilizing the molecular self-assembly of block co-oligomers with sub-10 nm domain sizes are widely discussed as a promising route for next generation photolithography. Double crystalline co-oligomers can be used to create well defined, high-fidelity nanostructures by controlling the competing driving forces microphase separation and crystallization. We report on the surface nanostructure formation and its temporal evolution during annealing of thin films of an amphiphilic double crystalline polyethylene-block-poly(ethylene oxide) co-oligomer (PE-b-PEO) on planar and patterned surfaces. Directing the self-assembly of such systems with physical or chemical guiding patterns can enable the formation of defined, large scale amphiphilic nanostructures, which could be of interest for various applications, e.g., biomaterials, photonics, and nanotechnology. However, there still remain several challenges regarding the characterization, de-

fect density, pattern fidelity, and post processing of such block copolymer nanopatterns. By investigating the directed self-assembly (DSA) of the PE-b-PEO using AFM in situ, we aim to tune the balance of the involved driving forces and in turn create optimized nano-templates.

CPP 17.13 Tue 11:00 P2

Influence of the surface roughness and surface chemistry to understand slide electrification — ●BENJAMIN LEIBAUER, WERNER STEFFEN, and HANS-JÜRGEN BUTT — Ackermannweg 10 55128 Mainz

In the last few years a lot of studies have shown that by contact electrification between water droplets and hydrophobic surfaces, it is possible to generate electricity in an environmentally friendly way.[1] The physical processes are still being discussed today and to extend the understanding Stetten et al.[2] have established an experimental setup that allows the drop charge of individual drops. In the work presented here we have studied with this setup the influence of the surface roughness and the chemistry of the substrates on hydrophobic to superhydrophobic substrates. We found that for the drop charge both parameters have an influence on at least the same order of magnitude.

[1] C. Wu, A. C. Wang, W. Ding, H. Guo, Z. L. Wang, *Advanced Energy Materials* 2019, 9, 1802906. [2] A. Z. Stetten, D. S. Golovko, S. A. Weber, H.-J. Butt, *Soft Matter* 2019, 15, 8667-8679.

CPP 17.14 Tue 11:00 P2

Dewetting dynamics and equilibrium droplet shapes for of visco-elastic substrates — ●KHALIL REMINI¹, LEONIE SCHMELLER², DIRK PESCHKA², BARBARA WAGNER², and RALF SEEMANN¹ — ¹Experimental Physics, Saarland University, Saarbrücken, Germany — ²Weierstrass-Institute, Berlin University, Berlin, Germany

In our study we are interested in the dewetting of liquid polymer layers (Polystyrene 18 kg/mol) with about 100 nm thickness from visco-elastic polydimethylsiloxane surfaces with elasticity ranging $E = 1.2$ MPa for Sylgard 184 to $E = 3$ kPa for Cy52-276. When heating the samples to temperatures where PS is liquid, holes nucleate in the initially uniform PS film. These holes grow during dewetting, coalesce and eventually form sessile droplets of a few micrometers in diameter sitting on the PDMS surface. Due to the particular situation of the adaptive PDMS substrate, we observe characteristic qualitative and quantitative differences in rim shapes, (dynamic) contact angles and dewetting velocities which are indicating differences in the underlying energy dissipation but might result also from potential phase separation of liquid and cross linked PDMS close to the three-phase contact line. To shed light on the impact of viscous and elastic properties and potential phase separation at the three phase contact line, we aim at a quantitative comparison of sessile (equilibrium) droplets on substrates having different elasticities and thus elastocapillary lengths.

CPP 17.15 Tue 11:00 P2

Messung von Kräften zwischen Tropfen und bewegten Oberflächen — ●MARISA FISCHER, SIMON SCHUBOTZ, JENS-UWE SOMMER, ANDREAS FERY und GÜNTER AUERNHAMMER — Leibniz-Institut für Polymerforschung Dresden e.V., 01069 Dresden, Germany

Um einen Tropfen über eine Oberfläche zu bewegen, wird eine Kraft benötigt, die von deren Eigenschaften abhängt. Das zur Messung dieser Kraft entwickelte Drop Adhesion Force Instrument (DAFI) erlaubt die freie Wahl der Geschwindigkeit der Drei-Phasen Kontaktlinie und der Größe des Tropfens [1]. Die Kraftmessung erfolgt mittels des Hookeschen Gesetzes, indem die Auslenkung einer im Tropfen befindlichen Glaskapillare gemessen wird.

Ein von der Bewegung des Tropfens aufgenommenes Video wird mit einem von uns entwickelten Analyseprogramm ausgewertet. Für die Übertragung größerer Kräfte wird ein Glasplättchen am Kapillarende befestigt, welches die Adhäsion zwischen Tropfen und Kapillare erhöht.

Mit dem entwickelten Aufbau wurden die Kräfte zwischen Wassertropfen und Polydimethylsiloxan (PDMS) sowie Poly(N-isopropylacrylamide) (PNiPAAm) Polymerbürsten untersucht. Dabei zeigte sich ein Zusammenhang zwischen dem Zustand der Oberfläche und der Kraft.

