

CPP 35: Poster Session II

Topics: Biopolymers, Biomaterials and Bioinspired Functional Materials (1-5); Complex Fluids and Colloids, Micelles and Vesicles (6-13); Composites and Functional Polymer Hybrids (14-23); Crystallization, Nucleation and Self-Assembly (24-32); Emerging Topics in Chemical and Polymer Physics, New Instruments and Methods (33-41); Hydrogels and Microgels (42-44); Modeling and Simulation of Soft Matter (45-50); Nanostructures, Nanostructuring and Nanosized Soft Matter (51-52); Polymer and Molecular Dynamics, Friction and Rheology (53-57); Responsive and Adaptive Systems (58-61); Wetting, Fluidics and Liquids at Interfaces and Surfaces (62-66).

Time: Wednesday 11:00–13:00

Location: P1

CPP 35.1 Wed 11:00 P1

Stability of biobased coatings on textiles — ●LUCIANA PLUNTKE^{1,2}, CONSTANTIN HARDER^{1,3}, SHOUZHENG CHEN^{1,4}, IULIANA RIBCA⁵, NADJA KÖLPIN¹, MARKUS OBERTHÜR², PETER MÜLLER-BUSCHBAUM³, MATS JOHANSSON⁵, and STEPHAN V. ROTH^{1,5} — ¹DESY, 22607 Hamburg, Germany — ²HAW, 20999 Hamburg, Germany — ³TUM School of Natural Sciences, Department of Physics, Chair for Functional Materials, 85748 Garching, Germany — ⁴University Hamburg, 20146 Hamburg, Germany — ⁵KTH Royal Institute of Technology, 10044 Stockholm, Sweden

Functionalizing textiles by spray-coating is in wide-spread use. Here, we focus on functional multi-layer protective coatings on light woven textile materials. The functionalization is achieved by spray-coating with bio-based materials.

We investigate the mechanical stability of these novel coatings and changes in the coating under external stress and standard abrasion conditions. Our aim is to determine the degree of stress that the coating can withstand under different types of mechanical stress until it loses its functionality. The results are important for implementing sustainable materials in textile industry.

CPP 35.2 Wed 11:00 P1

In situ GISAXS printing of biotemplated titania nanostructures — ●LINUS F. HUBER¹, MANUEL E. SCHEEL¹, STEPHAN V. ROTH³, and PETER MÜLLER-BUSCHBAUM^{1,2} — ¹Technical University of Munich, TUM School of Natural Sciences, Department of Physics, Chair for Functional Materials, James-Franck-Str. 1, 85748 Garching, Germany — ²MLZ, TUM, 85748 Garching — ³Deutsches Elektronen-Synchrotron (DESY), Notkestr. 85, 22607 Hamburg, Germany

Biotemplating is an effective method of nanostructuring hybrid inorganic-organic materials. This approach allows the tuning of material properties like porosity or domain sizes. Therefore, parameters like the electronic conductivity can be adjusted for different applications. In this work, differently structured Titania thin films are investigated for application in thermoelectric generators. Beta-lactoglobulin is a bovine whey protein that is used as a template during sol-gel synthesis. The Seebeck effect allows the conversion of waste heat into electrical energy. State of the art thermoelectric materials are rare, toxic and expensive. Biotemplated titania could provide a non-toxic and abundant alternative. 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 35.3 Wed 11:00 P1

A two-state Gaussian loop under tension: negative extensibility and ensemble inequivalence — ●GEUNHO NOH and PANAYOTIS BENETATOS — Department of Physics, Kyungpook National University, Republic of Korea

Loop formation is commonly observed in biopolymers and, in many cases, the loop structure is transient. Some examples of this structural rearrangement are the formation of denaturation bubbles in double-stranded DNA and the transient DNA looping associated with gene regulation. Here, we study the conformational statistics and the elastic behavior of a flexible polymer under tension with a two-state structure: looped or unlooped. We analyze two cases. In the first, the loop can zip to form a double-stranded chain. In the second, the dangling ends of a chain can bind to form a loop. In each case, we investigate the force-extension relation of the two-state loop in both the Helmholtz and the Gibbs ensembles. We also extend the two-level

system to a three-level Gaussian loop by introducing a third (intermediate) state. In contrast to the single Gaussian chain, the two- or three-level systems show qualitatively different tensile response and ensemble inequivalence. Interestingly they can have negative extensibility in the Helmholtz ensemble, and we point out that this is one of the simplest polymer models which exhibits such metamaterial-like behavior.

CPP 35.4 Wed 11:00 P1

Determination of the roast-dependent pore size in coffee beans using positron lifetime spectroscopy — ●ADRIAN LANGREHR, VASSILY BURWITZ, LUCIAN MATHES, and CHRISTOPH HUGENSCHMIDT — Forschungs-Neutronenquelle Heinz Maier-Leibnitz (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany

Positron Annihilation Lifetime Spectroscopy (PALS) is an established method to determine the type and concentration of open volume defects in crystals as well as to investigate the free volume in polymers. Using ²²Na as β^+ emitting radioisotope in the so-called "sandwich" geometry we present the capabilities of our four-detector setup with digital readout and signal processing. The efficient readout of this PAL spectrometer produces 12 lifetime spectra simultaneously. Our study encompasses the comparison of three different methods to combine information contained in these 12 spectra. To demonstrate a use case of a biomaterial we measured the positron lifetimes in coffee beans as a function of the degree of roasting. The application of the so-called Tao-Eldrup model allows us to study the influence of the roasting parameters on the mean pore size on the nanometer scale.

CPP 35.5 Wed 11:00 P1

Microgels for Enhanced Adsorption of Endothelial Cells on Artificial Networks — ●SOURAJ MANDAL and REGINE VON KLITZING — Soft Matter at Interfaces, Department of Physics, Technical University of Darmstadt, Germany

Artificial 3-D supply networks can be applied as a transport system for oxygen and nutrients, which can promote vascularization for organ-like 3-D cell culture systems. In the human body, the inner surface of such networks (blood vessels) is lined with a layer of endothelial cells and they play a vital role in cell maturation and angiogenesis (formation of new blood vessels). So far, the attachment of endothelial cells on the surface of the artificial network system is not sufficient. Addressing this problem, this study focuses on designing a suitable mediator between the inner walls of the artificial network and endothelial cells, which should be mechanically stable to flows of nutrient solutions. Here we employ Poly(N-isopropylacrylamide) (PNIPAm) microgel (MG) as cell-culturing surface mediator. However, the main challenges are (i) ensuring the firm adhesion of MGs on the surface of the artificial polymeric network, and (ii) seeding endothelial cells on top of them. As a primary approach, we synthesized positively charged MGs to attach them on plasma-treated silicon (Si) and 3-D printed polymeric surfaces. MG particles are characterized by their Zeta potential and hydrodynamic radius. As a rapid fabrication technique, spin coating was used to deposit a thin polymeric layer of MG particles on the substrates. AFM analyses showed a stable adhesion of MG particles on the flat surfaces even upon water washing and mechanical stress.

CPP 35.6 Wed 11:00 P1

Depletion induced phase behavior and equilibrium clusters in charged BSA and HSA protein solutions — ●MAXIMILIAN D. SENFT, FAJUN ZHANG, and FRANK SCHREIBER — Universität Tübingen, Germany

Understanding and predicting the phase behavior of proteins is an ongoing endeavor in many scientific research areas, including the phar-

maceutical industry. In addition to crystallization, liquid-liquid phase separation and condensate formation, which includes equilibrium clusters, dense liquid droplets, fibrils, and gels, appear to be closely related to many pathological conditions. The formation of equilibrium protein clusters in solution requires an interaction potential with competing contributions, i.e., long-ranged repulsion and short ranged attraction. Bovine and human serum albumin (BSA and HSA) carry negative charges at neutral pH which provide a long-range electrostatic repulsion between proteins. The attractive potential can be generated via the depletion interactions introduced by the non-adsorbing polymer polyethylene glycol in protein solutions. By tuning the ionic strength, polymer size and concentration, the competing potential can be continuously adjusted, resulting in equilibrium protein clusters due to the subtle balance to the different contributions of the interaction potential. Having performed systematic small angle scattering measurements, on BSA and HSA, together with quantitative modeling combined with protein phase diagrams a better understanding of depletion induced protein phase behavior and cluster state can be provided.

CPP 35.7 Wed 11:00 P1

Purely elastic instability of semi-dilute polymer solutions in shear flow — PEGAH SHAKERI^{1,2}, MICHAEL JUNG^{1,2}, and RALF SEEMANN^{1,2} — ¹Universität des Saarlandes, Saarbrücken, Germany — ²Max Planck-Institute for Dynamics and Self-Organization, Göttingen, Germany

Polymer solutions in the semi-dilute regime are of considerable industrial importance. The complex rheological properties of such highly viscoelastic fluids and the complexity of their flow characteristics, especially in curved geometries, require a thorough experimental characterization of the dynamics of such fluid flows. We experimentally investigate the flow of highly elastic polymer solutions above their overlap concentrations in a microfluidic serpentine channel using pressure measurements and particle image velocimetry. Our results show that the flow resistance increases significantly at high Weissenberg numbers but vanishing Reynolds numbers, indicating the occurrence of a purely elastic instability. We show that the onset of instability can be scaled by including shear-dependent rheological properties of the polymer solutions in the nonlinear stability analysis. As a result, a universal criterion as a function of normalized polymer concentration is provided for scaling the onset of pure elastic instability in the semi-dilute regime independent of the type and molecular weight of the polymer.

CPP 35.8 Wed 11:00 P1

Improved displacement efficiency in porous media by invasion of viscoelastic fluids — MICHAEL JUNG^{1,2}, PEGAH SHAKERI^{1,2}, and RALF SEEMANN^{1,2} — ¹Universität des Saarlandes, Saarbrücken, Germany — ²Max Planck-Institute for Dynamics and Self-Organization, Göttingen, Germany

Improving the displacement efficiency of capillary entrapments in porous media by adding high molecular weight polymers to the invading phase has a variety of industrial applications. Apart from an increased viscosity contrast compared to water flooding, the flow of viscoelastic polymer solutions exhibits unstable flow behavior even at small Reynolds numbers, which can lead to an additional displacement mechanism of the capillary entrapments. We use a microfluidic approach to reveal the underlying mechanism of this enhanced displacement by first considering a random array of cylindrical posts to identify fundamental differences in displacement processes for elastic and non-elastic fluids. Then, to focus directly on displacement processes driven solely by elastic stresses and to exclude the effects of viscous stresses, we consider a single capillary entrapment connected to two symmetric serpentine channels. We show that the unique viscoelastic fluid features, such as the emergence of a significant first normal stress difference, combined with the curved flow geometry, lead to purely elastic instability and elastic secondary flow, which in turn generate the stresses required to overcome the capillary threshold and displace capillary entrapment.

