# CPP 20: Poster Session I

Topics: Bioinspired Functional Materials (20.1-20.4), Biomaterials and Biopolymers (20.5-20.12), Polymers in Multi-Compartment and Aqueous Solutions (20.13-20.21), Modeling and Simulation of Soft Matter (20.22-20.24), Data-driven Methods in Molecular Simulations of Soft-Matter Systems (20.25-20.26), Polymer Networks and Elastomers (20.27-20.29), Polymer and Molecular Dynamics (20.30-20.33), Molecularly Functionalized Low-Dimensional Systems (20.34-20.35), Charged Soft Matter, Polyelectrolytes and Ionic Liquids (20.36-20.47), Crystallization, Nucleation and Self-Assembly (20.48), Interfaces and Thin Films (20.49-20.62).

Time: Monday 17:30–19:30                                                   Location: Poster A

### CPP 20.1   Mon 17:30   Poster A

**Dry adhesives of structured polydimethylsiloxane** — •Andreas Zheng[1], Volker Körstgens[1], Hsin-Yin Chiang[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]Rythm, 75009 Paris, France

Biocompatible, gecko-inspired dry adhesives are fabricated using polydimethylsiloxane (PDMS) in a 2-step fabrication process. First uncured PDMS is filled into a silicon mold of a regular hole pattern. After degassing and curing a PDMS replica containing a regular pillar pattern is obtained. In the second step the pillars of the PDMS replica are dipped into a thin film of liquid PDMS and attached onto an anti-adhesive film to achieve a mushroom-tip structure upon curing. The dimensions and the geometrical shapes of the achieved structures are investigated with optical microscopy. Adhesive forces of the PDMS patches in contact with different materials are measured with a tack test. Force-distance curves are obtained using a home-built instrument with a unique punch design developed for pressure sensitive adhesives. The dependence of adhesion forces on the structure of the PDMS patches is presented.

### CPP 20.2   Mon 17:30   Poster A

**Imitation of scattering networks by foam models** — •Dominic Meiers[1], Marie-Christin Angermann[1], and Georg von Freymann[1,2] — [1]Physics Department and Research Center OPTIMAS, University of Kaiserslautern, Kaiserslautern, Germany — [2]Fraunhofer Institute for Industrial Mathematics ITWM, Kaiserslautern, Germany

The wing scales of the beetle Cyphochilus show one of the highest whiteness and brightness found in nature, although they are only about 5 $\mu$m thick [1]. This brilliant whiteness is achieved by multiple light scattering in the inner disordered chitin network of the scales [2]. To model and optimize this network, a foam model generator (GeoDict) is used. This foam has an inner structure comparable to the beetle's network. By varying the parameters of generation, the optical properties are optimized in respect of whiteness and brightness. Therefore, the optical response is calculated by using a finite difference time domain method. Moreover, the foam structure is compared with the measurement-based model of the chitin network shown in [3]. Subsequent steps are the further improvement of the foam structure and its fabrication via 3D direct laser writing. Eventually, it might be possible to create artificial structures that are comparable to the beetle's wing scales in the near future.

[1] P. Vukusic, B. Hallam, J. Noyes, Science 315, 5810 (2007). [2] M. Burresi et al., Scientific Reports 4, 6075 (2014). [3] B. Wilts et al., Adv. Mater. 2017, 1702057 (2017).

### CPP 20.3   Mon 17:30   Poster A

**Entangled Nets from Surface Drawings** — •Benedikt Kolbe — Institute of Mathematics, Technische Universität Berlin

Imagine drawing a few lines on an arbitrary surface. What if the drawing for the rest of the surface can be filled in by invoking symmetries? Is there a way to enumerate different ways of scribbling? If the goal was to find molecular structures by drawing them on surfaces, what surfaces would we start with and why?

This talk will motivate and answer these questions, while focusing on a new technique to explicitly enumerate and construct all essentially different ways to decorate prominent examples of triply periodic minimal surfaces with a given symmetry. We will also touch upon what kind of 3D structures arise in this way.

There will be tie-ins to geometry, braid theory, combinatorial group and tiling theory, physics, and even some chemistry.

### CPP 20.4   Mon 17:30   Poster A

**Rearrangement of nanopatterns: Wetting of n-alkane Molecular Films** — Diego Diaz[1], Tomas P. Corrales[2], Maria J. Retamal[3], Marcelo Cisternas[1], Nicolas Moraga[1], Rodrigo Catalan[1], Mark Busch[4], Patrick Huber[4], Marco Soto-Arriaza[3], and •Ulrich G. Volkmann[1] — [1]Institute of Physics and CIEN-UC, P. Univ. Catolica de Chile, Santiago, Chile — [2]Department of Physics, UTFSM, Valparaiso, Chile — [3]Faculty of Chemistry and CIEN-UC, P. Univ. Catolica de Chile, Santiago, Chile — [4]TUHH, Hamburg, Germany

We present a study of the wetting properties of silicon samples coated with a single layer of n-alkane molecules self-assembled perpendicular to the surface. It is known that the filling fraction (between 10% to 50%) of molecules on the surface can be controlled by the withdrawal velocity of the silicon wafer from the coating solution. After sample preparation, the contact angle was measured of a 2 microliter drop of water placed on the patterned surface. The results of the apparent contact angle versus coverage can be grouped in two regimes that depend linearly on coverage, which is consistent with the Cassie wetting model. After drop evaporation, the molecules migrate to the center and the contact line of the area where the sessile drop was placed, leaving also a depletion zone. AFM studies showed that the original patterns restructure. Acknowledgements: Postdoctoral FONDECYT #3160803 (MJR), FONDECYT #1141105 (UGV) and #1171047 (MSA), FONDECYT INICIACION #11160664 (TPC), CONICYT Fellowships (RC, MC) and CONICYT-PIA ACT 1409.