[1] D. W. Pilat u. a., *Langmuir* 2012, **28**, 49, 16812-16820

CPP 17.16 Tue 11:00 P2

In-situ Monitoring of Hard-Core Soft-Shell Microgels During Monolayer Drying — ●JULIAN RINGLING, KEUMKYUNG KUK, and MATTHIAS KARG — Heinrich-Heine-Universität, Düsseldorf, Germany

Hard-core soft-shell (HCSS) microgels are interesting colloids with the potential to be used as model systems to understand crystallization and melting processes [1]. They spread at the air/water interface and self-assemble into 2D monolayers in which the cores do not touch directly due to shell-shell repulsion. Compression of such a monolayer allows control over the inter-particle distance by compressing the soft and deformable shell [2]. After transferring a compressed monolayer to a substrate, various structures can be observed [3]. Understanding and controlling the formation of those structures is essential for the use of the system as a model for crystallization.

Previously our group discovered a difference in monolayer structure at the air/water interface in comparison to the dried monolayer after transfer onto a substrate when using micron-sized silica-poly(N-isopropylacrylamide) HCSS microgels. To understand the phase transition/structural change occurring, we have monitored this phase transition/structural change using fluorescence and light microscopy. Here we present results from in-situ observations of drying 2D colloidal monolayers focussing on the effect of different parameters on drying and assembly behaviour.

[1] G. Wie et al., *Soft Matter*, 2013, 9, 9924-9930

[2] J. Tang et al., *ACS Omega*, 2018, 3, 12089 -12098

[3] S. Ciarella et al., *Langmuir*, 2021, 37, 5364-5375

CPP 17.17 Tue 11:00 P2

Investigation of Cononsolvency Phase Transition of Poly(sulfobetaine)-based Diblock Copolymer Thin Films — ●PEIXI WANG¹ and PETER MÜLLER-BUSCHBAUM^{1,2} — ¹Technische Universität München, James-Frank-Straße 1, 85748 Garching, Germany — ²Heinz Maier-Leibnitz Zentrum (MLZ), Lichtenbergstr. 1, 85748 Garching, Germany

Co-nonsolvency occurs if a mixture of two good solvents causes the collapse or demixing of polymers into a polymer-rich and solvent-rich phase in a certain range of compositions of these two solvents. The non-ionic thermo-responsive polymer, poly(N-isopropylmethacrylamide) (PNIPMAM), which features a lower critical solution temperature (LCST) in aqueous solution, has been widely used to investigate its collapse transition behavior in a mixture of two competing good solvents. However, co-nonsolvency response of its block copolymer containing the zwitterionic poly(sulfobetaine)s, especially poly(4-((3-methacrylamidopropyl)dimethylammonio)butane-1-sulfonate) (PSBP)* which exhibits an lower upper critical solution temperature (UCST) and shows a strong swelling transition in aqueous media, is newly studied. We focus on the co-nonsolvency behavior of PSBP-b-PNIPMAM thin films in water/acetone mixtures by in situ time-of-flight neutron reflectometry (TOF-NR) and spectral reflectance (SR). Furthermore, Fourier transform infra-red (FTIR) spectroscopy is applied to investigate the interactions between the polymer thin film and water/co-solvent, which is closely related to their deuteration level.

CPP 17.18 Tue 11:00 P2

Core-shell microgels synthesized in continuous flow: Deep insight into shell growth by temperature-dependent FTIR spectroscopy — ●PASCAL FANDRICH¹, MARCO ANNAGARN¹, LARS WIEHEMEIER¹, INA EHRRING¹, TILMAN KOTTKE², and THOMAS HELLWEG¹ — ¹Physical and Biophysical Chemistry, Bielefeld University, 33615 Bielefeld, Germany — ²Biophysical Chemistry and Diagnostics, Bielefeld University, 33615 Bielefeld, Germany

While core-shell microgels have been intensively studied in their fully synthesized state, the formation mechanism of the shell growth has not been completely understood. Such insight is decisive for a customization of microgel properties for applications. In a novel approach, we synthesized microgels based on a N-isopropylmethacrylamide (NiP-MAM) core and a N-n-propylacrylamide (NnPAM) shell in a continuous flow reactor. The shell growth is studied depending on the solution's time of residence inside the reactor. PCS experiments reveal a significant decrease of the volume phase transition temperatures of the core and the shell respectively, with increasing residence time. At early stages, a decreased swelling capacity is found before a discrete NnPAM shell is formed. Temperature-dependent FTIR spectroscopy shows that the decreased swelling capacity originates from a pronounced interpenetrated network between NnPAM and NiPMAM. AFM images resolve a raspberry-like structure after 3 min, pointing to an aggregation of NnPAM domains before the distinct shell forms.