CPP 35.9 Wed 11:00 P1

Supraparticles: Aggregation of colloids in evaporating dispersion drops — MELIS YETKIN¹, YASHRAJ MANISH WANI², ARASH NIKOUBASHMAN², MICHAEL KAPPL¹, and HANS-JÜRGEN BUTT¹ — ¹Department of Physics at Interfaces, Max-Planck-Institute for Polymer Research, Germany — ²Institute of Physics, Johannes Gutenberg University Mainz, Germany

Evaporating dispersion drops from superamphiphobic surfaces opens

a way to fabricate supraparticles (SPs) with complex structures. The structure formation can be controlled by tailoring the interaction forces between particles and process conditions. In this study, the structure of the SPs was investigated by tuning the shape of the primary building blocks and the process conditions. Ellipsoidal polystyrene (PS) particles of different aspect ratios were obtained by stretching a polymeric film of spherical particles above the glass transition temperature. Aqueous dispersion drops of the ellipsoidal particles were evaporated from silicone nanofilaments-based superamphiphobic surfaces under varying humidity conditions, during which the evaporation process was monitored by a camera. The interaction between the building blocks, and hence the final morphology of the SPs, were altered by the addition of surfactant sodium dodecyl sulfate (SDS). Control experiments with spherical PS building blocks were conducted in parallel. The study elucidated the effect of primary building block shape on the final morphology of supraparticles and the transition between a shape-dominated regime and an interaction-dominated regime.

CPP 35.10 Wed 11:00 P1

Temperature dependent measurements of the diffusion- and Soret-coefficient in a binary polystyrene/toluene mixture — JANNIK KANTELHARDT and WERNER KÖHLER — Physikalisches Institut Universität Bayreuth, Germany

In this work we investigate the dependence of the diffusion- and Soret-coefficient in respect to different ambient temperatures with a temperature range from 10°C to 50°C in steps of 5°C. The here investigated system, a solution of polystyrene (PS) in toluene with a weight fraction of $c_{PS}=1\%$, has in a similar concentration also been used in the binary companion cell of the DCMIX4 microgravity campaign on ternary mixtures. Furthermore, binary and ternary polystyrene solutions are candidates for the forthcoming GIANT FLUCTUATIONS project of ESA for the investigation of non-equilibrium fluctuations under microgravity conditions.

The measurements were performed with a Thermal-Diffusion-Forced-Rayleigh-Scattering (TDFRS) setup. Through a writing beam a holographic grating is created inside the mixture where a small amount of an inert dye is added. The grating heats the sample periodically which leads to temperature gradients. Through the Soret-effect concentration gradients appear and both lead to changes in the refractive index. The signal is measured with a readout beam under Bragg diffraction.

CPP 35.11 Wed 11:00 P1

Diffusion, Thermodiffusion and turbidity of thermoresponsive Poly(N-acryloylglycinamide) in water. — ROMAN REH¹, NIKOLA MAJSTOROVIC², SEEMA AGARWAL², and WERNER KÖHLER¹ — ¹Universität Bayreuth, Physikalisches Institut, Germany — ²Universität Bayreuth, Macromolecular Chemistry II, Germany

We report about measurements on Poly(N-acryloylglycinamide) (PNAGA) in aqueous solution. Diffusion-, Thermodiffusion- and Soretcoefficients were measured with the polymer in linear form and as a crosslinked microgel. Furthermore, temperature dependent measurements on turbidity were done with the linear polymer. Experiments on diffusion were performed with the Optical-Beam-Deflection technique where a vertical temperature gradient is applied to the sample and information about the time dependent distribution of temperature and concentration in the sample is gathered by recording the position of a laser beam, which traverses the sample and gets deflected. This is because the refractive index changes with temperature and concentration, which on its part changes due to thermodiffusion. Turbidity measurements show a UCST-behavior and a hysteresis in the temperature of the cloud point, depending on the direction of the temperature ramp, which is in accordance with results from literature. Thermodiffusion- and Soretcoefficients at different temperatures are described with an exponential Piazza function [S. Iacopini et al., Eur. Phys. J. E **19**, 59-67 (2006)] and are comparable for the linear polymer and the microgel, showing a systematical behaviour and a change in sign in the region of about 35 to 40 °C.

CPP 35.12 Wed 11:00 P1

Measurement of diffusion and thermodiffusion of polydisperse polymers by means of a compact optical beam deflection setup — MAREIKE HAGER, ROMAN REH, and WERNER KÖHLER — Universität Bayreuth, Physikalisches Institut, Germany

We have performed diffusion and thermodiffusion experiments on solutions of polydisperse polymers by means of a newly developed double-pass optical beam deflection (OBD) instrument. The aim is to develop a model for the description of the multimodal OBD signals and to de-

velop the technique into a method for polydispersity analysis. The double-pass OBD instrument utilizes a laser beam that is reflected behind the Soret cell and passes the sample volume a second time. In the cell a vertical temperature gradient is applied that leads to thermodiffusion in the sample and, thus, to a concentration gradient and a gradient of the refractive index. The laser beam that traverses the cell twice is deflected and detected on a camera where the time dependent laser position is recorded. From the measured OBD signal the diffusion, thermodiffusion and Soret coefficients can be extracted. The multimodal time traces are evaluated with an adapted version of the CONTIN program for the solution of inverse problems. It is shown that diffusion coefficients extracted in this way agree with literature data. The results of the measurements of samples with two polymers of different sizes are in accordance with the results for the single components. Based on these results, polymers with a broad molar mass distribution can now be investigated.

CPP 35.13 Wed 11:00 P1

Mixture of magnetic and non-magnetic ellipsoids — ●ELENA PYANZINA¹, ANNA AKISHEVA¹, TATYANA BELAYEVA¹, MARINA GUPALO¹, and SOFIA KANTOROVICH² — ¹Ekaterinburg, Russia — ²University of Vienna, Vienna, Austria

In this contribution, mixtures of magnetic and non-magnetic ellipsoids were studied. We chose systems with the ratio of the semi-axes equal to 3 and 5 and different concentrations, as well as the direction of the magnetic moment along the main axis. The ratios of magnetic and non-magnetic particles considered were as follows: 30/70, 50/50 and 70/30. The initial susceptibility of such systems was calculated since the magnetic response of the system is very important for various applications. It turned out that with an increase in the magnitude of the magnetic moment, a structural transition occurs in the system: first, the initial susceptibility increases, and then it becomes almost zero. This is because the basic state of elongated ellipsoids is an antiparallel pair, which becomes stable with an increase in the magnitude of the magnetic moment. And its total magnetic moment is quite small, and the susceptibility of such an object is much lower than that of a pair of particles with a head to tail orientation. The behavior of mixtures of ellipsoids with similar systems of magnetic disks (like ellipsoids with a magnetic moment perpendicular to the main axis) was also compared. It turned out that at large values of the magnetic moment, the disks form "stacks" in which the magnetic moments are directed head to tail, and ellipsoids form flat structures with a thickness of one ellipsoid, with an antiparallel orientation of the moments.

CPP 35.14 Wed 11:00 P1

Mesoporous polymers as electrode material in hybrid organic-inorganic lithium-ion batteries — ●TOM WICKENHÄUSER¹, LUCAS UEBERRICKE², ANGELINA JOCIC², ERIK MISSELWITZ², ELISA THAUER¹, YUQUAN WU¹, MICHAEL MASTALERZ², MILAN KIVALA², and RÜDIGER KLINGELER¹ — ¹Kirchhoff Institute for Physics, Heidelberg University, Germany — ²Institute of Organic Chemistry, Heidelberg University, Germany

We report on the characterisation of mesoporous polymers as electrode materials in hybrid organic-inorganic lithium-ion batteries. In particular, dendritic pyrene tetraone (D-PTO) and triphenylamine (TPA) is investigated as cathode material and non-planar covalent carbon networks are studied as anode material in lithium half-cells. Cyclic voltammetry as well as galvanostatic cycling measurements were done to investigate on ionic and electric transport mechanisms. For redox active dendritic pyrene tetraone, the mesoporous character of the amorphous polymer is confirmed and the specific surface areas range up to nearly 700 m²g⁻¹. Galvanostatic cycling measurements show a specific capacity of 137 mAhg⁻¹ and a capacity retention of 86% after 50 cycles.

CPP 35.15 Wed 11:00 P1

Design, fabrication and nano-scale characterization of novel SEI layers — ●ZHUIJUN XU¹, YAJUN CHENG², YONGGAO XIA², and PETER MÜLLER-BUSCHBAUM^{1,3} — ¹TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — ²Ningbo Institute of Materials Technology and Engineering, Chinese Academy of Sciences, 315201, Ningbo, China — ³MLZ, TUM, 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. SEI can be enhanced by synergetic additives in commercial electrolytes. Herein, amphiphilic block copolymers/inorganic materials-PS-b-PEO/LiNO₃ as additives, which bear some clear advantages including absorbing mechanical stress, conducting lithium ion and controlling the lithium dendrite growth, are mixed with commercial electrolytes and applied in the lithium metal battery. Remarkably, Li symmetric cells have a long-term cycling life over 300 h with a capacity of 3 mAh cm⁻². Moreover, full battery with lithium metal anode and LiFePO₄ exhibits a stable and high capacity of 138 mAh g⁻¹ at 1 C. 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.

CPP 35.16 Wed 11:00 P1

Less is more: tiny amounts of insoluble multi-functional microporous additive plays a big role in lithium secondary batteries — ●RUOXUAN QI¹, PETER MÜLLER-BUSCHBAUM^{1,2}, and YAJUN CHENG³ — ¹TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — ²MLZ, TUM, Garching, Germany — ³NIMTE, CAS, Zhejiang Province, P. R. China

Binders play an important role in multi-component electrodes for rechargeable batteries, which suffer from poor electronic and ionic conductivity. Binder-free electrodes provide another way to resolve problems, where sophisticated structure construction is required. A new concept of electrode processing alternative to binder-containing and binder-free electrodes was established. A multi-functional PIM-1 (a polymer with intrinsic microporosity) additive was used instead of PVDF to form mechanically processable Li secondary battery cathodes. Due to its unique nanoporous structure built by the spiro-containing rigid aromatic polymer chain, only a tiny amount of PIM-1 in the LiNi_{0.8}Co_{0.1}Mn_{0.1}O₂ cathode is needed to retain good performance, far below the typical composition for PVDF. Homogeneous dispersion of carbon black is achieved by PIM-1, which stabilizes the electrode and increases the electronic conductivity. Different from PVDF, mechanical buffering by stiff PIM-1 yields crack-free electrodes after cycles. Moreover, an inorganic rich cathode-electrolyte interface layer is formed via a desolvation process promoted by PIM-1, because of its strong binding ability with lithium ions, which is beneficial for cyclic stability and rate capability.