### CPP 20.5   Mon 17:30   Poster A

**Microrheology of hydrogel-like biological materials** — •Elke Bradt[1], Sabine Hild[1], Erwin K. Reichel[2], Thomas Voglhuber-Brunnmaier[2], and Milan Kracalik[1] — [1]Johannes Kepler University, Institute of Polymerscience, Linz, Austria — [2]Linz Institute of Technology, Institute for Microelectronics and Microsensors, Linz, Austria

Rheology of biofluids introduces a new inside into medical technology and is crucial for the associated physiological function. Typical example for biofluids is synovial liquid, which can be found in joints. The viscosity and elasticity of synovial fluids are essentially determining the ability to maintain the joint spacing, reduce slip resistance, and protect cartilage from abrasion. Biological elastic liquids show pronounced extensional viscosity, they are therefore often analyzed using capillary breakup rheometry. Comparing to this method microrheological investigation e.g. passive microrheology based on dynamic light scattering is in the meantime a common technique using commercial equipment. In order to be conform with actual ethics in medicine research, for preliminary studies (optimization of measuring conditions like tracer selection, temperature, pH) model liquids are important. In this work different model liquids, which are physiologically similar to synovial liquid, have been explored and measured using passive microrheology. The differences in viscoelastic behavior between model liquids and synovial liquid were evaluated.

### CPP 20.6   Mon 17:30   Poster A

**Protein exchange on Gold Nanoparticles – Tailored Polymers as model systems** — •Carmen Radeke[1,2], Jonas Schubert[1,3], Munish Chanana[4,5], and Andreas Fery[1,3] — [1]Department of Nanostructured Materials, Leibniz-Institut für Polymerforschung Dresden e. V. — [2]Department of Biopolymers, University of Bayreuth, 95440 Bayreuth, Germany — [3]Physical Chemistry of Polymer Materials, Technische Universität Dresden, D-01062 Dresden, Germany — [4]Institute of Building Materials (IfB), ETH Zurich, 8093 Zurich, Switzerland — [5]EMPA Dübendorf, 8600, Dübendorf, Switzerland.

Understanding the behavior of NPs in biological systems is one of the

major challenges on the way to new therapeutics and diagnosis tools in medicine. Therein, the generation of an undefined protein corona is a crucial point, as by this, the physicochemical properties of the NPs and therefore also their behavior change drastically. To address these problems, we used a defined protein corona on Au NP as model system. This has the advantage that a fluorescent labeled protein shell can be detected when being exchanged. To understand the influence of physicochemical parameters (e.g. molecular weight, functional groups and concentration of free protein) of protein exchange under physiological conditions, we simplified the system by using polymer and polypeptides as model systems.

CPP 20.7    Mon 17:30    Poster A

**Adsorption of finite semiflexible polymers and their loop and tail distributions** — •Tobias A. Kampmann and Jan Kierfeld — TU Dortmund University, Germany

We discuss the adsorption of semiflexible polymers to a planar attractive wall and focus on the questions of the adsorption threshold for polymers of finite length and their loop and tail distributions using both Monte-Carlo simulations and analytical arguments. For the adsorption threshold, we find three regimes: (i) a flexible or Gaussian regime if the persistence length is smaller than the adsorption potential range, (ii) a semiflexible regime if the persistence length is larger than the potential range, and (iii) for finite polymers, a novel crossover to a rigid rod regime if the deflection length exceeds the contour length. In the flexible and semiflexible regime, finite size corrections arise because the correlation length exceeds the contour length. In the rigid rod regime, however, it is essential how the global orientational or translational degrees of freedom are restricted by grafting or confinement. For the loop and tail distributions, we find power laws with an exponential decay on length scales exceeding the correlation length. This allows us to explain that, close to the transition, flexible and semiflexible polymers desorb by expanding their tail length.

CPP 20.8    Mon 17:30    Poster A

**Non-Classical Interactions of Phosphatidylcholine with Mucin for Protection of Intestinal Surfaces: A Microinterferometry Study** — •Federico Amadei and Motomu Tanaka — Institute of Physical Chemistry, Heidelberg, Germany

Albeit many studies demonstrated that the accumulation of phospholipids in the intestinal mucosal surfaces is essential for the protection of colon epithelia against pathogenic bacteria, the mechanism of interactions between phospholipids and the surface protein mucin is not well understood. In this study, the significance of phospholipid-mucin interactions was quantified by the combination of an in vitro intestinal surface model and label-free microinterferometry. The model of intestinal surfaces consists of planar lipid membranes deposited on solid substrates that display mucin proteins at defined anchoring densities. Following the characterization of the systems by quartz crystal microbalance and fluorescence staining, the vertical Brownian motion of cell-sized particles on model surfaces was monitored by using RICM. In case of latex particles bearing different surface charges, the calculated potential curvature monotonically increased according to the increase in surface potential, suggesting the dominant role of electrostatic interactions with negatively charged mucin in the potential confinement. However, the particles coated with phospholipids exhibited a clear nonlinearity: the particles coated with zwitter-ionic phosphatidylcholine is most sharply confined on mucin surfaces. Our data suggested the presence of another underlying molecular level interaction that is stronger than electrostatic interactions.