CPP 17.19 Tue 11:00 P2

How ultrasound accelerates microgel adsorption kinetics —

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Poly-N-isopropylacrylamide (PNIPAM) based microgels (MGs) are surface-active and offer great opportunities as stabilizers of emulsions and foams. Due to their thermosensitive response, the MGs enable also destabilization on demand. However, emulsion formation implies energy input by stirring or ultrasonication. To understand this formation process, it is important to understand the interfacial adsorption of the MGs. A fast trigger to affect the adsorption process is given by ultrasonication. The present study shows the effect of ultrasound on the adsorption kinetics of PNIPAM MGs at the water-oil interface monitored by drop shape tensiometry. The adsorption kinetics of MGs accelerates with increasing ultrasonication intensity. The variation of different parameters, such as ultrasonic frequency, MG crosslinker density, concentration and phase composition, indicates that both acoustic streaming as well as ultrasound induced deswelling of MGs due to breakage of hydrogen bonding cause this acceleration.

CPP 17.20 Tue 11:00 P2

Interaction of soft microgel with solid silica particles at the air-water interface — •CARINA SCHNEIDER, SEBASTIAN STOCK, KEVIN GRÄFF, FRANZISKA JAKOB, and REGINE VON KLITZING — Department of Physics, TU Darmstadt, Hochschulstraße 8, 64289, Darmstadt

Emulsions stabilized by multiple particle systems are interesting in various research fields, e. g., in the food industry or interfacial catalysis. The interaction of two or more nano-particle systems of different properties at liquid interfaces is important for the coalescence behavior of emulsion droplets stabilized by these particle mixtures. For instance, a mixture of hydrophilic microgel particles (MGs) and hydrophobic silica nano-particles (SiNP) is able to stabilize water in oil emulsions, which is not possible with MGs alone. Therefore, it is of special interest to understand the interaction of those particles at the interface. In this context, their lateral compression may simulate the droplet interfaces under coalescence conditions. For this purpose, we spread mixtures of poly-NIPAM MGs and spherical SiNPs at the air-water interface of a Langmuir trough and determined the compression isotherms. For deeper insights into the lateral structure formation, the particle layers were transferred onto Silicon wafers and scanned by atomic force microscopy. For low compressions, the elastic MG network dominates the isotherm while SiNP are situated between the MGs with low impact. For higher compressions, the inelastic SiNP structures are pushed onto the MGs and take over the resistance to the outer pressure.

CPP 17.21 Tue 11:00 P2

Adsorption kinetics of microgel particles at the air/water interface — •KAI LUCA SPANHEIMER, DANIEL JÄGER, SEBASTIAN STOCK, and REGINE VON KLITZING — Department of Physics, TU Darmstadt, Hochschulstraße 8, 64289 Darmstadt

Interest in microgel particles (MGs) based on poly-N-isopropyl acrylamide (PNIPAM) as surface-active material remains high. The nano-micrometer sized, cross-linked polymer particles are able to adsorb to water/air or water/oil interfaces spontaneously. Combined with their ability to act as carriers for drugs, recent studies showed, that they may act as transport vehicles for amphiphilic catalysts to the interface, resulting in improved interfacial catalysis, e. g., in Pickering emulsions. Despite much research on the interaction of MGs with various low and higher molecular weight material, the adsorption of MG/catalyst complexes at the interface is not yet well understood. In the presented work, the adsorption kinetics at the air/water interface is measured via change in surface tension over time by drop shape analysis. In order to disentangle different effects in case of MG/catalyst complexes the adsorption kinetics of pure MGs and mixtures of MGs with simple anionic and cationic surfactants as model systems for the catalysts is studied and compared with the adsorption of MG/catalyst complexes.

CPP 17.22 Tue 11:00 P2

A molecular dynamics approach to understand and control the catalyst enrichment at the IL/vacuum interface in SILP systems — MATTIA LIVRAGHI¹, CHRISTIAN WICK^{1,2}, •DAVID MATTHEW SMITH^{1,3}, and ANA-SUNČANA SMITH³ — ¹PULS Group, Institute for Theoretical Physics and Interdisciplinary Center for Nanostructured Films (IZNF), Friedrich-Alexander Universität

Erlangen-Nürnberg (FAU), 91058 Erlangen, Germany — ²Competence Unit for Scientific Computing (CSC), FAU, 91058 Erlangen, Germany — ³Group of Computational Life Sciences, Division of Physical Chemistry, Ruder Bošković Institute, 10000 Zagreb, Croatia

Supported Ionic Liquid Phase Catalysis (SILP) improves the catalytic turnover by smearing a thin IL layer onto a support material, reducing the need for slow reactant transport inside viscous ILs. Next generation SILP technology will rely on confining the catalyst to the vacuum interface, spatially localising the chemical reaction. This will require a deep understanding of the interface enrichment and structuring of the individual chemical components. We investigated ionic liquids made of iodide and polyethylene glycol imidazolium cations. Therefore, we parameterized atomic charges for the new ILs using multiple conformations during the RESP fitting procedure, compatible with the GAFF force field, and validated our simulations against experimental data. The (also newly parameterized) catalysts are Nickel(II) coordination compounds with task-specific carbene ligands. We investigate the influence of the structures of the ligands and the IL's chain on controlling the catalyst's distribution in and affinity for the IL-vacuum interface.