CPP 35.17 Wed 11:00 P1

Positrons probe advanced and functionalized porous materials — ●AHMED GAMAL ATTALLAH, ERIC HIRSCHMANN, MAIK BUTTERLING, MACIEJ OSKAR LIEPKE, and ANDREAS WAGNER — Institute of Radiation Physics, Helmholtz-Zentrum Dresden-Rossendorf

Positron annihilation lifetime spectroscopy (PALS) is an effective porosimetry technique complementing standard gas intrusion methods. PALS is able to detect open and closed pores, and resolve depth-dependent porosity. It can operate under variable pressures, temperatures, and atmospheres to monitor structural changes during in situ conditions. In this contribution, PALS results of various functionalized porous materials including polymer grating, structural changes in metal-organic-frameworks (MOFs), effect of additives in food ingredients (maltodextrin) on water uptake, and impact of modification of low-k dielectrics on stiffness will be presented. In polymer grafting, the mechanism of polymer grafting on MCM-48-type mesoporous silica nanoparticles forming core-shell composite structure is understood from PALS. Uniquely in MOFs, PALS was able to prove that the temperature-driven transformed metal-organic framework DUT-8(Ni) is still porous possessing closed porosity that is not accessible by other techniques. Sucrose in maltodextrin is the third topic where in situ humidity experiment during PALS revealed that adding 10 % sucrose to maltodextrins has a negligible effect on hygrocapacity at relative humidity > 50 %. Finally, the improved mechanical stability of low-k materials by adding methyl terminal groups that cause less interconnected pores has been verified by positron annihilation.

CPP 35.18 Wed 11:00 P1

Insights into the morphology-structure-property relationship of mesoporous ZnO films during humidity sensing — ●TING TIAN¹, SHANSHAN YIN¹, SUO TU¹, APOSTOLOS VAGIAS², ANNALENA OECHSLE¹, TIANXIAO XIAO¹, SIGRID BERNSTORFF³, and PETER MÜLLER-BUSCHBAUM^{1,2} — ¹Technical University of Munich, TUM School of Natural Sciences, Department of Physics, Chair for Functional Materials, 85748 Garching — ²MLZ, TU München, 85748 Garching — ³Elettra-Sincrotrone Trieste S.C.p.A., Strada Statale 14

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Moisture can strongly influence the conductivity of ZnO semiconductors via the physisorption and chemisorption of water molecules on the ZnO surface. Mesoporous ZnO structures can facilitate the absorption process by providing a large surface area and active sites. However, little effort has been devoted yet to gain an in-depth understanding of the effect of water on the morphology and electrical property. In the present work, different mesoporous ZnO thin films were synthesized by exploiting different diblock copolymers. Benefiting from the different inorganic frameworks, these thin films show significantly different structural properties and defects density. To explore the morphology-structure-property relationship, in situ Fourier-transform infrared spectroscopy (FTIR) was used to confirm the water absorption. Simultaneously, in situ grazing-incidence small-angle X-ray scattering (GISAXS) measurements were performed to investigate the morphology evolution, and in situ electrochemical impedance spectroscopy (EIS) was used to monitor the conductivity changes.

CPP 35.19 Wed 11:00 P1

Morphology transformation pathway of block copolymer-directed cooperative self-assembly of ZnO hybrid films monitored in situ during slot-die coating — •TING TIAN¹, SHANSHAN YIN¹, SUO TU¹, CHRISTIAN L. WEINDL¹, KERSTIN S. WIENHOLD¹, SUZHE LIANG¹, MATTHIAS SCHWARTZKOPF², STEPHAN VOLKHER ROTH², and PETER MÜLLER-BUSCHBAUM^{1,3} — ¹Technical University of Munich, TUM School of Natural Sciences, Department of Physics, Chair for Functional Materials, 85748 Garching — ²James-Franck-Str. 1 — ³MLZ, TUM, 85748 Garching

Co-assembly of diblock copolymers (DBC) and inorganic precursors that takes inspiration from the rich phase separation behavior of DBCs can enable the realization of a broad spectrum of functional nanostructures with the desired sizes. In a DBC assisted sol-gel chemistry approach with polystyrene-block-poly(ethylene oxide) and ZnO, hybrid films are formed with slot-die coating. Pure DBC films are printed as control. In situ grazing-incidence small-angle X-ray scattering (GISAXS) measurements are performed to investigate the self-assembly and co-assembly process during the film formation. Combining complementary ex situ characterizations, several distinct regimes are differentiated to describe the morphological transformations from the initially solvent-dispersed to the ultimately solidified films. The precursor reduces the degree of order, prevents crystallization of the poly(ethylene oxide) block, and introduces additional length scales in the hybrid films.

CPP 35.20 Wed 11:00 P1

Evaluation of different textile mount designs for printing on textiles in commercial SLA 3D printers for scientific investigation — •TIMO GROTHE¹, ELISE DIESTELHORST¹, JAN LUKAS STORCK¹, DANIEL KOSKE¹, NATALIE FRESE², and MARTIN WORTMANN² — ¹Faculty of Engineering and Mathematics, Bielefeld University of Applied Sciences, Interaktion 1,33619 Bielefeld, Germany — ²Faculty of Physics, Bielefeld University, Universitätsstraße 25, 33615 Bielefeld, Germany

The technology of 3D printing has already reached the commercial sector. But it is not only the industry that is interested in 3D printing; the scientific world is also investigating the possibilities of this multifaceted technology. Here, in addition to the fused deposition modeling (FDM) process, the cornerstone stereolithographic (SLA) process in particular has become the focus of scientific attention. Especially in combination with textiles, some unique composites with outstanding properties can be produced. In order to be able to print these in commercially available printers, some textile mounts were developed and their applicability as well as usability were investigated. Not only the printing result and the adhesion between resin and different textiles were investigated by abrasion tests, but also the application of the individual holders was evaluated. Finally, the produced composites were examined with a scanning helium ion microscope to show, in combination with the other examination methods, that both the textile-resin composites have exceptional abrasion resistance and that the textile holders make it much easier to produce them.

CPP 35.21 Wed 11:00 P1

Polymer Composite Films with Induced Structural Anisotropy for Thermoelectric Application — •CHRISTIAN GRADL¹, MARIE SIEGERT¹, and JENS PFLAUM^{1,2} — ¹Experimental Physics VI, University of Würzburg, 97074 Würzburg — ²ZAE Bayern, 97074 Würzburg

Thermoelectric generators offer a prospective opportunity to handle the increasing energy demand by utilizing waste heat. Organic thin films represent a promising candidate because of benefits like non-toxicity, cost-effectivity or versatile implementation. For an efficient thermoelectric device, the thermoelectric figure of merit $zT = \sigma S^2 T / \kappa$ needs to be high. So the Seebeck coefficient S and the electrical conductivity σ should achieve high values, whereas the thermal conductivity κ has to be low. Taking advantage of the intrinsically low κ , we combine the polymer PEDOT:PSS with additives like silver nanowires, the crystalline organic TTT₂I₃ or VO₂ needles, by which a higher σ is aspired without pronounced detriment of the Seebeck coefficient. TTT₂I₃ and VO₂ are fabricated via microspacing in-air sublimation. Controlled orientation of the additives induced by the substrate is a main topic of our research. Further we investigate the alignment of additives embedded in polymer thin films prepared via doctor-blading to improve the efficiency for thermoelectric application. The results on characterizing the electrical and thermal properties of the organic-metallic composites with respect to their anisotropy will be presented.

CPP 35.22 Wed 11:00 P1

Morphological studies in semicrystalline polymers and polymer nanocomposites using spin diffusion — •DORIT HARTMANN, ANNA NITSCHKE, YURY GOLITSYN, HORST SCHNEIDER, and KAY SAALWÄCHTER — Department of Physics / NMR Group, University of Halle, Betty-Heimann-Str. 7, 06120 Halle, Germany

ABSTRACT: The properties of synthetic polymers can be selectively modified by adding nanoparticles, which is why polymer nanocomposites have a wide range of applications. The interaction of the polymer chains with the surface of silica particles leads to the formation of a multiphase structure, characterized by a gradient of molecular dynamics. [1] Studies of polymer nanocomposites using spin diffusion (SD) experiments in conjunction with the numerical simulations have shown that the interphases exhibit complex morphology with dynamic heterogeneities. [2] In this work, we investigate the effect of magnetic field strength on spin diffusion in semicrystalline poly(ϵ -caprolactone) and a poly(2-vinyl pyridine)-silica nanocomposite. The experiments were performed at two different field strengths of 0.47 T and 4.7 T (proton Larmor frequency of 20 MHz and 200 MHz, respectively) and were supported by spin diffusion calculations. In addition, this paper aims to provide an overview of the different data acquisition and analysis strategies for high- and low-field instruments. **REFERENCES:** [1] Horst Schneider, Kay Saalwächter, and Matthias Roos. *Macromol.* (2017), 50, 8598-8610. [2] Horst Schneider, Matthias Roos, Yury Golitsyn, Kerstin Steiner, and Kay Saalwächter. *Macromol. Rapid Commun.* (2021), 2100061.

CPP 35.23 Wed 11:00 P1

Two-step electrochemical Au nanoparticle formation in polyaniline — •BIN ZHAO and SEBASTIAN GUTSCH — institut für mikrosystemtechnik, freiburg, germany

In this study, we report on an electrochemical insertion of Au nanoparticles in polyaniline (PANI) using a two-step process. In the first step, tetrachloroaurate anions (AuCl₄⁻) are attached on the protonated imine sites of PANI while holding the potential at +0.8 V. The applied electrochemical potential prevents any reduction of the PANI/AuCl₄⁻ complex. After rinsing of excess AuCl₄⁻, a controlled reduction is carried out via cyclic voltammetry. Therefore, we investigate the introduction of Au species into PANI via precise electrochemical control in a flow cell system. The PANI/Au composites are characterized using scanning electron microscopy (SEM) and Rutherford backscattering spectrometry (RBS) to quantify the amount of introduced Au. It is demonstrated that the PANI/AuCl₄⁻ complex is not aggregating prior to the electrochemical reduction process. However, the controlled reduction of these PANI/Au complexes leads to the subsequent formation of Au nanoparticles, whose density and size dispersion depend on the Au loading in PANI. Furthermore, additional Au deposition cycles increase both the Au nanoparticle density and size. We propose a two-step growth model based on our experimental results. The results are discussed with respect to the formation of atomic Au clusters reported in previous works.

CPP 35.24 Wed 11:00 P1

Accelerating self-assembly of colloidal particles at air-water interface by laser induced heating of upconverting particle — •LOKESH CHINNAKANA MURUGA, GOKUL NALUPURACKAL, SRESTA ROY, SNIGDHAVEV CHAKRABORTY, JAYESH GOSWAMI, and BASUDEV ROY — Indian Institute of Technology Madras, Chennai, India -

600036

Particles can be assembled at the air-water interface due to optically induced local heating. This induces convection currents in the water which brings particles to the surface. We improve the technique by employing an upconverting particle (UCP), which, when illuminated with 975 nm light, not only emits visible emission but also generates heat owing to the poor efficiency of the upconversion process. This induces strong convection currents which makes particles dispersed in the suspension assemble at the interface and immediately under the UCP. We show assembly of polystyrene particles of 1 μm diameter and diamonds of 500 nm diameter bearing Nitrogen-Vacancy (NV) centers around the UCP. We also show, for the first time, that the microdiamonds are assembled within about 30 nm at the bottom of the UCP by utilizing non-radiative energy transfer that reduces the lifetime of the 550 nm emission from about 90 μs to about 50 μs .