CPP 20.9    Mon 17:30    Poster A

**In situ GISAXS analysis of spray deposited metal-biopolymer thin films** — •Wiebke Ohm[1], Michał Kamiński[1], Pallavi Pandit[1], Calvin Brett[1,2], Shun Yu[2], Nitesh Mittal[2], Daniel Söderberg[2], and Stephan V. Roth[1,2] — [1]Deutsches Elektronen-Synchrotron Hamburg, Notkestraße 85, 22607 Hamburg — [2]KTH Royal Institute of Technology, Department of Fibre and Polymer Technology, Teknikringen 56-58, SE-100 44 Stockholm, Sweden

Conductive polymer substrates based on metal coated cellulose layers offer a renewable and sustainable replacement for synthetic polymer substrates, which is essential for many applications in nanotechnology. In order to reach this target, we follow a route combining cellulose nanofibril thin films with silver nanowire (Ag NW) coating offering the additional advantage of transparency. For effective industrial fabrication, not only the controlled arrangement of the precursors during the deposition process is essential but also the use of an industrial

compatible deposition process. Air-brush spray deposition is a versatile deposition technique that fulfils industrial demands and was thus chosen for preparation of metal-cellulose thin films.

We investigated all spray deposited cellulose/Ag NW layer form aqueous and alcoholic solution. In situ grazing incidence small angle x-ray scattering (GISAXS) in combination with microscopy techniques of the final layers revealed the inner structure and arrangement of these films. The conductivity and transparency as function of surface coverage are investigated for Ag NW deposited on different substrates. First GISAXS results of aligned Ag NW will be presented.

CPP 20.10    Mon 17:30    Poster A

**Raman spectroscopy on bioinorganic model complexes** — •Dieter Rukser[1], Florian Biebl[1], Melissa Teubner[1,2], Benjamin Grimm-Lebsanft[1], Patricia Liebhäuser[2], Sarah Neville[3], Alexander Hoffmann[2], Linda Doerrer[3], Sonja Herres-Pawlis[2], and Michael Rübhausen[1] — [1]Center for Free Electron Laser Science, Universität Hamburg — [2]Instiut für anorganische Chemie, RWTH Aachen — [3]Inorganic Chemistry, Boston University

Elucidating charge-transfer dynamics of transition metal complexes is crucial for the understanding of a multitude of biochemical processes. Raman spectroscopy is a useful tool to study model complexes mimicking these processes.

By resonant excitation of the transition state, the electron transfer is accessible through vibrational modes, which are coupled to metal-ligand charge transfer (MLCT) and ligand-metal charge transfer (LMCT) states.

We have studied bioinorganic copper complexes using resonant as well as time-resolved Raman spectroscopy. For complexes stable at temperatures below -60 °C we have designed a Peltier cooled cryostat for our UT-3 Raman spectrometer, allowing operando oxygenation and measurement of the samples at temperatures down to -90 °C.

For samples that are damaged by laser radiation, we have designed several jet-based delivery systems. Jet diameters down to 10 $\mu m$ and flow rates of 15 $\mu$L/min allowed us to measure small sample volumes for several hours.

CPP 20.11    Mon 17:30    Poster A

**Simulations of linear and cyclic RGD peptides at a free surface of the polymer brushes** — •Olga Guskova[1,2], Ulla König[1], Petra Uhlmann[1], and Jens-Uwe Sommer[1,2] — [1]IPF Dresden — [2]DCMS, TU Dresden

Motivated by recent experiments [1,2] aiming at biomimetic design of new polymeric surfaces relevant for the biotechnological applications, the behaviour of short peptides with the RGD motif, mimicking the cell adhesion proteins, is simulated using DFT/MD combination. Three peptides are modeled: linear GRGDS, linear GRGDSPK and cyclic cRGDyK in aqueous solutions and being chemically attached to the PAA brush surface. For free peptides, the net charge and the charge pattern are characterized and the most reactive amino-groups are predicted based on the ESP charges. The free energy of hydration calculated by thermodynamic integration shows the negative values and changes in the row GRGDS>GRGDSPK>cRGDyK. Secondary structures of linear peptides have "normally allowed" $\beta$-regions, $\beta$-turns and coil-like structures, whereas the cyclic chain is sterically restraint. The secondary structures and the radial distribution functions of water around the charged peptide groups are calculated for the chains attached to PAA backbone. We compare the shielding and exposure of bound GRGDS, GRGDSPK and cRGDyK peptides and the availability of the RGD sequence and R-side chain at the brush surface.

[1] E. Psarra et al. ACS Omega, 2017, 2, 946.
[2] U. König et al. Biointerphases 2017 (submitted).

CPP 20.12    Mon 17:30    Poster A

**A Theoretical Study of the Interaction of Calcite with Amino Acids** — •Robert Stepić[1,2], Zlatko Brkljača[1,2,3], Ana-Sunčana Smith[1,2,3], and David M. Smith[2,3] — [1]FAU, Institute for Theoretical Physics I, PULS Group, Erlangen, Germany — [2]Cluster of Exellence: Engineering of Advanced Materials, Erlangen, Germany — [3]Rudjer Bošković Institute, Zagreb, Croatia

Calcite is one of the most widespread minerals on earth which interacts favourably with a variety of biomolecules. This interaction can mediate the growth of calcite resulting in formation of biominerals with remarkable mechanical properties useful in a number of applications. In this work we utilize a bottom-up approach and study the interaction of protein building blocks, amino acids, with the stable (104) surface of calcite. We also probe the interactions with different morphologies

deriving from (104) surface which incorporate kinks and edges. Amino acids are studied in their native zwitterionic and protected forms. Our method of choice for this study encompasses fully atomistic molecular dynamics simulations using state of the art force fields for these types of systems. We employ enhanced sampling techniques with biasing potentials to obtain free energy profiles along the axis perpendicular to the surface. This enables us to estimate the free energies of binding of amino acids to the calcite and also gives us the information on the molecular details of the interaction. These results provide a force field benchmark and reference data on binding energies of specific amino acids which could help interpret the experimental data on peptide and protein mediated calcite functionalization and growth.