CPP 17.23 Tue 11:00 P2

Morphology control of titania thin films in a low temperature process — •GUANGJIU PAN¹, SHANSHAN YIN¹, NIAN LI¹, TIANFU GUAN¹, RENJUN GUO¹, SUZHE LIANG¹, YUQIN ZOU¹, CAROLINE EHGARTNER², NICOLA HÜSING², and PETER MÜLLER-BUSCHBAUM^{1,3} — ¹TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — ²Materialchemie, Chemie und Physik der Materialien, Universität Salzburg, 5020 Salzburg, Austria — ³MLZ, TU München, 85748 Garching, Germany

A low-temperature routine to realize inorganic electron-transport layers (ETLs) is important for the commercialization of perovskite solar cells. Fabricating ETLs at low temperature is energy saving and compatible with flexible substrates. In this work, titania thin films are synthesized at low temperature (below 100 Celsius degree) with a polymer template sol-gel method based on the amphiphilic diblock copolymer polystyrene-b-polyethylene oxide (PS-b-PEO), in combination with selective incorporation of the titanium precursor ethylene glycol-modified titanate (EGMT). Tailoring titania film morphology in the low-temperature process is achieved by managing phase separation of the polymer template. The ratio of polymer, precursor, solvent, and catalyst for the sol-gel solution is varied to tune the thin film morphologies. The surface morphologies of titania films are probed via scanning electron microscopy and GISAXS. The optical properties of the films are examined with ultraviolet-visible spectroscopy.

CPP 17.24 Tue 11:00 P2

Soft Matter Food Physics: Oat Drink Foams — •JUDITH HEGE, ANTONIA-LOUISA SCHLICHTING, JANA REEH, and THOMAS A. VILGIS — Max Planck Institute for Polymer Research, Mainz, Germany

For various applications, oat drink needs to provide a capacity to form stable, creamy, homogeneous foams. Such macroscopic foam properties are based on molecular interactions at the air-water interfaces and protein kinetics within the lamellae. However, the underlying structure-function relationships between molecular interactions and macroscopic foam properties are not yet fully understood, especially for multicomponent systems like plant-based drinks. Therefore, this study probed foams formed by an oat drink containing only water, oats, canola oil and salt.

Investigations focused on the influence of enzyme treatment, canola oil addition, heat treatment and homogenization parameters on foam properties. Accordingly, time-dependent foam height measurements were performed and supported by light microscopy, photography, and particle size measurements to compare the findings on the macroscopic scale with bubble size evolution and oil droplet distribution.

This study showed that protease treatment resulted in a higher foaming capacity, but lower foam stability and that heat treatment lessened the foam stability. Furthermore, addition of small contents of canola oil increased the foaming capacity, however, higher canola oil contents reduced foam stability. Furthermore, a longer duration and higher speed of homogenization treatment caused a more homogeneous emulsion and increased foaming capacity as well as foam stability.

CPP 17.25 Tue 11:00 P2

Spatial resolution of particle transport at interfaces — •KEVIN HÖLLRING¹, ANDREAS BAER¹, DAVID M. SMITH², and ANA-SUNČANA SMITH^{1,2} — ¹PULS Group, FAU Erlangen-Nürnberg, Germany — ²Group for Computational Life Sciences, Ruder Bošković Institute,

Zagreb, Croatia

Confined geometries play an important role in various applications, where it is generally important to be able to predict particle transport and mobility. Commonly used techniques like the Einstein-approach using the Mean Square Displacement (MSD) as well as Auto-correlation-function (ACF) related techniques rely on strong assumptions about spatial isotropy and homogeneity tied to conditions on local symmetry, that are not satisfied in these confined geometries, making it especially hard to resolve interface-orthogonal particle dynamics. Still other techniques like jump-diffusion are only able to approximate relative mobility and require calibration for each system.

We propose a theoretical model for resolving absolute interface-perpendicular diffusion based on the time particles spend within sub-spaces of confined systems that accurately predicts diffusion for simple point-like particles like water. In addition, we also present an extension to that model taking into account internal deformational degrees of freedom that can affect the observed particle lifetime.

By application of the proposed models to water as well as Imidazolium-based ionic liquids, we confirm their accuracy and versatility in the analysis of complex particle dynamics thus also proving their applicability to confined geometries.