CPP 35.25 Wed 11:00 P1

Following the directed self-assembly of crystallizable block co-oligomers via in situ AFM — ●ALEXANDER MEINHARDT¹, PENG QI², IVAN MAXIMOV³, and THOMAS F. KELLER¹ — ¹Centre for X-ray and Nano Science (CXNS), Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — ²Paul Scherrer Institut, Villigen, Switzerland — ³Solid State Physics and NanoLund, Lund University, Lund, Sweden

Bottom up nanofabrication utilizing the molecular self-assembly of block co-oligomers with sub-10 nm domain sizes is 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 the 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. On a planar Si surface we observed the self-assembly of PE-b-PEO into locally ordered lamellar surface structures extending over several micrometers. Directed self-assembly (DSA) of this PE-b-PEO system by physical guiding patterns can enable the formation of large scale nanostructures interesting for future applications. First DSA experiments indicate that the formed PE-b-PEO based surface nanostructures depend on the pitch of the guiding pattern. We furthermore aim to use in situ AFM to shed light on the pitch-dependent structural evolution during dedicated temperature-controlled annealing procedures.

CPP 35.26 Wed 11:00 P1

Intracrystalline dynamics of polybutylene succinate and poly(3-Hydroxybutyrate) — ●MOHD AFIQ BIN ANUAR, YU QIANG, THOMAS THURN-ALBRECHT, and KAY SAALWÄCHTER — Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle, Germany

The dynamics behavior of polymers chain in crystal lamellae plays a critical role for its semicrystalline morphology [1, 2]. It is influenced by this intracrystalline dynamics (ICD) explaining the factors that limit its crystal thickness during isothermal crystallization. In this work, two different behaviours of semicrystalline polyesters, namely polybutylene succinate (PBS) and poly(3-Hydroxybutyrate) (P3HB), are discussed. A combination of nuclear magnetic resonance (NMR) techniques shows that isothermally crystallized PBS exhibit slow ICD longer than 1s which is similar to the reported crystal-fixed polymer, polycaprolactone [1]. Meanwhile, in P3HB crystal chain, the ICD with correlation jump motion around 0.5s/monomer at 120°C was detected. This is in contrast to previous reported [3] demonstrating a crystal-mobile behavior. Small-angle X-ray scattering measurement reveal that the P3HB crystal lamellae are significantly thicker than in PBS, confirming that P3HB and PBS can be classified as crystal-mobile and crystal-fixed, respectively. Details regarding morphology are shown in the poster.

References: [1] Schulz, M., et al., *Macromolecules* 2018, 51, 8377. [2] Schulz, M., et al., *Nat. Common.* 2022, 13, 1. [3] Xia, Z., et al., *Soft Matter* 2021, 17, 4195.

CPP 35.27 Wed 11:00 P1

Non-linear mechanical properties of polycaprolactone polymer/oligomer blends with defined entanglement density and crystalline thickness — ●TONGHUA LIU, ALBRECHT PETZOLD, and THOMAS THURN-ALBRECHT — Von-Danckelmann-Platz 3, 06120, Halle(Saale)

The mechanical properties of semi-crystalline polymers are determined by the semi-crystalline morphology and the entanglements in the amorphous regions. Here we use polymer/oligomer blends to control the entanglement density independently of the crystallinity. This system is also used as a model to study effects on the non-linear mechanical properties. The aim of the project is to develop a quantitative method for the determination of the entanglement density in the amorphous region as well as to investigate its relation to yielding, modulus and strain hardening. The commonly used method is tensile testing, but cavitation and necking cannot be avoided. Instead, we use plane-strain compression tests, which allow the direct determination of the true stress and avoids problems like cavitation. A separation of viscous and elastic contributions can be achieved by inserting relaxation measurements during the deformation. Our preliminary results indicate a strong effect of the crystallinity on the modulus and yield stress. The relation between strain hardening and entanglement density will be discussed.

CPP 35.28 Wed 11:00 P1

New experimental methods for structure analysis of soft matter — ●ERIC EUCHLER¹, ANNA KATHARINA SAMBALE¹, REGINE BOLDT¹, KAI UHLIG¹, LAURA NEUMANN¹, KONRAD SCHNEIDER¹, MATTHIAS SCHWARTZKOPF², STEPHAN ROTH^{2,3}, and MARKUS STOMMEL^{1,4} — ¹Leibniz-Institut fuer Polymerforschung, Dresden, Germany — ²Deutsches Elektronen Synchrotron DESY, Hamburg, Germany — ³KTH Royal Institute of Technology, Stockholm, Sweden — ⁴Technical University Dresden, Dresden, Germany

Recently developed stretching devices for synchrotron measurements are available to investigate deformation-induced phenomena, such as strain-induced crystallization in natural rubber or void formation in biological tissues, at quasi-static and impact loading. In addition to measurements in transmission, novel studies of thin layers on flexible substrates can be realized by performing in situ grazing-incidence (GI) experiments.

Beside structure analysis in solid parts, the flow-induced structure formation in polymer melts is of particular interest to better understand the impact of melt processing parameters on macroscopic material properties, such as Young's modulus and tensile strength. For this purpose, a new experimental setup has been designed and built to study time- and temperature-dependent structure evolution events in thermoplastics. Within a temperature-controlled flow channel, polymer melts can be monitored with a microfocus X-ray synchrotron beam and first results obtained for two different thermoplastic materials proofed the experimental concept under quiescent melt conditions.

CPP 35.29 Wed 11:00 P1

Towards experimental detection of crystallization in individualized polymer chains — ●WING KIT OR, ALAA HASSAN, and MARTIN TRESS — Peter Debye Institute for Soft Matter Physics, Leipzig University, Leipzig, Germany

Although crystallization of polymers has been investigated since decades, it is not yet fully understood. One way to gain more insight is to study the difference between bulk polymer and confined polymer chains with focus on how crystallization characteristics change depending on the size and type of confinement. Until now, most studies have used confinement in thin films or nanopores but the approach to study crystallization and aggregation in individual chains was accessible only to computer simulations. Since detection of phase transitions in individual polymer chains poses a severe challenge to most experimental methods, the measurement of ensembles of individual chains is desirable. However, maintaining the individual character requires a sophisticated method to separate them. Here, we use block copolymer micelle lithography (BCML) to deposit a regular pattern of well-separated gold nanodots on a silicon substrate in order to chemically graft end-functionalized polymer chains on these nanodots to individualize them. Instead of common thermodynamic methods (which require considerably more sample material), we employ dielectric spectroscopy using a nanostructured electrode arrangement since it is much more sensitive. Albeit being typically considered a dynamics method, it also allows to examine density changes and thus phase transitions of polymers.

CPP 35.30 Wed 11:00 P1

Uniaxially Aligned Merocyanine Films by Graphene Nanoribbon Templated Growth — ●PHILIPP WEITKAMP, NORA GILDEMEISTER, LUKAS BÖHNER, DIRK HERTEL, and KLAUS MEERHOLZ — Physikalische Chemie, Universität zu Köln, Deutschland

We herein report the unique and novel approach of achieving a poly-

crystalline thin film consisting of uniaxially aligned domains by using 7-armchair graphene nanoribbon (7-aGNR) monolayers as van-der-Waals template. For this purpose, a merocyanine dye was evaporated on 7-aGNRs, transferred on quartz glass substrates. The alignment of the formed molecular aggregate along the GNR alignment direction was proven by polarisation dependent absorbance spectroscopy. The J- and H-transition, formed by the dye aggregate, were correlated with distinct axes of the crystal structure. By combining this correlation with polarisation dependent absorbance measurements and X-ray diffraction experiments we elucidated the three-dimensional structure of the formed aggregate thin film. The growth mode of these films was investigated as a function of the applied layer thickness. Atomic force microscopy-based morphology analysis and X-ray diffraction experiments were used to reveal the anisotropic on-surface crystallisation along the 7-aGNR long axes direction. Furthermore, we found that the delocalisation length of the aggregate increases with increasing in-plane order. Finally, we demonstrated that the in-plane alignment leads to an anisotropic charge carrier transport by implementing the templated merocyanine thin film as active layer in a top-gated organic field effect transistor.

CPP 35.31 Wed 11:00 P1

Long chain Polyamides: Influence of methylene sequence length and external forces on structural features — ●RENE SATTLER^{1,2}, VARUN DANKE³, and MARIO BEINER^{1,2} — ¹Fraunhofer IMWS, Walter-Hülse-Str. 1, D-06120 Halle (Saale), — ²Martin-Luther-Universität Halle-Wittenberg, Naturwissenschaftliche Fakultät II, D-06099 Halle (Saale) — ³Evonik Operations GmbH, Research Development & Innovation, Paul-Baumann-Str. 1, D-45722 Marl

Crystallographic studies towards the influence of methylene sequence length on a series of even-even polyamides PA 10.n (with n = 12, 14, 16 and 18) are performed. Temperature-dependent X-ray diffraction measurements show that the triclinic α phase is the preferred phase at room temperature after slow cooling from melt. In PA 10.12 and PA 10.14 a reversible Brill transition to the (pseudo)hexagonal high temperature γ phase is observed. However, the Brill transition temperature is strongly dependent on n and shifting to higher temperatures with increasing methylene sequence length. For the two higher members a Brill transition is absent. The analysis of annealed, uniaxial oriented fibers reveals that the crystalline state achieved under ambient conditions is influenced by external forces. This is due to relatively small energetic differences between the α and β polymorphs. All the uniaxial oriented PA 10.n samples show a β polymorph which is most prominent for PA 10.12 and PA 10.14. The higher members show a mixture of the β polymorph superimposed with a certain fraction of the α polymorph.

CPP 35.32 Wed 11:00 P1

Bond order parameters in crystallization of short polymer chains in thin films: SAMC simulation — ●EVGENIYA FILIMONOVA, TIMUR SHAKIROV, and VIKTOR IVANOV — Martin Luther University of Halle-Wittenberg, Institute of Physics, 06120, Halle (Saale), Germany

We study the crystallization of polymer melts in thin films using a coarse-grained model and stochastic approximation Monte Carlo (SAMC) simulation. Our goal is to reveal physical factors which are responsible for one of two possible scenarios of surface-induced polymer crystallization: heterogeneous nucleation or prefreezing. We have developed an approach that allows us to identify the translational and orientational local ordering by means of comparing our system configurations with reference crystalline structures of different symmetries. In addition to calculating the usual order parameters (Steinhardt parameters, common neighbors analysis, nematic order parameter, etc.), we suggested new order parameters based on scalar products of bonds between nearest neighbors. We observe a coexistence of an isotropic structure in the center of the film with ordered structures at the walls at intermediate values of energies (in microcanonical analysis). A change in the crystal structure accompanying a change in density at different energies is also shown. Financial support of the International Graduate School AGRIPOLY supported by the European Social Fund (ESF) and the Federal State Saxony-Anhalt is acknowledged.