CPP 20.13   Mon 17:30   Poster A

**SANS Study on the Pressure-Dependence of the Cononsolvency Effect in Aqueous PNIPAM Solutions** — •Bart-Jan Niebuur[1], Kora-Lee Claude[1], Ralf Schweins[2], Vitaliy Pipich[3], Marie-Sousai Appavou[3], Alfons Schulte[4], and Christine M. Papadakis[1] — [1]TU München, Physik-Department, Garching, Germany — [2]Institut Laue-Langevin, Grenoble, France — [3]JCNS at MLZ, FZ Jülich, Garching, Germany — [4]University of Central Florida, Department of Physics, Orlando, U.S.A.

The solubility of the thermoresponsive polymer poly(N-isopropylacrylamide) (PNIPAM) in aqueous solutions decreases drastically when small amounts of methanol are added, resulting in a reduced cloud point, an effect called cononsolvency. If high pressure is applied, the cononsolvency effect is destroyed, meaning that the cloud point is clearly higher in comparison with PNIPAM solutions in pure water at the same pressure. Using small-angle neutron scattering, the phase behavior of semi-dilute PNIPAM solutions in mixtures of water and methanol is studied in temperature scans at various pressures, revealing the behavior of the concentration fluctuations near the respective cloud points. The results show that high pressure strongly broadens the phase transition, revealing changes in the polymer-solvent interaction. Very small-angle neutron scattering allowed us to study the effect of methanol on the mesoglobule formation and the size of the mesoglobules in the segregated state of PNIPAM at high pressure.

CPP 20.14   Mon 17:30   Poster A

**The structural, thermal and dynamic behavior of the thermoresponsive polymer Poly(N-isopropylmethyacrylamide)** — •Chia-Hsin Ko[1], Kora-Lee Claude[1], Dirk Schanzenbach[2], Bart-Jan Niebuur[1], Xiaohan Zhang[1], Dionysia Aravopoulou[3], Apostolos Kyritsis[3], Henrich Frielinghaus[4], Peter Müller-Buschbaum[1], André Laschewsky[2,5], and Christine M. Papadakis[1] — [1]TU München, Physik-Department, Garching, Germany — [2]Universität Potsdam, Institut für Chemie, Potsdam-Golm, Germany — [3]National Technical University of Athens, Greece — [4]Forschungszentrum Jülich GmbH, JCNS at MLZ, Garching, Germany — [5]Fraunhofer-Institut für Angewandte Polymerforschung, Potsdam-Golm, Germany

Poly(N-isopropylmethacrylamide) (PNIPMAM) is a thermoresponsive polymer, exhibiting lower critical solution temperature (LCST) behavior in aqueous solution with a cloud point at ~43 °C. We investigate the temperature- and concentration-dependent phase behavior of PNIPMAM in D2O using turbidimetry, differential scanning calorimetry (DSC), small-angle neutron scattering and dynamic light scattering. We find that the phase transition consists of two steps, namely (i) hydrophobic aggregation at ~39 °C, as evident from turbidmetry and SANS and (ii) the chain collapse and water release at ~44 °C, as evident from DSC and SANS.

CPP 20.15   Mon 17:30   Poster A

**Thermodynamics of polyNIPAM – simulation study** — •Vladimir Palivec, Denis Zadrazil, and Jan Heyda — University of Chemistry and Technology, Prague, Czech Republic

Among thermoresponsive polymers, Poly-N-isopropyl acrylamide (PNIPAM), plays a prominent role, both in simulations, theory, and in applications. Nevertheless, the microscopic description of a PNIPAM chain collapse transition above the LCST is still puzzling and challenges the computational chemists for last decades. In this contribution, we have employed large-scale atomistic computer simulations of single PNIPAM chain in explicit water. We have analyzed swollen-to-collapse transition thermodynamics and the values were compared with in house performed experimental data, such as calorimetric or volumetric.

CPP 20.16   Mon 17:30   Poster A

**NiPAM-salt interactions in aqueous solutions** — •Jakub Polák, Vladimír Palivec, Adam Kovalčík, Pavel Vrbka, Daniel Ondo, and Jan Heyda — Department of Physical Chemistry, University of Chemistry and Technology, Prague, Czech Republic

This contribution is focused on a physico-chemical characterization of N-isopropyl-acrylamide (NiPAM) in aqueous solutions of sodium and guanidinium salts. To describe the NiPAM-salt interaction, two properties were chosen. The preferential binding of salt over that of water to the NiPAM surface, which was determined by vapor pressure osmometry (VPO), and the partial molar volume of NiPAM in salt solutions determined from large set of density measurements.

Firstly acquired data for preferential binding were used to evaluate the Salting out (Setschenow) constants and compared to literature values for similar amides. Secondly the relevant Kirkwood-Buff integrals were calculated, by joining data from osmometric and densimetric measurements. Last, the thermodynamic properties of NiPAM were compared with data for thermoresponsive polymer polyNiPAM obtained from our recently derived thermodynamic model and its combination with the Kirkwood-Buff theory of solutions.

CPP 20.17   Mon 17:30   Poster A

**Morphology of Amphiphilic Bottlebrush Copolymers in Dilute Aqueous Solution** — •Jia-Jhen Kang[1], Kaltrina Shehu[1], Junpeng Zhao[2], Stergios Pispas[2], and Christine M. Papadakis[1] — [1]TU München, Physik-Department, Garching, Germany — [2]Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, Athens, Greece

Densely grafted copolymers, or polymeric bottle brushes, present a complex architecture. We investigate polymeric bottle brushes having diblock or random copolymers as side arms. These comprise poly(ethylene oxide) and poly(propylene oxide), where the former is water-soluble and the latter becomes hydrophobic at elevated temperatures, which leads to increased turbidity both for diblock and for random side arms [1]. In the present study, we aim to characterize their temperature-dependent conformation and self-assembly in dilute aqueous solution using dynamic light scattering and small-angle X-ray scattering. Comparing the data of the bottle brushes with analogous linear polymers, we gain insight into the effects caused by the complex architecture.