CPP 17.26 Tue 11:00 P2

In-situ investigation during gold HiPIMS deposition onto polymers — ●YUSUF BULUT^{1,2}, KRISTIAN RECK³, MATTHIAS SCHWARTZKOPF¹, JONAS DREWES³, SUZHE LIANG², TIANFU GUAN², THOMAS STRUNKUS³, FRANZ FRAUPEL³, PETER MÜLLER-BUSCHBAUM^{2,4}, and STEPHAN V. ROTH^{1,5} — ¹DESY, 22607 Hamburg — ²TU München, Physik Department, Lehrstuhl für Funktionelle Materialien, 85748 Garching — ³CAU, Chair for Multicomponent Materials, Faculty of Engineering, 24143 Kiel — ⁴MLZ, TU München, 85748 Garching — ⁵KTH Royal Institute of Technology, Department of Fibre and Polymer Technology, SE-100 44 Stockholm

Gold deposition via high power impulse magnetron sputtering (HiPIMS) allows to coat thin metal layers on heat sensitive materials such as polymers allowing for increased adhesion and density. HiPIMS allows deposition at a lower total deposited thermal energy in comparison to conventional magnetron sputtering, but this energy is delivered in a very short pulse exhibiting very high power and ionization. The consequences for the nucleation and growth processes during HiPIMS deposition are not sufficiently known. Therefore, we investigate the morphology evolution of thin gold layers on four polymer templates, namely polystyrene (PS), polyvinylalcohol (PVA), polystyrene sulfonic acid (PSS) and poly-4-vinylpyridin (P4VP). These polymers show different functional moieties and thus are expected to influence the growth of the gold layer. We present first results of our in situ investigations combining grazing-incidence small angle X-ray scattering (GISAXS), grazing incidence wide angle X ray scattering (GIWAXS).

CPP 17.27 Tue 11:00 P2

High-concentration Lithium-ion Electrolyte Overcomes the Challenges of High-temperature Lithium Batteries — ●TIANLE ZHENG¹, YAJUN CHENG², and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — ²Ningbo Institute of Materials Technology & Engineering, Chinese Academy of Sciences, Ningbo, 315201, Zhejiang Province, P. R. China

Traditional Li-ion batteries, on the other hand, are severely constrained in high-temperature applications due to the low thermal stability of the electrolyte/electrode interface and electrolyte decompositions in the cell. Herein, we demonstrate a new electrolyte that achieves an excellent stable long-term cycling at 100°C, well beyond the typical 60°C limits of normal conventional Li-ion batteries. The high concentrated lithium oxalyldifluoroborate (LiODFB) is selected as the only lithium salt with a carefully designed high thermal stability solvent group. As a result, this unique high-concentration electrolyte can promote to form a stable and inorganic solid electrolyte interface (SEI) layer on the electrode at elevated temperature, leading to improved performance in MCMB/Li and lithium iron phosphate (LFP)/Li half-cells, and achieve reversible capacities of 160 and 350 mA h/g, respectively, with Coulombic efficiencies (CEs) > 99.3%. Subsequently, we further investigate the mechanism of high concentration LiODFB electrolytes by molecular dynamics (MD) simulations and XPS characterization techniques, exploring a new way for future high-temperature electrolytes for Li-ion batteries.

CPP 17.28 Tue 11:00 P2

Sol-gel based tailored lithium-ion battery electrodes — ●IVANA PIVARNÍKOVÁ^{1,2}, RALPH GILLES¹, and PETER MÜLLER-BUSCHBAUM^{1,2} — ¹MLZ, TU München, 85748 Garching — ²TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching

Silicon based materials have been considered as one of the most promising candidates for the next-generation lithium-ion battery anodes, thanks to its low cost, non-toxicity and high theoretical gravimetric capacity (4200 mAh/g). One of the concepts for a suitable application is to design the mesoporous Si-based material via copolymer assisted sol-gel synthesis. This wet chemical method consists of the formation of the organic-inorganic composites by a self-assembly mechanism, where the organic phase (PEO-b-PPO-b-PEO non-ionic triblock copolymer) serves as a template for the inorganic structure (SiOx). The tetraethoxysilane (TEOS) is used as a Si precursor. The solution mix is spin-coated onto the cleaned Si substrates and the removal of the template is done by calcination at high temperature (400 °C). The properties of the thin films can be tuned by adjusting the synthesis conditions such as concentration of the reaction compounds, choice of the deposition technique, choice of the final calcination step or choice of additives. The aim is to reach the desired thickness, porosity, conductivity and mechanical stability for a successful Li-ion battery anode application. The produced thin films are characterized by scanning electron microscopy (SEM), grazing incidence small-angle X-ray scattering (GISAXS), profilometry and ellipsometry measurements.