CPP 35.33 Wed 11:00 P1

Investigating the thermodynamics and kinetics of catechin pyrolysis for environmentally friendly binders — ●JAKOB KRAUS and JENS KORTUS — Institute of Theoretical Physics, TU Bergakademie Freiberg, Leipziger Str. 23, D-09599 Freiberg, Germany

The thermodynamics and kinetics of the pyrolysis of (+)-catechin, a building block of the condensed tannins found in recipes for sustainable binders, are evaluated at the CCSD(T) level and compared to other methods from quantum chemistry. Using the climbing image nudged elastic band method coupled with transition state optimization, minimum energy paths and highest-energy transition states are identified for the first two pyrolysis steps, a catechol splitoff with subsequent dehydrogenation. While the catechol splitoff path was very smooth, the dehydrogenation featured an additional transition state in the form of an OH group rotation. The combined reaction was judged endothermic in the range of 0 K to 1250 K, and exergonic at 1000 K and above. It is shown that the catechol splitoff is the rate-determining step of the pyrolysis of catechin, which is equivalent to kinetic inhibition at all investigated temperatures.

CPP 35.34 Wed 11:00 P1

Pyrolysis of ellagic acid - a thermodynamic and kinetic study by means of quantum chemistry — ●PHILIP SCHÖNE, JAKOB KRAUS, and JENS KORTUS — TU Bergakademie Freiberg (Institut für Theoretische Physik) Leipziger Str. 23, 09599 Freiberg, Deutschland

By performing ab-initio calculations, thermodynamic and kinetic data on the pyrolysis of ellagic acid were computed. The reaction path consists of two decarboxylations and two hydrolyses. The pyrolysis of ellagic acid can take place via the formation of either hexahydroxydiphenic acid or urolithin m5. Using select DFT functionals and quantum chemical methods, data for each reaction were calculated between 0 K and 1200 K. The occurring decarboxylations were found to be very similar to each other, being exothermic and exergonic reactions that become increasingly so with rising temperature. The hydrolyses show the opposite behavior, being slightly endothermic and endergonic reactions that become increasingly so with rising temperature. With the help of the climbing image nudged elastic band method, mechanisms for all reactions could be proposed and highest energy transition states could be identified. For the decarboxylations, these represent H transfers from the carboxylic group to the neighboring C atom. For the hydrolyses, the highest energy transition states correspond to H transfers from water to the nascent carboxylic group. Moreover, the rate-determining steps in the pyrolysis of ellagic acid were determined, which are the hydrolyses of urolithin m5 and luteic acid.

CPP 35.35 Wed 11:00 P1

Transversal piezo-force-microscopy with the use of interdigitated electrodes — ●MAXIMILIAN LITTERST, ANDREY BUTKEVICH, and MARTIJN KEMERINK — Institute for molecular systems engineering and advanced materials, Heidelberg, Germany

Piezoresponse force microscopy (PFM) is a simple method to measure the piezoelectric effect of many materials with an atomic force microscope (AFM). Usually, a voltage is applied between the tip and the substrate to trigger a vertical displacement of the material via the converse, longitudinal, piezoelectric effect, which results in a vertical displacement of the tip. The transversal piezoelectricity can result in a torsion of the tip, it is however often very difficult to find a direct connection between the two.

Here, we present how interdigitated electrodes (IDEs) can be used to apply an electric field in the film-plane, resulting in a vertical displacement of the film due to the converse, transversal, piezoelectric effect. In addition, the longitudinal component can be measured via the torsional tip motion. This does not only provide a direct way to measure the transverse piezoelectricity, but also opens new possibilities for the device preparation.

CPP 35.36 Wed 11:00 P1

Ca substitution instead of Sr in La_{0.58}Sr_{0.4}Co_{0.2}Fe_{0.8}O_{3- δ} as a cathode electrode for IT-SOFCs — ●MAJID JAFARI¹, FATEMEH YADOLLAHI FARISANI², NORBERT MENZLER³, CHRISTIAN LENSER⁴, and FABIAN GRIMM⁵ — ¹Plön, Germany — ²Isfahan university of technology, Isfahan, Iran — ³Forschungszentrum Jülich, Jülich, Germany — ⁴Forschungszentrum Jülich, Jülich, Germany — ⁵Forschungszentrum Jülich, Jülich, Germany

La_{0.58}Ca_{0.4}Co_{0.2}Fe_{0.8}O_{3- δ} (L58CCF) was synthesized and evaluated as a cathode electrode for intermediate temperature solid oxide fuel cells (IT-SOFC) based on the Y₂O₃-stabilized ZrO₂ (YSZ) electrolyte. The effect of sintering temperature on the L58CCF performance was investigated. The best Area specific resistances (ASRs) for the L58CCF sintered at 950 °C were 1.218, 0.447, 0.228, 0.156, 0.099 $\Omega.cm^2$ at 600, 650, 700, 750, 800 °C, respectively.

CPP 35.37 Wed 11:00 P1

Antiperovskites (Li₂Fe)ChO as cathode material for lithium-ion batteries and investigation of the reaction mechanism — •BOWEN DONG¹, LENNART SINGER¹, MOHAMED ABDULLAH ABDULLAH MOHAMED², SILKE HAMPEL², NICO GRÄSSLER², and RÜDIGER KLINGELER¹ — ¹Kirchhoff Institute for Physics, Heidelberg University, Germany — ²Leibniz Institute for Solid State and Materials Research (IFW) Dresden e.V., Germany

Due to its unique structure, antiperovskite (Li₂Fe)ChO (Ch = S, Se) have emerged as a promising Li-ion battery (LIB) cathode material with excellent rate capability and a good discharge capacity. We report synthesis of antiperovskites by a direct ball-milling process and evaluate the phase stability, cycling performance, and rate performance. The effect of post-synthesis heat treatment on the resulting materials as well as on its battery performance is studied. Cyclic voltammetry studies reveal a high-voltage decomposition process which progressively yields the formation of Fe_xCh_y. Galvanostatic measurements exhibit outstanding electrochemical cycling performance of antiperovskite-based cathodes of 250 mAh/g at 0.1 C. Further, we suggest a route to avoid the progressing conversion of (Li₂Fe)ChO (Ch=S, Se) to Fe_xCh_y which effectively improves the cell performance of antiperovskites.

CPP 35.38 Wed 11:00 P1

Rational Design of Novel Photoswitches with Generative Models — •ROBERT STROTHMANN, CHRISTIAN KUNDEL, JOHANNES MARGRAF, and KARSTEN REUTER — Fritz-Haber-Institut der MPG, Berlin, Germany

The sheer vastness of chemical spaces poses a daunting challenge to molecular discovery through high-throughput screening based on exhaustive sampling. Generative models (GMs) are an emerging machine learning (ML) approach that enables a more guided discovery. Implicitly learning chemical design rules from large reference data sets and suitable descriptors of a targeted functionality, GMs directly propose promising, yet diverse candidates.

Here we explore the use of GMs for the design of novel molecular photoswitches. In a first step, large general molecular databases are used to train a GM to generate chemically valid photoswitches. In a second step, the creation process needs to be conditioned towards performant switching capabilities. In the absence of sufficient corresponding experimental reference data, this conditioning is based on synthetic first-principles data. For that purpose computationally efficient descriptors are used in a multi-objective fashion to account for the desired key aspects of the switching process.

CPP 35.39 Wed 11:00 P1

Correlating molecular properties to nonlinear optical activity: Prerequisites for white light generation. — •FERDINAND ZIESE, LENA ALBOHN, KEVIN EBERHEIM, and SIMONE SANNA — Institut für Theoretische Physik Heinrich-Buff-Ring 16, 35392 Gießen, Germany

Recent studies have demonstrated white light generation from molecular clusters with adamantane-like cores and different ligands [1,2]. To understand the origin of this behavior, we have investigated structural, electronic, and (nonlinear) optical properties from first principles for isolated molecules and dimer structures [3]. In this contribution, we focus on the comparison between isolated molecules and molecular dimers. We correlate the structural and electronic properties with the optical response and investigate the effect of symmetry and heterogeneous composition.

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[2] N. W. Rosemann, J. P. Eufner, E. Dornsiepen, S. Chatterjee, S. Dehnen, *J. Am. Chem. Soc.* 2016 138 (50), 16224-16227

[3] S. Schwan, A. J. Achazi, F. Ziese, P. R. Schreiner, K. Volz, S. Dehnen, S. Sanna, D. Mollenhauer, *J. Comput. Chem.* 2022

CPP 35.40 Wed 11:00 P1

Effect of electron and laser irradiation on the structure of halogen substituted adamantane clusters — •LENA ALBOHN, SIMONE SANNA, KEVIN EBERHEIM, and FERDINAND ZIESE — Institut für Theoretische Physik Heinrich-Buff-Ring 16, 35392 Gießen, Germany

Functionalized adamantane molecular clusters are highly nonlinear optical materials which are able to convert infrared radiation into a directed emission supercontinuum. While the origin of the optical nonlinearity is still under debate, the amorphous habitus of the materials

seems to be a prerequisite for the white-light generation.

Unfortunately, many adamantane-based or organotetrel clusters crystallize in an ordered structure characterized by intense second-harmonic generation instead of white-light emission. In order to render the molecular crystals amorphous, electron or laser irradiation has been suggested. In order to explain the mechanisms leading to the structural modification, we model electron or laser irradiation from first principles. Thereby, we employ halogen substituted adamantane clusters as a model system. Our calculations reveal that laser and electron irradiation have a similar effect on the compounds. Depending on the irradiation dose, intermolecular rearrangements as well as intramolecular deformations (photochemical rearrangement) may occur, thus facilitating the white-light emission.

CPP 35.41 Wed 11:00 P1

Structural properties of a semi-dilute suspensions of magnetic multicore nanoparticles — •EKATERINA NOVAK¹, ANDREY KUZNETSOV², ELENA PYANZINA¹, MARINA GUPALO¹, TATYNA BELYAEVA¹, and SOFIA KANTOROVICH² — ¹Ekaterinburg, Russia — ²University of Vienna, Vienna, Austria

During the last thirty years, magnetic soft matter systems have become highly promising candidates for medical applications such as magnetic hyperthermia and magnetic drug targeting. The subject of this work, magnetic multicore nanoparticles (MMNPs), are rigid clusters of single-domain magnetic nanocrystals (cores or grains) embedded in a polymer or other non-magnetic matrix. While the grains typically have a characteristic linear size of the order of 10 nm, the size of MMNPs can range from tens to a few hundred nanometers. Here, using Langevin dynamics computer simulations, we investigated diluted suspensions of MMNPs composed by grains, whose positions are fixed within the particle body, but their magnetic moments are free to rotate, corresponding to the grains with negligibly low magnetic anisotropy.

We calculated cluster size distributions and compared them to their counterparts in a system of single-domain magnetic nanoparticles. A drastic difference was found: for two MMNPs to aggregate they need to form a bridge of a stable array of grains from both multicores that are connected via dipolar interactions. The more bridges the two MMNPs form, the more stable is their aggregate.