[1] J. Zhao et al., J. Polym. Sci.: Part A: Polym. Chem. 48, 2320 (2010) and Macromolecules 43, 1771 (2010).

CPP 20.18   Mon 17:30   Poster A

**Morphological study of drug delivery systems based on poly(2-oxazoline) bottle brushes** — •Kaltrina Shehu[1], Jia-Jhen Kang[1], Clemens Sachse[2], Rainer Jordan[2], and Christine M. Papadakis[1] — [1]TU München, Physik-Department, Garching, Germany — [2]TU Dresden, Professur für Makromolekulare Chemie, Dresden, Germany

Nano carriers for drug delivery have traditionally been based on the self-assembly of amphiphilic block copolymers. These typically form spherical micelles which can incorporate hydrophobic drugs. It has been shown, however, that it is an advantage if the polymeric nanoparticles are elongated. Densely grafted copolymers, or polymeric bottle brushes, form unimolecular elongated nanoparticles. If their side arms are amphiphilic, they may incorporate hydrophobic drugs. Poly(2-oxazoline)s are highly biocompatible and may be rendered hydrophilic or hydrophobic by the choice of the side group, and are thus of interest for this application. Here, we investigate the concentration and temperature-dependent size, shape and inner structure of a polymeric bottle brush, having a poly(2-isopropenyl-2-oxazoline) backbone and poly(2-ethyl-2-oxazoline) side chain in dilute aqueous solution using dynamic light scattering (DLS) and small angle X-ray scattering (SAXS).

CPP 20.19   Mon 17:30   Poster A

**A wide range of surface forces of PSS terminated polyelectrolyte multilayers** — •Heba Soker Mohamad, Sven Neuber, Annkatrin Sill, and Chistiane A. Helm — Institut für Physik, Uni. Greifswald, Felix-Hausdorff-Str. 6 17489 Greifswald

Films built from the Poly (styrenesulfonate) (PSS) and poly (diallyl-methylammonium) (PDADMA) in 0.1 Mol/L NaCl are investigated. Film build-up starts with a parabolic growth regime, followed by a linear growth regime. In the former positive PDADMA and negative PSS monomers are balanced; in the latter an excess of PDADMA

monomers is balanced by Cl- ions. Colloidal probe measurements show that in the former PSS-terminated films are flat and negative, in the latter they are electrically neutral at 0.1 Mol/L NaCl and are positively charged at other ion concentrations . If exceeds 1 Mol/L steric forces are found. Thus, by choosing the growth regime and suitable post-preparation treatment the surface forces can be tuned.

CPP 20.20   Mon 17:30   Poster A
**Scattering Behavior of Distorted Semi-Flexible Polymers and Semi-Flexible Random Copolymers** — ●Reinhard Sigel — Max-Planck-Institut für Eisenforschung, Düsseldorf

Models for the interpretation of scattering experiments for two classes of polymer systems are discussed. In distorted semi-flexible polymers, the orientation correlation of the chain gets lost at distortions (kinks). A statistical combination of different monomers results in a random copolymer, where the orientation correlation is affected by the persistence lengths of the respective homo-polymers. In a dilute solution condition, the description of both polymer systems can be traced back to suitable averages of form factors from the literature. To handle the contrast difference in random copolymers, the approach of Endo and Shibayama (Polymer J. 42, 157-160, 2010) for flexible chains is extended to the case of semi-flexible chains.

CPP 20.21   Mon 17:30   Poster A
**One-Pot Synthesis of Copper Oxide Nanowires and PVDF/CuO Composite Films for Piezoelectric Energy Harvesting Application** — Samiran Garain[1], ●Karsten Henkel[1], Dipankar Mandal[2], and Dieter Schmeisser[1] — [1]Angewandte Physik-Sensorik, Brandenburgische Technische Universität Cottbus-Senftenberg, K.-Wachsmann-Allee 17, 03046 Cottbus, Germany — [2]Organic Nano Piezoelectric Devices Laboratory, Jadavpur University, Kolkata-700032, India

Copper oxide (CuO) is an attractive p-type oxide semiconductor with narrow band gap that has intriguing properties such as non-toxicity, chemical stability, electrocatalytic activity, abundant availability and low production cost. Polymeric materials have attracted great interest owing to their high flexibility, light weight, low cost production and high resistance against corrosion. Poly(vinylidene fluoride) (PVDF) is a commonly used piezoelectric polymer due to its excellent flexibility and piezoelectric properties. In this work, we adopted a one-pot synthesis of CuO nanowires by facile and selective chemical etching process of Cu substrate. XPS, XRD, SEM data ascribed the formation of polycrystalline CuO nanowires over the entire Cu surface. It has been observed that the uniformity, shape and size of the nanowires could be conveniently controlled by etching time and etchant concentration. We have also prepared piezoelectric nanogenerator based on the flexible PVDF/CuO composite film, where the traditional electrical poling treatment was avoided. In addition, dielectric properties have been studied to demonstrate the role of interfacial polarization.

CPP 20.22   Mon 17:30   Poster A
**Molecular dynamics simulation of hyperbranched polymers as a twofold distributed polymer system** — ●Peter Friedel[1], Shamila Firdaus[1,2], Albena Lederer[1,2], and Susanne Boye[1] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., Dresden, Germany — [2]Technische Universität Dresden, Dresden, Germany

The properties of hyperbranched polymers are determined by a molar mass and a configuration distribution which makes the experimental characterization difficult.