CPP 17.29 Tue 11:00 P2

Silicon-germanium based coating of anodes for Lithium-ion batteries — ●KEXIN WU¹, CHRISTIAN L. WEINDL¹, and PETER MÜLLER-BUSCHBAUM^{1,2} — ¹TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — ²MLZ, TU München, 85748 Garching

Lithium-ion batteries (LIBs) have received increasing attention over several decades as an indispensable role in energy storage. The application of silicon anodes is hindered by their volumetric expansion after full lithiation, which causes collapse with three failure mechanisms including electrode pulverization, disconnection between the electrode and current collector, and continuous breaking and re-growth of the solid electrolyte interface (SEI) layer. To tackle this critical issue, the construction of hierarchical structures is a promising way to increase the stability of active materials. In our studies, Si/Ge hierarchical structures are built by chemical templating of pre-nanostructure self-assembled polystyrene nanoparticles, using an amphiphilic polystyrene-block-polyethylene oxide (PS-b-PEO) diblock copolymer as structure-directing agent. The diblock copolymers undergo microphase separation, which is further modified by solvent vapor annealing with dichloromethane (DCM) and SiCl₄. By pyrolysis, mesoporous thin films are achieved. The desirable morphological and crystallographic studies are accomplished by GISAXS SEM, AFM, and GIWAXS) The study is completed by galvanostatic cycling tests and impedance spectroscopy.

CPP 17.30 Tue 11:00 P2

Modeling of Nano-Porous Electrode Systems via Molecular Dynamics — ●PHILIPP STÄRK — SC Simtech, Uni Stuttgart, Germany

We use grand canonical Monte Carlo combined with atomistic-level MD to simulate open electrode systems at a constant potential. Using a multi-scale approach, our aim is to aid in the design of energy storage devices/electrocatalysis applications. In order to achieve this goal, we use different constant potential approaches to characterise the atomistic mechanisms behind charging and electro-catalytic product transport.

CPP 17.31 Tue 11:00 P2

Charging of dielectric surfaces in contact with aqueous electrolyte – the influence of CO₂ — ●PETER VOGEL¹, NADIR MÖLLER¹, PRAVASH BISTA², STEFAN WEBER², HANS-JÜRGEN BUTT², BENNO LIEBCHEN³, and THOMAS PALBERG¹ — ¹Institut für Physik, Johannes Gutenberg Universität, 55128 Mainz (Germany) — ²Max Planck Institut für Polymerforschung, 55128 Mainz (Germany) — ³Institut für Physik kondensierter Materie, Technische Universität Darmstadt, 3 64289 Darmstadt (Germany)

The charge state of dielectric surfaces in aqueous environments is of fundamental and technological importance. We use super-heterodyne light scattering in a custom-made cell to study the influence of dis-

solved CO₂ on the charging of three, chemically different surfaces. We compare an ideal, CO₂-free reference state to ambient CO₂ conditions. Systems are conditioned under conductometric control at different low concentrations of NaCl. As expected for constant charge densities, ζ -potentials drop upon increasing the salt concentration in the reference state. Presence of CO₂ leads to an overall lowering of ζ -potentials. Moreover, for the inorganic dielectric, the salt dependent drop is significantly weakened, and it is inverted for the organic dielectrics. We suggest that at ambient conditions, the charge state of dielectric surfaces is related to dielectric charge regulation caused by the salt concentration dependent adsorption/desorption of CO₂.

CPP 17.32 Tue 11:00 P2

Characterization of Nd complexes and processing of photonic crystal structures — ●MIRIAM GERSTEL¹, MUHAMMAD SHAHARUKH¹, INGO KÖHNE², PAUL MERTIN³, RUDOLF PIETSCHNIG², BERND WITZIGMANN³, JOHANN PETER REITHMAIER¹, and MOHAMED BENYOUCHEF¹ — ¹Institute of Nanostructure Technologies and Analytics (INA) — ²Institute of Chemistry — ³Institute of Computational Electronics and Photonics, CINSaT, University of Kassel, Germany

Lanthanide (Ln) ions are unique for applications in lighting, sensing, and display technologies. In our approach, we investigate the potential of using Ln(III) complexes as attractive luminescent materials due to its characteristics of narrow emission bands and wide emission spectrum. Two different types of Nd(III) complexes are investigated: Nd complexes with phosphonate ligands with varying aromatic residues and complexes where the Nd ion is incorporated in a polyoctahedral silsesquioxane cage. Optical properties of Nd complexes are determined by photoluminescence (PL) spectroscopy, which reveals three emission bands of Nd(III) ions in the NIR region. To achieve a low-density molecular distribution on the sample surface, the complexes are dissolved in dichloromethane and drop-casted on a flat surface. For light enhancement, molecules will be immobilized on photonic crystal cavities (PhCs). The fabrication of PhCs by electron-beam lithography, inductively coupled plasma reactive ion etching and selective wet etching techniques is discussed. This work is supported by the state of Hesse in the frame of LOEWE priority project SMolBits.

CPP 17.33 Tue 11:00 P2

Fabrication of photonic crystals for integration of molecules — ●ÖZLEM URKAN¹, RANBIR KAUR¹, MUHAMMAD SHAHARUKH¹, INGO KÖHNE², RUDOLF PIETSCHNIG², JOHANN PETER REITHMAIER¹, and MOHAMED BENYOUCHEF¹ — ¹Institute of Nanostructure Technologies and Analytics (INA), Kassel, Germany — ²Institute of Chemistry, Kassel, Germany

The control of light-matter interaction is an enabling technique for many emerging quantum technology applications. Photonic crystals (PhCs) are of particular interest since they can confine light in small mode volumes producing a strong interaction between light and emitters located in or near the cavity. Emitters such as lanthanide (Ln) molecules offer the potential of scalable quantum systems due to their characteristic narrow linewidth and wide emission spectrum.