CPP 35.42 Wed 11:00 P1

Characterisation and transport within tetra-PEG*tetra-PCL amphiphilic end-linked polymer model networks — •LUCAS LÖSER¹, CAROLIN BUNK², FRANK BÖHME², and KAY SAALWÄCHTER¹ — ¹Inst. F. Physik * NMR, Martin-Luther-Universität Halle-Wittenberg, Halle/D — ²Leibniz-Institut für Polymerforschung Dresden e.V., Hohe Str. 6, Dresden/D

A new approach for the synthesis of model-like amphiphilic co-networks is introduced, and their structure is analyzed by static 1H time-domain nuclear magnetic resonance (NMR) methods [1]. The heterocomplementary end-linking reaction of two well-defined star precursors [2] is implemented to obtain amphiphilic gels. We link PEG stars with hydrophobic poly-ε-caprolactone stars (tetra-PCL), resulting in the formation of an amphiphilic network. NMR is shown to be capable of distinguishing different chain species in the swollen PEG-PCL networks, allowing quantification of network connectivity defects arising from the end-linking reaction, as well as accurate quantification of inelastic material. The mesh size of the networks is studied by Pulsed-Field Gradient (PFG) NMR, using dextrans as hydrophilic probe molecules for the network swollen in selective solvents. Furthermore, we performed measurements using small-angle x-ray scattering and 1H MAS recoupling NMR for information on the properties of the selectively swollen networks, e.g., estimates for the correlation length of PCL domains, and chem. shift-specific information about the chain dynamics. [1] Bunk et al.; *Macromolecules* 2022, 55, (15), 6573-6589 [2] Sakai, T. et al.; *Macromolecules* 2008, 41, (14), 5379-5384

CPP 35.43 Wed 11:00 P1

Hybrid hydrogel films for scalable H2 production — •MORGAN LE DÛ¹, JULIJA REITENBACH¹, MANUEL A. REUS¹, KUN SUN¹, ZERUI LI¹, SIGRID BERNSTORFF², CRISTIANE HENSCHEL³, ANDRÉ LASCHWESKY³, CHRISTINE M. PAPADAKIS⁴, and PETER MÜLLER-BUSCHBAUM^{1,5} — ¹TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — ²Elettra-Sincrotrone Trieste, Basovizza, Italy — ³Fraunhofer-Institut für Angewandte Polymerforschung, Potsdam-Golm, Germany — ⁴TUM School of Natural Sciences, Soft Matter Physics group, Garching, Germany — ⁵Heinz

Maier-Leibnitz-Zentrum (MLZ), TUM, Garching, Germany

The water splitting reaction can produce hydrogen-based energy from solar radiation. A promising photocatalyst for this reaction is Pt loaded graphitic carbon nitride (g-CN). It shows a high H₂ evolution efficiency in aqueous solution. Previous works proposed to introduce hydrogels as host matrix and water storage to facilitate homogeneous spreading. This work aims to develop this system industrially scalable in a polymer thin film configuration. Poly(N-isopropylacrylamide) thin films exhibit good swelling capacity in water vapor atmosphere and appear suitable for a hybrid thin film system. A new isomer poly(N-vinylisobutyramide) seems also promising due to its higher lower critical solution temperature in aqueous solution. Therefore, a comparison of both polymers is based on in situ spectral reflectance and FT-IR measurements. The films have been spray coated to proceed grazing incident small angle x-ray scattering where g-CN/Pt blended polymer films microstructure was analysed under light irradiation.

CPP 35.44 Wed 11:00 P1

Effect of type of initiator and purification on the properties of thermo-responsive PNIPAM microgels — ●JOANNE ZIMMER, SEBASTIAN STOCK, SOURAJ MANDAL, CARINA SCHNEIDER, LUCA MIRAU, and REGINE VON KLITZING — Soft Matter at Interfaces, Institute for Condensed Matter Physics, TU Darmstadt, Germany

Microgels (MG) are polymeric networks in the size range of micrometers boasting properties of both colloids and polymers. Depending on their composition MG can respond to external stimuli such as temperature or pH. An example of a thermo-responsive polymer is Poly(N-isopropylacrylamide) (PNIPAM). PNIPAM MG can be synthesized by surfactant-free precipitation polymerization comprising NIPAM monomers, the crosslinker N,N'-methylenebisacrylamide (BIS) and a radical initiator. Depending on the radical initiator, either negatively or positively charged MG are generated. The subject of this work is the evaluation of the MG charge on the thermo-responsive swelling behavior and elastic properties using Dynamic Light Scattering and Atomic Force Microscopy. In addition, the type of MG purification and its effect on the resulting MG properties is investigated. It was shown, that the presence of undesired low-molecular weight products strongly impacts the MG interfacial adsorption behavior what we wish to understand. In this regard, sufficient removal was only achieved if, apart from the standard purification via dialysis, subsequent centrifugation steps were carried-out. The MG bulk properties (hydrodynamic radius, Zeta-potential) remained unchanged before and after centrifugation.

CPP 35.45 Wed 11:00 P1

Diketopyrrolopyrroles on graphite: Carpets self-assembled via hydrogen bonding — MOUFDI HADJAB^{1,2}, VLADYSLAV SAVCHENKO², NINA TVERDOKHLEB², and ●OLGA GUSKOVA² — ¹Mohamed Boudiaf University of M'sila, Algeria — ²IPF Dresden, Germany

We investigate the initial stages of the adsorption and thin-film formation of N-unsubstituted difuryl-diketopyrrolopyrroles (DPP) on graphite. Molecules in a particular conformational state (cis-cis, cis-trans or trans-trans) build the adsorption layers during in-silico self-assembly on surface through intermolecular hydrogen bonding. Here, the vacuum deposition of the molecules is reproduced in the all-atom MD setup [1]. We found out the formation of stable carpets made of molecular stripes. These carpets can be characterized as monomolecular layers in contrast to the structures, formed using droplet deposition [2]. The most stable stripes are made of cis-cis conformers, which is explained by stronger intermolecular hydrogen bonding. The stripe growth is accompanied by the reduction of the Eg gap. At the same time, the binding energy of the molecules does not show a clear dependence on the stripe length, which is a signature of the isodesmic self-assembly. Additionally, we quantify the intermolecular and the molecule/graphite energies for the hydrogen-bonded DPP molecules and compare the results with known experimental data. This work is supported by DFG, grant GU1510/5-1. [1] Guskova O.A., et al. J. Phys. Chem. C 2013, 117, 33, 17285. [2] Hadjab M., Guskova O. Herald of TvSU. Ser. Chem. 2021, 4, 46, 118.

CPP 35.46 Wed 11:00 P1

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

Tetraphenyl compounds with formula X(C₆H₅)₄ (X being a tetravalent atom of the 14th group such as C, Si, Ge, Sn, Pb), crystallize either in a tetragonal crystalline structure or in an amorph 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 amorph phase is a white light emitter. Tetraphenyl molecules feature indeed the delocalized π -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(C₆H₅)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 35.47 Wed 11:00 P1

Scaling Properties of Tree-like Self-Similar Polymers — ●RON DOCKHORN¹ and JENS-UWE SOMMER^{1,2} — ¹Leibniz-Institut für Polymerforschung Dresden e.V., D-01069 Dresden, Germany — ²Technische Universität Dresden, Institut für Theoretische Physik, D-01069 Dresden, Germany

In this study, regular polymeric Vicsek- and T-fractals are compared to dendrimers in means of theory and simulations. Albeit all structures exhibit exponential growth both for the number of monomers inside the structures and also for the terminal groups their structural properties differ significantly. Computer simulations are performed to investigate the scaling properties of the tree-like self-similar polymers utilizing the Bond-Fluctuation-Model with the Metropolis method as well as with the Wang-Landau algorithm. The radius of gyration, the heat capacity and the θ -point of those systems is investigated to examine the coil-globule transition of the polymeric fractals. A mean field theory for the scaling exponent in different solvent regimes is applied and found in fair agreement to the simulation data. A cross-over from almost linear chain behavior to spherical shape is observed, which can be tuned by the intrinsic functionality of the building blocks. The polymeric fractals can be an alternative to dendrimers in the class of hyperbranched polymers.

CPP 35.48 Wed 11:00 P1

Statistical Analysis of the Dimerization of Polyglutamine Chains — ●CHRISTIAN LAUER and WOLFGANG PAUL — Martin-Luther-Universität Halle-Wittenberg, Halle (Saale), Germany

We are presenting a numerical investigation of the dimerization of polyglutamine homo-peptides of varying length. We use the intermediate resolution protein model PRIME20 and study it with a flat-histogram type Monte Carlo simulation. This gives us access to the thermodynamic equilibrium of this model over the complete control parameter range, which for our simulations is the temperature. For densities comparable to typical in vitro experimental conditions we find that the aggregation and folding of the polyglutamine chains occur concurrently. However, as a function of chain length the sequence of establishment of intra- and intermolecular hydrogen bonding contacts changes. Chains longer than about $N = 24$ polyglutamine repeat units fold first and then aggregate. This agrees well with the experimental finding, that beyond $N = 24$ the single polyglutamine chain is the critical nucleus for the aggregation of amyloid fibrils. A finite size scaling of the ordering temperatures reveals that for this chain length (and longer chains) folding occurs at physiological (respectively larger) temperatures whereas shorter chains are disordered at physiological conditions.

CPP 35.49 Wed 11:00 P1

Construction of a polarizable force field for molecular dynamics simulation of a NaOTF Water-in-Salt electrolyte — ●MAJID REZAEI, SUNG SAKONG, and AXEL GROSS — Institute of Theoretical Chemistry, Ulm University, 89069 Ulm, Germany

A NaOTF Water-in-Salt (WiS) electrolyte is modeled using classical molecular dynamics (MD) simulations. For this, four different force fields are employed to account for atomic polarization at different levels: a non-polarizable all-atom force field where the polarization effect

is only implicitly included in the Van der Waals interaction parameters; the same force field with uniformly scaled ionic charges which, in a mean-field approximation, mimics electron polarization; a partially polarizable force field where ion polarization is explicitly accounted for via Drude oscillators while water is modeled by the non-polarizable SPC/E model; and a fully polarizable force field where the Drude oscillator model is used to account for both water and ion polarization. The primary goal of this study is to evaluate the simulation stability when using the above force fields and to investigate how the electrolyte properties are sensitive to the force field parameters. The results are then used to construct a force field that best reproduces the electrolyte properties obtained from ab initio molecular dynamics (AIMD) calculations. For this purpose, we use the partially polarizable model, which we believe is accurate enough to reproduce various properties of the studied electrolyte while the computational effort is affordable. The optimized force field will then be used to study the structure and dynamic properties of a NaOTf WiS solution under different conditions.