The developement of a simple simulation approach which may describe the properties of such a twofold distributed hyperbranched polymer system is the aim of the following denoted procedure. Starting with a well optimized monomer unit one may build up a set of hyperbranched polymer models (e.g., the specific poly(2,2-bis(hydroxymethyl)propionic acid) polymer system) with different molar masses and configurations (from linear over hyperbranched up to dendritic ones). Performing corresponding molecular dynamics simulations of every model of this set diluting it in an explicit solvent (i.e. THF) and equilibrating the whole NpT ensemble up to a standard state one is able to evaluate the corresponding trajectories (time averaged radii of gyration, monomer densities, pair distance distributions etc.).

These results may be weighted summarized and represent the properties of the called polymer system which are comparable to the experimental findings and to corresponding MC simulations (NVT ensemble with implicit solvent).

CPP 20.23   Mon 17:30   Poster A
**Event-chain simulations of many semiflexible polymers** — ●Tobias A. Kampmann and Jan Kierfeld — TU Dortmund University, Germany

We applied the extended, parallel EC algorithm to a system of many (semiflexible) harmonic chains, where the simulation efficiency is comparable to optimized molecular dynamics simulations, while still incorporating the essential features of the actual dynamics. This novel algorithm allows the simulation of melts of hard needle polymers - chains of infinitely thin rods - where reptational behaviour can be clearly observed. When the polymers interact via a short range, attractive square well potential bundled structures arise. It is not known, neither experimentally nor theoretically, what the actual thermodynamic equilibrium state of such a system is and whether this state can be achieved kinetically at all, depending on the initial conditions. Possible equilibrium structures are a single thick bundle or networks of smaller bundles. In any case, tightly packed bundles are created, which are difficult to equilibrate with traditional local moves. The use of EC algorithms thus appears to be advantageous.

CPP 20.24   Mon 17:30   Poster A
**Assignment of polymer geometries in STM images via statistical analysis of fitted patterns** — ●Florian Günther[1,2,3], Dmitry Skidin[1,3], Francesca Moresco[1,3], Gianaurelio Cuniberti[1,3], Sibylle Gemming[2,3,4], and Gotthard Seifert[1,3] — [1]TU Dresden, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Germany — [3]Center for Advancing Electronics Dresden, Germany — [4]TU Chemitz, Germany

To study the physical properties of a system on the atomic scale, the geometry is an important issue. For soft materials, however, the geometry is a priori unknown and hard to access experimentally.

In this work, we study the donor-acceptor polymer poly-dithienyl-diketopyrrolopyrrole (pTDPP) for which we analysed the impact of the torsion angles on the stability of the system. For this, we used density functional theory (DFT) methods using different functionals as well as the computationally efficient density functional based tight binding (DFTB) approach.

Moreover, we consider scanning tunnel microscopy (STM) images of pTDPP obtained via on-surface polymerization at Au(111). Here, we use an empirical fitting of frequently occurring patterns and analyse the obtained distances and angles statistically. In doing so, we could clearly assign certain geometries of the polymer found by simulation to the STM patterns.

CPP 20.25   Mon 17:30   Poster A
**Machine learning of correlated dihedral potentials for atomistic molecular force fields** — ●Pascal Friederich[1], Manuel Konrad[1], Timo Strunk[2], and Wolfgang Wenzel[1] — [1]Karlsruhe Institute of Technology, Karlsruhe, Deutschland — [2]Nanomatch GmbH, Karlrsuhe, Deutschland

Computer simulation increasingly complements experimental efforts to describe nanoscale structure formation. Molecular mechanics simulations and related computational methods fundamentally rely on the accuracy of classical atomistic force fields for the evaluation of inter- and intramolecular energies. One indispensable component of such force fields, in particular for large organic molecules, is the accuracy of molecule-specific dihedral potentials which are the key determinants of molecular flexibility. We show in this work that non-local correlations of dihedral potentials play a decisive role in the description of the total molecular energy - an effect which is neglected in most state-of-the-art dihedral force fields. We furthermore present an efficient machine learning approach to compute intramolecular conformational energies. At the example of $\alpha$-NPD, a prototypical molecule used in organic electronics, we demonstrate that this approach improves the agreement between semi-empirical energies and traditional force fields by one order of magnitude to a mean absolute deviation smaller than 0.37 kcal/mol (16.0 meV) per dihedral angle.

CPP 20.26   Mon 17:30   Poster A
**Quantifying how coarse-graining reduces the size of chemical compound space** — ●Kiran Kanekal, Kurt Kremer, and Tristan Bereau — Max Planck Institute for Polymer Research

Increasing the efficiency of materials design and discovery remains a significant challenge, especially given the prohibitively large size of chemical compound space. Efficient sampling of chemical compound space can be achieved *in silico* with the use of transferable coarse-

grained (CG) models that retain the essential properties of a higher resolution method. In addition to reducing computational expense, use of a chemically transferable CG model enables different molecular fragments to map to the same bead type. This further increases sampling efficiency, effectively reducing the size of chemical compound space. For example, the MARTINI[1] force field consists of 14 different neutral bead types, allowing for 119 unique representations consisting of 1-bead and 2-bead CG molecules. We previously showed that over 400,000 molecules could be mapped to these 119 MARTINI representations, demonstrating a drastic reduction of chemical compound space[2]. However, it is unclear as to how much variability exists within the subset of molecules and functional groups that map to a single bead type. In this work, we investigate these subsets for each MARTINI bead type to quantify the effective range of chemical space that is covered by that bead type. We further propose new criteria for the rational design of CG models that allows for the optimization of their chemical transferability. [1] Fink and Reymond, J. Chem. Inf. Model. 2007, 47, 342. [2] Menichetti et al., J. Chem. Phys. 2017, 147, 125101.