This work focuses on the fabrication of PhCs by electron-beam lithography, inductively coupled plasma reactive ion etching and selective wet etching techniques and investigating different process parameters influencing the quality of PhCs. The morphological and optical properties of PhCs are characterized by scanning electron microscopy and micro-photoluminescence spectroscopy. In order to enhance the light emission, Ln molecules will be immobilized on the processed PhC cavities.

This work is supported by the state of Hesse in the frame of LOEWE priority project SMolBits

CPP 17.34 Tue 11:00 P2

Propandehydrierungskatalysatoren mit den Eisen(III)oxid-Nanopartikeln — ●IRINA BELOVA — Moscow, Russia

Propylen ist ein sehr wichtiger Industrirohstoff, aber das Wachstum seiner Produktion hat mit dem Wachstum des Verbrauchs nicht Schritt gehalten. Das größte Potenzial im Bereich der Propylenherstellung haben die Reaktionen der direkten und oxidativen Dehydrierung von Propan. Wir haben versucht, einen Propan-Dehydrierungskatalysator als Eisen-Nanopartikel auf Aluminiumoxid zu erhalten. Um Nanopartikel zu bilden, griffen wir auf die Bildung von Eisenkomplexen mit Phenanthrolin zurück. Bei der Reaktion der direkten Propandehydrierung gibt es bei diesen Katalysatoren eine geringe Selektivität. Dabei schreitet Cracken schreitet aktiv voran. Es gibt jedoch immer noch eine Propandehydrierung. Wir planen, mit Sauerstoff gemischtes Propan

benutzen. Wir erwarten, dass die *milde* Oxidation von Propan mit Sauerstoff besser verläuft.

CPP 17.35 Tue 11:00 P2

Polydisperse curved polymer brushes — ●MARIOS GIANNAKOU and FRIEDERIKE SCHMID — University of Mainz

In the past, polymer brushes have been investigated in the monodisperse limit or in flat geometries. These circumstances however aren't as experimentally relevant, as monodisperse brushes are difficult to construct and brushes are found in curved geometries most of the times. Here, we attempt to resolve this issue by extending the already established mean-field theory describing polymer brushes developed by Cates et.al.. We develop a numerical method that allows us to investigate cylindrical and spherical geometries for arbitrary polydispersities. We then explore the uniform, Schulz-Zimm and monodisperse polymer distributions, and comment on the results.

CPP 17.36 Tue 11:00 P2

Temperature-dependent conformation behavior of isolated Poly(3-hexylthiophene) chains — ●SANWARDHINI PANTAWANE and STEPHAN GEKLE — Biofluid Simulation and Modeling Theoretische Physik VI Universität Bayreuth 95440 Bayreuth Germany

We use atomistic as well as coarse-grained molecular dynamics simulations to study the conformation of a single Poly(3-hexylthiophene) chain as function of temperature. We find that mainly bundle and toroid structures appear with bundles becoming more abundant for decreasing temperatures and even more after adding solvent (THF), leading to a prominent swelling of the molecular size at a temperature of about 220K. This swelling is in close agreement with the interpretation of recent spectroscopic experiments (Panzer et al. J Phys Chem Lett 8, 114 (2017)). We further relate the temperature dependence of P3HT to that of simple Lennard-Jones model polymers in vacuum.

CPP 17.37 Tue 11:00 P2

Dynamic Origin of the Entropic Force on a Semi-Confined Chain — ●RODRIQUE BADR¹, LAMA TANNOURY², and LEONID KLUSHIN³ — ¹Johannes Gutenberg University, Mainz, Germany — ²Martin Luther University, Halle-Wittenberg, Germany — ³American University of Beirut, Beirut, Lebanon

Thermodynamics predicts that the free energy of confinement

$$F = B \frac{L}{D}$$

for a chain confined in a tube with thin and thick walls is the same in both cases. This equivalence implies that the force acting to eject the chain from semi-confinement is also the same. Thermodynamics, however, does not explain the dynamical origin of the force, but one can understand the force as originating from contacts with the surface of the boundary. Intuition suggests that the thin boundary should amount to fewer contacts and thus lead to a smaller ejection force when compared to the case of a thick boundary. Using coarse-grained molecular dynamics (MD) simulations, we support and validate the thermodynamic prediction that the magnitude of the ejection force is the same for different thicknesses of the boundary.

The forces are also found to be in good agreement with the scaling laws predicted by the thermodynamic approach. Finally, the results from our MD simulations provide an explanation of the origin of this equivalence of entropic forces, through the analysis of the radial distribution of contributions from the boundary to the ejection force.