CPP 35.50 Wed 11:00 P1

Kirkwood-Buff theory approach towards cosolvent effects on single polymer chain collapse transition — ●MARTIN MELČÁK, JAKUB SMUTEK, and JAN HEYDA — Department of Physical Chemistry, University of Chemistry and Technology, Prague, Technická 5, CZ-16628 Praha 6, Czech Republic

The so-called smart materials are unique for their ability to rapidly and fully reversibly change physical or chemical properties upon exposure to external stimuli, such as temperature, light, pH, or solvent quality. In this contribution, we have taken under focus the prominent example of thermoresponsive polymer, which conformation can be near critical temperature modulated by the addition of small doses of cosolvents. To reveal the microscopic origin of the thermodynamic effect, we employed coarse-grained molecular dynamics simulations of a single polymer chain in mixed solution. The studied model can effectively describe changes in polymer chain conformation as well as the responses of the local solution composition in polymer proximity. Utilizing this fact, we have described and analyzed system thermodynamics in the framework of Kirkwood-Buff theory, which combines the polymer and environmental perspective of cosolvent effect on the polymer transition. Within a single unifying concept, our model is thus capable to quantitatively describe cosolvent effects in three interaction regimes, namely: depleted, weakly binding, and bridging regime.

CPP 35.51 Wed 11:00 P1

Fabrication of Plasmonic Au Nanostructures for Electrocatalysis — ●GINA ROSS and BJÖRN BRAUNSCHWEIG — Institut für Physikalische Chemie, WWU Münster, 48149 Münster, Germany

Nanosphere lithography (NSL) is a classical technique to fabricate reproducible 2D masks. These masks can be used to structure surfaces in a well-defined fashion. We have used spherical polystyrene (PS) particles to generate closed-packed hexagonal layers on a substrate surface that serves as a quasi 2D mask. The latter is subsequently coated with Au to fabricate Au nanopyrramids which are received by dissolution of the PS particles. Their deposition as a mask was done with the Langmuir-Blodgett transfer at the air-water interface. For that a suspension of polystyrene particles was spread on the water subphase containing no additional salt or surfactant. The fraction of PS particles sinking into the bulk subphase was drastically reduced by a 1:1 suspension of water and ethanol, and by dispensing the PS suspension onto the air-water interface with a glass slide at an angle of 45° relative to the interface. Au deposition and mask removal with an ultrasonic bath led to the formation of Au nanopyrramids. We expect the interaction of these nanostructures with electromagnetic radiation to result in a local field enhancement which promises to improve chemical reactions sensitive to electric field gradients. For that reason we have investigated the ability of Au plasmonic structures to promote CO₂ electrocatalysis.

CPP 35.52 Wed 11:00 P1

Luminescence properties of Nd complexes and processing of photonic crystal structures — ●MIRIAM GERSTEL¹, INGO KÖHNE², PAUL MERTIN³, BERND WITZIGMANN³, JOHANN PETER REITHMAIER¹, RUDOLF PIETSCHNIG², and MOHAMED BENYOUCHEF¹ — ¹Institute of Nanostructure Technologies and Analytics — ²Institute of Chemistry, CINSaT, University of Kassel, Germany — ³EEl Department, Friedrich-Alexander University of Erlangen-Nürnberg, Germany Lanthanide ion luminescence exhibits characteristic narrow emission bands along with relatively long emission lifetimes which makes them

attractive for applications in lighting, sensing, and display technologies. We investigate the optical characteristics of phosphonate ester-supported nitrite and chloride neodymium(III) complexes as solid bulk material and in solution. Optical properties of Nd complexes are determined by photoluminescence (PL) spectroscopy, which reveals emission bands of Nd(III) ions in the NIR region. PL measurements of equimolar solutions reveal information about the emission strength of the complexes with different ligand types. Temperature-dependent PL spectra enable the assignment of the emission lines observed around 880 nm. For light enhancement, molecules are 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 and the DFG grant-BE 5778/4-1.

CPP 35.53 Wed 11:00 P1

Insights into structure and dynamics of polycaprolactone-based star-shaped polymer electrolytes from molecular dynamics simulations — ●MIRKO FISCHER¹, DIDDO DIDDENS², and ANDREAS HEUER¹ — ¹Institute of Physical Chemistry, Westfälische Wilhelms-Universität Münster, Münster 48149, Germany — ²Forschungszentrum Jülich GmbH, Helmholtz Institute Münster, Münster 48149, Germany

Solid polymer electrolytes (SPEs) are promising candidates to substitute classical organic electrolytes in lithium-ion batteries, as they are chemically and mechanically more stable and have improved safety. However, they exhibit low ionic conductivity, which can be generally improved by developing novel polymer architectures. Experiments have shown that the biodegradable Grafted Cyclodextrin-Polycaprolactone (GCD-PCL) has higher transfer numbers than classical poly(ethylene oxide). In this work, we present results of molecular dynamics (MD) simulations to understand the ion transport in GCD-PCL. In order to directly compare our simulations with experiments, we used the time-temperature superposition of mean residence times and mean squared displacements of lithium ions to calculate the ionic conductivity at low temperatures, which would otherwise require larger time scales than are accessible through MD simulations.

CPP 35.54 Wed 11:00 P1

Organisation of Nanoparticles with Polymer Brushes: Computer Simulation Studies — ●BHUVAN POUDEL, HSIAO-PING HSU, and KURT KREMER — Max Planck Institute for Polymer Research, Mainz, Germany

For polymer brushes containing nanoparticles, the interplay between concentration of nanoparticles and interaction between monomers and nanoparticles affects the ordering of nanoparticles and the structural and dynamical properties of the respective polymer brushes. We perform molecular dynamics simulations of polymer brushes based on the bead-spring model and treat nanoparticles as hard spheres with a diameter six times larger than the monomer size. Initially, nanoparticles are randomly distributed inside or above the polymer brushes. By tuning the attractive interaction between monomers and nanoparticles, we study the assembly of nanoparticles within the polymer brushes as a function of nanoparticle concentration. The appropriate choice of monomer-nanoparticle interaction and concentration of nanoparticles gives rise to a single (ordered) layers of nanoparticles whose equilibrium positions fluctuate within their diameters.

CPP 35.55 Wed 11:00 P1

Tribological Properties of Selected Vanadium Oxides Investigated with *ReaxFF* molecular dynamics — ●MILJAN DASIĆ^{1,2}, ILIA PONOMAREV¹, TOMAŠ POLCAR¹, and PAOLO NICOLINI¹ — ¹Department of Control Engineering, Faculty of Electrical Engineering, Czech Technical University in Prague, Technická 2, Prague 6, 16627, Czech Republic — ²Scientific Computing Laboratory, Center for the Study of Complex Systems, Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia

Providing effective lubrication at high temperatures/pressures and in oxidative environments is relevant for various industrial applications, such as turbomachinery and cutting tools. Promising solutions are oxidation-resistant hard coatings consisting of binary or ternary films (e.g., Cr-N, Ti-N, Cr-Al-N, Ti-Al-N) doped with vanadium. The amount of oxygen present in an oxidative environment can be varied, leading to different vanadium oxide stoichiometries. We investigated tribological performance of under-oxidized vanadium lubricants, selected based on available experiments. We conducted a *ReaxFF*

molecular dynamics study on selected stoichiometries $\{V_2O_3, V_3O_5, V_8O_{15}, V_9O_{17}, VO_2\}$ at elevated temperatures $\{600, 800, 1000\}$ [K] and pressures $\{1, 2, 3, 4\}$ [GPa]. Our tribosystem consists of two rigid V_2O_5 layers, and a vanadium oxide in-between. At a fixed temperature, we did not notice significant changes of the friction coefficient with stoichiometry. All considered stoichiometries provide effective lubrication. Our study is relevant and interesting for the design of vanadium doped oxidation-resistant hard coatings.

CPP 35.56 Wed 11:00 P1

interfacial rheology of PNIPAM aqueous solutions at air-water interface: effect of cross-linking and oscillation frequency — ●ATIEH RAZAVI, REGINE VON KLITZING, and AMIN RAHIMZADEH — Hochschulstraße 8, 64289 Darmstadt, Germany

PNIPAM microgels are swollen and dispersible in water at temperatures below their VPTT. Microgels tend to adsorb at the liquid-air interface, thus reducing the surface tension. The degree of crosslinking influences the required time to reach the steady state. Higher crosslinker content results in a longer transient time in the order of several minutes (depending on the solution concentration). Upon the formation of a new interface, this transient time together with the mechanical properties of microgels play key roles in the interfacial elasticity of the air-water interface. The dynamic surface elasticity of aqueous solutions of PNIPAM has been measured by the oscillating barrier method as a function of time and concentration in different surface elongation frequencies. Results shows the apparent dilational elastic and loss moduli deduced from the pendant drop shape analysis at the air*water interface, as a function of pressure for the three cross-linking densities: 1, 5 and 10 mol%. In all cases, the apparent elastic modulus is much larger than the apparent loss modulus. The magnitude of the different elastic moduli goes through a maximum of elasticity for pressure values of about 15 mN/m. This behavior is a direct consequence of the particular structure of microgels, i.e. a dense and rigid core surrounded by a deformable shell made of dangling chains. The effect of oscillation frequency is still challenging and open question.

CPP 35.57 Wed 11:00 P1

Diffusion controlled pairwise associations of telechelic polymer chains — ●MICHAEL LANG and RON DOCKHORN — Leibniz-Institut für Polymerforschung Dresden, Institut Theorie der Polymere, Hohe Straße 6, 01069 Dresden, Germany

We study the pairwise association of telechelic chains in polymer melts. We derive the life time distributions of open stickers that return to the same partner as before (return walks) and the life time distribution of open stickers that exchange their binding partners (exchange walks) for both entangled and non-entangled chains. These distributions contain the full information of the bond association dynamics and allow to develop a generalization of the law of mass action in the diffusion controlled limit. The model predictions are tested by Monte-Carlo simulations and compared with preceding work on associations in networks.

CPP 35.58 Wed 11:00 P1

Architecture effect on the behavior of gradient and triblock terpolymer OEGMA-BuMA-DEGMA — ●WENQI XU¹, EIRINI MELAMPANAKI¹, FEIFEI ZHENG¹, ANNA P. CONSTANTINO², THEONI K. GEORGIU², and CHRISTINE M. PAPADAKIS¹ — ¹TUM School of Natural Sciences, Technical University of Munich, Garching, Germany — ²Department of Materials, Imperial College, London, England

Triblock terpolymers with hydrophilic, hydrophobic, and thermoresponsive blocks feature micellization, aggregation, and gelation in response to temperature changes and are therefore promising in various biomedical applications [1]. Gradient terpolymers can serve as a cost-effective alternative. Here, we investigate a triblock and a gradient terpolymer composed of hydrophilic oligo(ethylene glycol) methyl ether methacrylate (OEGMA), hydrophobic *n*-butyl methacrylate (BuMA), and thermoresponsive di(ethylene glycol) methyl ether methacrylate (DEGMA). Dynamic light scattering and synchrotron small-angle X-ray scattering revealed that the gradient terpolymer forms spherical micelles, whereas the triblock terpolymer is apt to form elongated micelles. With increasing temperature, the former grow in radius and the latter in length, which may be due to the increasing hydrophobicity of the DEGMA block.