CPP 20.27   Mon 17:30   Poster A
**The elasticity of real polymer networks without entanglements** — •Michael Lang[1], Toni Müller[1,2], and Jens-Uwe Sommer[1,2] — [1]Institut Theorie der Polymere, Leibniz-Institut für Polymerforschung Dresden, Hohe Straße 6, 01069 Dresden, Germany — [2]Technische Universität Dresden, Institut für Theoretische Physik, Zellescher Weg 17, 01069 Dresden, Germany

We develop a method that allows to analyze directly the local contributions of individual strands to rubber elasticity. This method is used to quantify the impact of cyclic defects on elasticity for 4-functional model networks that were prepared at a different polymer volume fraction and with a different degree of polymerization between the crosslinks. Using the bond fluctuation model for simulations, entanglements and excluded volume can be switched off separately, which allows for a direct quantification of the effect of excluded volume on the phantom modulus of a network. We test our estimate of the phantom modulus with the modulus as measured from shearing the networks without excluded volume. For networks with excluded volume switched on, we find that excluded volume renormalizes fluctuations but has virtually no impact on the elasticity of the networks. However, the inactive material, which is connected to the network through a single point now couples partially to the shear deformation of the elastically active network, such that considering a zero contribution of the inactive material underestimates the phantom modulus.

CPP 20.28   Mon 17:30   Poster A
**Development of a self-healing silicone rubber for high-voltage cable accessories** — •Lena Barnefske[1], Andreas Petersen[2], Gerd Heidmann[2], and Heinz Sturm[1] — [1]Bundesanstalt für Materialforschung und -prüfung, Berlin, Germany — [2]Institut Prüffeld für elektrische Hochleistungstechnik GmbH, Berlin, Germany

Self-healing materials are modified materials which respond on a damage phenomenon by using a damage management, called self-healing. In the scope of this research it is important that such materials are developed for a specific damage phenomenon as well as on a specific application. One of the biggest problems in high-voltage silicone rubber insulation cable accessories is the damage on electrical treeing, initiated by partial discharges. This damage leads at one point to a breakdown of the insulation. Furthermore, these cable accessories are often difficult to access. This aspects open up a question whether novel and promising self-healing materials might be a solution to this problem.

Our research focuses on a highly homogeneous material design, which is composed by a silicone rubber matrix with polydimethylsiloxane-polyorganosiloxane filler particles. Particles are able to release polydimethylsiloxane after destruction for healing. With our contribution we would like to present first results on the characterization on the damage mode induced by electrical treeing under high-voltage with scanning electron microscopy to define parameters for further developments on the material.

CPP 20.29   Mon 17:30   Poster A
**Intercalation of p-aminobenzoic acid into layered cobalt hydroxide salt using a hydrothermal methodology: synthesis, characterization, and evaluation as potential modifier of polyethylene of absorption ultraviolet ray properties** — •neffer gomez[1], swami maruyama[1], fernando wypych[1], and an-

dreas leuteritz[2] — [1]Universidade Federal do Parana,curitiba, brazil — [2]leibniz institutes für polymerforschung

This paper aims to synthesize nanocomposites based in hydroxide salts intercalated with organic ultraviolet (UV) absorbent molecule for use in the lining of cables that could be apply in the electrical center. The synthesis procedure was performed using urea hydrolysis of Co (II) nitrate melts at 160 °C and its modification carry-out in an oven at 90 and 120 °C in a simple process. The modified structure and thermal stability of the hydroxide salt with formula (Co(OH)1,7(PABA)0,3).0,443H2O were characterized by XRD, FTIR, TGA, Raman, DSC, UV-Vis, MEV. Its studies suggest that HNCo-AB may have potential application as a UV absorber, because it improves this property when mixing with polyethylene,when the UV spectra shows a big band that covered the region between 400-200 nm.

CPP 20.30   Mon 17:30   Poster A
**Molecular Modeling of Polycarbonate Materials: Glass Transition and Mechanical Properties** — •Karol Palczynski[1], Andreas Wilke[2], Manfred Paeschke[2], and Joachim Dzubiella[1] — [1]Institut für Weiche Materie und Funktionale Materialien, Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner Platz 1, 14109 Berlin, Germany — [2]Bundesdruckerei GmbH, Kommandantenstraße 18, 10969 Berlin, Germany

Linking the experimentally accessible macroscopic properties of thermoplastic polymers to their microscopic static and dynamic properties is a key requirement for targeted material design. Classical molecular dynamics simulations enable us to study the structural and dynamic behavior of molecules on microscopic scales, and statistical physics provides a framework for relating these properties to the macroscopic properties. We take a first step towards creating an automated workflow for the theoretical prediction of thermoplastic material properties by developing an expeditious method to parameterizing a simple yet surprisingly powerful coarse-grained bisphenol-A polycarbonate model which goes beyond previous coarse-grained models and successfully reproduces the thermal expansion behavior, the glass transition temperature as a function of the molecular weight, and several elastic properties.