CPP 17.38 Tue 11:00 P2

Computational study of the rheology of nanoparticle-polymer composites — ●LEON HILLMANN, NIKLAS BLAGOJEVIC, and MARCUS MÜLLER — Institute for Theoretical Physics, Georg-August-Universität Göttingen, Germany

Matrix-filler interactions in nanoparticle-polymer composites play a crucial role in the manufacturing process as well as the properties of the final material. Therefore, understanding the interplay between the parameters, such as shape, concentration, and size, is paramount for the design process of new composites. Computer simulations of these materials, however, pose several challenges due to the vast differences in the length scales involved, ranging from atomistic forces up to large-scale self-assembling structures. Here, a single nanoparticle embedded in polymer melt, represented by a highly coarse-grained, Gaussian, bead-spring model, is studied by dissipative particle dynamics (DPD) simulations. The nanoparticle-polymer interaction is adjusted with iterative Boltzmann inversion to match predictions of the density profile from atomistic simulations. Measurements of the nanoparticle's veloc-

ity autocorrelation function are then used to determine the memory kernel in a generalized Langevin equation. To what extent does the motion of the nanoparticle provide information about the viscoelastic properties of the surrounding melt? To this end, a numerical solution of the corresponding inverse problem is presented, which arises from a reformulation of the problem as the inversion of a triangular Toeplitz matrix. The results are finally compared with the predictions made by the Rouse model for unentangled polymer melts.

CPP 17.39 Tue 11:00 P2

Anomalous Diffusion of Diisocyanate in Cross-linked Silicone — ●MARTIN WORTMANN¹, KLAUS VIERTTEL², NATALIE FRESE¹, WALDEMAR KEIL³, CLAUDIA SCHMIDT³, and BRUNO HÜSGEN² — ¹Bielefeld University, Bielefeld, Germany — ²Bielefeld University of Applied Sciences, Bielefeld, Germany — ³Paderborn University, Paderborn, Germany

In industrial applications of polyurethane vacuum casting, silicone casting molds are used to replicate complex three-dimensional master patterns for prototypes and small series production. The undesired diffusion of isocyanate from the casting resin into the silicone causes gradual degradation of the casting molds. In this contribution, we present mathematical models for the anomalous diffusion process and a comprehensive description of the underlying chemical and physical mechanisms. The polymerization of the isocyanate with residual moisture to polyurea within the silicone matrix leads to a time dependence of both the surface concentration and the diffusion coefficient. The resulting concentration distribution over time and cross-section is modelled by analytical solutions to the diffusion equation.

CPP 17.40 Tue 11:00 P2

Molecular Dynamics Simulation of Free chain Diffusion into a Regular Network — ●JUDE ANN VISHNU¹ and FRIEDERIKE SCHMID² — ¹Johannes Gutenberg University, Mainz, Germany — ²Johannes Gutenberg University, Mainz, Germany

Thermo-sensitive hydrogels have attracted considerable attention in the field of bio chemistry and bio-medicine. Earlier works show that microfluidics can be used to create core-shell particle with decoupled

elasticity and surface adhesiveness. However these experiments could not achieve proper control over the core-shell interconnectivity. We use MD simulations to understand and quantify the diffusive interpenetration of these shell polymers into a core gel. The simulation uses a Regular network to model the gel which is diffusively invaded via a polymer solution. We look into the interfacial profile and the ways to control this core-shell connectivity. The density profiles show a clear dependence of penetration on shell polymer concentrations. This is also seen in the degree of interfacial integration and diffusion depths. Finally the analysis of diffused free chain within the gel shows the emergence of large clusters leading to percolation. These results give us insight into how the factors like the core-shell polymer contact time, shell polymer concentration, etc can help us fine tune the core-shell connectivity in experiments.

CPP 17.41 Tue 11:00 P2

Nucleation of separating liquid phases in elastic polymer networks — ●CHARLOTTA LORENZ, CARLA FERNÁNDEZ-RICO, and ERIC DUFRESNE — Soft and Living Materials, ETH Zurich, Zurich, Switzerland

Arrested phase separation is a key mechanism used by living systems to create well-controlled nanostructures. One of the most salient examples is structural color as present in some bird and insect species. Besides fascinating optical properties, phase-separating composite systems can have astonishing mechanical properties: For example, liquid inclusions can stiffen polymer networks. These mechanical properties have been less studied compared to the optical properties. To study the mechanical properties we use a sample system of a polymer network made of PDMS and fluorinated oil. We aim to control mechanical properties by tuning the structure of the phase-separated domains. Structure of the phase separating domains can be influenced by their nucleation. We vary typical parameters which could determine the nucleation such as the mesh size of the polymer network and total liquid fraction. We employ small-angle X-ray scattering, tensile tests and indentation experiments to study nucleation and mechanical properties of phase-separating samples. Our studies can result in mechanically highly flexible, self-assembled materials, which are comparatively fast and easy to produce.