[1] A. P. Constantinou, L. Wang, S. Wang, T. K. Georgiou, Polym. Chem. 2022., doi: 10.1039/D2PY01097F

CPP 35.59 Wed 11:00 P1

Adaptive Air-Water Interfaces with Spiropyran and Arylazopyrazole Photoswitches — ●MICHAEL HARDT and BJÖRN BRAUNSCHEWIG — University Münster, Center for Soft Nanoscience, 48149 Münster, Germany

Interfaces that respond to stimuli such as light or temperature are of great interest for new intelligent materials. Using molecular switches that respond to orthogonal triggers, the properties of fluid interfaces can be preconditioned and a low level of adaptivity can be integrated that extends the possibilities of soft matter interfaces beyond responsive functions.

In this contribution, we report on the adaptive behavior of air-water interfaces that are decorated by spiropyran (SP) and arylazopyrazole (AAP) photo-responsive surfactants. The SP surfactants increase their surface activity when irradiated with UV light that causes a ring-closure reaction. *E/Z* photo-isomerization of the AAP surfactants drives a substantial decrease in surface activity and thus desorption from the interface when the AAP surfactants are switched from their *E* to the *Z* state. In addition, at low pH the short thermal lifetime of the *Z* state as well as of the SP form offers the use of thermal relaxation as an alternative trigger, while also irradiation with green light can partially recover the initial properties. Interfacial properties and molecular kinetics were studied in detail using surface tensiometry and vibrational sum-frequency generation (SFG).

CPP 35.60 Wed 11:00 P1

A thermo- and photoresponsive polymer for schizophrenic switching of amphiphilic self-assembled micelles — ●PEIRAN ZHANG¹, RENÉ STEINBRECHER², ANDRÉ LASCHEWSKY^{2,3}, PETER MÜLLER-BUSCHBAUM⁴, and CHRISTINE M. PAPADAKIS¹ — ¹Soft Matter Physics Group, TUM School of Natural Sciences, Technical University of Munich — ²Institute of Chemistry, University of Potsdam — ³Fraunhofer IAP, Potsdam-Golm — ⁴Chair for Functional Materials, TUM School of Natural Sciences, Technical University of Munich

Schizophrenic switching, namely the exchanging of hydrophilic and hydrophobic segment of an amphiphilic diblock copolymer, leads to self-assembly of micelles and inverse micelles, which can be used in the drug delivery application [1]. We aim to achieve such behavior by means of diblock copolymers composed of a thermo-responsive block with a fixed LCST (lower critical solution temperature) and a photo-responsive block with a tunable LCST, which is accomplished by cis-trans isomerization of the incorporated azobenzene group. As a first step, we use turbidimetry and dynamic light scattering (DLS) to investigate a homopolymer precursor with respect to the cloud point and the chain size in the cis- and trans-form of the azobenzene group, which is realized by 365 nm UV light and 470 nm blue light, respectively.

[1] C. M. Papadakis, P. Müller-Buschbaum, A. Laschewsky, Langmuir 2019, 35, 9660-9676.

CPP 35.61 Wed 11:00 P1

Effect of pressure on the micellar structure of PMMA-*b*-PNIPAM in aqueous solution — ●PABLO A. ALVAREZ HERRERA¹, GEETHU P. MELEDAM¹, CRISTIANE HENSCHL², LEONARDO CHIAPPISI³, ANDRÉ LASCHEWSKY², and CHRISTINE M. PAPADAKIS¹ — ¹TU München, School of Natural Sciences, Garching Germany — ²Universität Potsdam, Institut für Chemie, Potsdam-Golm, Germany — ³Institut Laue-Langevin, Grenoble, France

In aqueous solution, amphiphilic diblock copolymers consisting of a permanently hydrophobic and a thermo-responsive block self-assemble into core-shell micelles. In particular, poly(methyl methacrylate)-*b*-poly(*N*-isopropylacrylamide) (PMMA-*b*-PNIPAM) forms micelles featuring a hydrophobic PMMA core and a thermo-responsive PNIPAM shell. This phase transition can be also induced by changing the pressure. Here, we study the effect of pressure on the micellar structure of PMMA-*b*-PNIPAM in aqueous solution by small-angle neutron scattering (SANS). In temperature-resolved experiments, we find that the micellar shell strongly dehydrates after crossing the co-existence line at 0.1 MPa. At 75 MPa, on the contrary, it remains hydrated and the micelles are highly-correlated within the aggregates. We also characterized the micellar structure in a pressure-resolved experiment at 31.8 °C. In this case, we find that, after crossing the co-existence line, the micellar shell appreciably shrinks, even though it remains partially hydrated. We conclude that the micellar structure in the two-phase region strongly depends on pressure.

CPP 35.62 Wed 11:00 P1

Synthesis of diblock copolymer brush surfaces to control the adaptation time to water — ●BENJAMIN LEIBAUER¹, ANDRES DE

LOS SANTOS PEREIRA², OGNEN POP-GEORGIEVSKI², HANS-JÜRGEN BUTT¹, and RÜDIGER BERGER¹ — ¹Max-Planck institute for polymer research, Ackermannweg 10, 55128 Mainz — ²Institute of macromolecular chemistry cas, Heyrovskeho nam. 1888, 162 00, Praha 6

The Young's model describes the wetting behavior of an ideal surface. Recently, Butt et al. presented a model, which connects adaptation processes of the surface to dynamic contact angles. We developed an experimental setup, which allows measuring adaptation processes. The adaptation model was experimentally verified by Li et al. using surfaces coated with films of statistical copolymers. We synthesize polymer brush surfaces with the aim to control the adaptation time scale upon wetting and dewetting systematically. We used the surface-initiated atom transfer radical polymerization / ATRP to selectively synthesize diblock copolymer brushes. We prepared poly(2-hydroxyethyl methacrylate) (PHEMA) as a hydrophilic block from the surface and we grafted polystyrene (PS) as hydrophobic block on top of the PHEMA block. By regulating the architecture and thickness of the polymer brush we can tune surface adaption to wetting.

CPP 35.63 Wed 11:00 P1

Droplets sliding on compressed soft surfaces — ●YOUNG CHAO, HANSOL JEON, and STEFAN KARPITSCHKA — Max Planck Institute for Dynamics and Self-Organization, 37077 Göttingen, Germany

The motion of droplets on rigid substrates is mainly slowed up by the viscous dissipation inside the liquid phase. However, this does not hold for droplets sliding on soft substrates: viscoelastic dissipation inside solid phase now dominates the motion, leading to "viscoelastic breaking". A recent study revealed that droplets move anisotropically on soft, pre-stretched solids, which is incompatible with the classical visco-elastocapillary wetting theory. Here, we impose a compression rather than a stretch on the soft solid, and explore how pre-compression influences the droplet speed. Intriguingly, we observe a non-monotonic dependence of the sliding speed on the pre-strain: a minimal speed exists as the solid is consecutively compressed. This may enrich our current understanding of elastocapillarity, for instance, in tissue engineering where soft materials are frequently squeezed.

CPP 35.64 Wed 11:00 P1

Understanding wetting and drying of nanoporous media through optical and dilatometry experiments — ●LAURA GALLARDO^{1,2,3}, JUAN SÁNCHEZ^{1,2,3}, YANNICK TETZNER^{1,2,3}, and PATRICK HUBER^{1,2,3} — ¹Institute of Materials Physics and Technology, Hamburg University of Technology, Germany — ²Photon Sciences, Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — ³Center for Hybrid Nanostructures CHyN, Hamburg University

While imbibition kinetics is well-understood in nanoporous materials [1], their drying dynamics is still under investigation [2]. In this study, we present time-dependent macroscopic dilatometry experiments on the deformation of nanoporous monoliths upon spontaneous, capillarity-driven infiltration of water as well as drying. During both processes, we find characteristic dynamical regimes that can be quantitatively described in terms of Laplace pressure effects and changes in the surface stress at the inner pore walls [3]. In the particular case of transparent nanoporous Vycor glass, additional imaging experiments are conducted, allowing direct optical access to the filling front. The

observed wetting-drying dynamics are consistent with our analysis of the strain regimes. Our study demonstrates that it is possible to monitor the interplay of imbibition and drying dynamics by simple dilatometry measurements, provided proper humidity control. [1] Gruener, et al (2009), Phys. Rev. E Stat. Nonlin. Soft Matter Phys., 79(6). [2] Al-Madani, R. (2018), Conference paper: YUCOMAT2018. [3] Gor, G. Y., et al. (2017). Appl. Phys. Rev., 4(1), 011303

CPP 35.65 Wed 11:00 P1

Studying Solid-liquid Contact Charge Separation Dynamics using Mirror Charge — ●PRAVASH BISTA¹, HANS-JÜRGEN BUTT¹, and STEFAN A.L WEBER^{1,2} — ¹Max-Planck-Institut für Polymer research Mainz — ²Johannes Gutenberg University of Mainz

Charge separation as water drops slide over a hydrophobic solid surface is a well known phenomenon (Slide electrification). Nevertheless, a macroscopic understanding of dynamics in solid-liquid contact charge separation is still incomplete. To address that, we introduce a method based on "mirror charge" detection to locally measure the change in surface charge density ($\Delta\sigma$). Here, we placed a grounded metal electrode parallel beneath the substrate. As a spontaneously charged drops move over a surface, they attract opposite charge in the metal electrode causing a flow of capacitive current. Analysing this current, we studied $\Delta\sigma$ dynamics with increasing slide length and drop number as multiple deionized water drops slid down the inclined hydrophobic surface (trichloro(1H,1H,2H,2H-perfluorooctyl)silane, PFOTS-functionalized glass). Using the results, we estimated a set of parameters to describe the $\Delta\sigma$ dynamics in slide electrification. Further, we used these parameters in a numerical simulation where we numerically reproduced the experimental results.

CPP 35.66 Wed 11:00 P1

Towards wetting on switchable and adaptive conducting polymer surfaces — ●JUNQI LU¹, ALDILENE SANTOS FRANCA¹, NIKOLAOS KARADIMITRIOU², HOLGER STEEB², and SABINE LUDWIG¹ — ¹IPOC-Functional Polymers, Institute of Polymer Chemistry, University of Stuttgart, Germany — ²Institute of Mechanics (MIB) & SC SimTech, University of Stuttgart, Germany

Conducting polymers (CPs) are discussed in a huge variety of electronic devices including electrochromic windows, batteries, actuators and chemical-biology sensors, mainly because of switchable electronic and optical properties. Compared to other conducting materials, CPs have advantages of light-weight, low cost, non-toxicity, flexibility, easy processing, and low voltage operation. In our group, poly(3-hexylthiophene) (P3HT) and poly(3,4-ethylenedioxythiophene):poly(styrene sulfonate) (PEDOT:PSS) are mostly studied. In the case of P3HT, the doping states can be precisely controlled by electrochemical or chemical doping, which results e.g. in an increase of conductivity over 6 orders of magnitude with a maximum of 224 S/cm. [1] On the other hand, PEDOT:PSS can be controlled by electrochemical means, but also by humidity, as used e.g. for actuators. [2] In this contribution, we will show our preliminary data on the wetting behavior on such switchable and adaptive CP surfaces.

Ref.: [1] Chem. Mater. 2020, 32, 14, 6003; [2] Adv. Mater. 2021,33, 2007982