CPP 20.31   Mon 17:30   Poster A
**Structure-Property Relationships of Hyperbranched Polyamine ester/Ka-DCA nanocomposites.** — •Shereen Omara[1,2], Mona H Abdel Rehim[2], Gamal Turky[2], Sherif Madkour[1], and Andreas Schönhals[1] — [1]Bundesanstalt für Materialforschung und-prüfung (BAM), — [2]National Research Centre (NRC), 33 El Behouth St., Dokki, Giza, P.O.12622, (Egypt)

Hyperbranched polyamine ester (HPAE)/ kaolinite nanocomposites were papered via an ex situ (solution-based) method. The kaolinite has been modified by dodecylamine (DCA). SAXS measurements revealed that the Ka interlayer space increased from 0.71 to 3.6 nm-1. A partly exfoliated structure of the HPA/Ka-DCA nanocomposites was proved by SAXS and TEM. By a combination of BDS and SHS, the relaxation properties of the nanocomposites were investigated in dependence on frequency and temperature. The activation energies of $\gamma$-relaxation for the nanocomposites were lower than the values found for the pure HPAE. The segmental dynamics ($\alpha$- relaxation) was found to be screened out by the conductivity contribution, while it was retrieved by SHS employing AC-chip calorimetry. The confinement effect of the Ka-DCA nanofillers reduces the glass transition temperature Tg and enhances, meanwhile, the electrical conductivity of the polymer. By comparing the temperature dependence of the dynamic glass transition measured with SHS and that of the dc conductivity measured by BDS, a decoupling in their temperature dependencies was found.

CPP 20.32   Mon 17:30   Poster A
**Dynamic Properties of Multiblock Copolymers** — •Fabian Berressem, Friederike Schmid, and Arash Nikoubashman — Institute of Physics, Johannes Gutenberg University Mainz

The ability of copolymers to self-assemble into well-defined nanostructures has been of enormous importance in academic studies as well as in industry. This remarkable property makes it possible to create large volumes of materials with specific nanostructures and tailored properties. Previous research has focused mainly on diblock copolymers, as these macromolecules are relatively easy to produce. However, recent advances in chemical synthesis have made it possible to create more complex polymers such as multiblock copolymers. Self-assembled structures of multiblock copolymers contain many loops and bridges,

which can drastically alter the rheological properties of the polymer melts compared to simple diblock copolymer systems. The microscopic arrangement of the individual polymers, and thus the distribution of loops and bridges, strongly depends on the specific polymer properties as well as the employed manufacturing processes, e.g., solvent casting or spray coating. Therefore, it is crucial to consider the self-assembly of the chains on a microscopic level to fully understand the macroscopic flow properties of the melts. To this end, we combine self-consistent field theory and molecular dynamic simulations of Lennard-Jones chains. Our simulations reveal that the number of loops and bridges increases with the number of blocks in a copolymer. Further we study how the order of the self-assembled structures is improved by applying external fields, such as substrate patterning or shear.

### CPP 20.33   Mon 17:30   Poster A

**Evaluating thermal diffusion forced rayleigh scattering experiments with polydisperse polymers** — •Bastian Pur and Werner Köhler — Physikalisches Institut, Universität Bayreuth, 95440 Bayreuth, Germany

The Soret effect (thermophoresis) describes a diffusion flux that is driven by a temperature gradient in a multicomponent mixture. By means of thermal diffusion forced rayleigh scattering (TDFRS), which is a holographic grating technique, one can obtain the collective (Fickian) diffusion coefficient $D$, the thermal diffusivity $D_{th}$, the Soret coefficient $S_T$ and the thermal diffusion coeffcient, also known as the thermophoretic mobility, $D_T$. Measurements with binary mixtures, e.g. polymer solutions, can be evaluated with an working equation deduced from the linear response theory. This works well for monodispers polymers, but there are discrepancies due to polydispersity. Polydispersity was obtained by dynamic light scattering experiments, which yields the hydrodynamic radii distribution. From the initial rise of the concentration signal of TDFRS measurements, we can calculate the thermal diffusion coefficient $D_T$, even for polydisperse polymers.

### CPP 20.34   Mon 17:30   Poster A

**Quantum currents and pair correlation of electrons in a chain of localized dots** — •Klaus Morawetz — Münster University of Applied Sciences,Stegerwaldstrasse 39, 48565 Steinfurt, Germany — International Institute of Physics (IIP)Av. Odilon Gomes de Lima 1722, 59078-400 Natal, Brazil — Max-Planck-Institute for the Physics of Complex Systems, 01187 Dresden, Germany

The quantum transport of electrons in a wire of localized dots by hopping, interaction and dissipation is calculated and a representation by an equivalent RCL circuit is found. The exact solution for the electric-field induced currents allows to discuss the role of virtual currents to decay initial correlations and Bloch oscillations. The dynamical response function in random phase approximation (RPA) is calculated analytically with the help of which the static structure function and pair correlation function are determined. The pair correlation function contains a form factor from the Brillouin zone and a structure factor caused by the localized dots in the wire. Eur. Phys. J. B 90 (2017) 53

### CPP 20.35   Mon 17:30   Poster A

**Covalent dye functionalization of single-walled carbon nanotubes** — •Gririraj Manoharan[1], Henrik Flötotto[2], Petra Bösel[1], René Wieczorek[1], Jan Kurzhals[1], Paul Kögerler[2], Wolfgang Harneit[1], Claire Besson[3], and Carola Meyer[1] — [1]Fachbereich Physik, Universität Osnabrück, Deutschland — [2]Institut für Anorganische Chemie, RWTH Aachen, Deutschland — [3]Department of Chemistry, The George Washington University, Washington, DC 20052, USA

Dye-functionalized carbon nanotubes (CNTs) have great potential for application in light-harvesting devices, in optical sensors, and in biosensing. Covalent attachment allows for high selectivity and stability of the reaction. It can be applied after a CNT has been contacted with electrodes to avoid surface or contact contamination. Our goal is to use CNTs as containers to place spin carriers next to shallow NV centers in diamond for quantum sensing.

We present covalent functionalization of single-walled CNTs with the Alexa Fluor® 594 dye, characterizing the individual steps of the chemical route. Dye-functionalized CNTs are dispersed on oxygen-terminated diamond and located by their fluorescence for co-localization with NV centers. An open question is whether a CNT in the vicinity of a shallow NV center quenches NV luminescence. We check this by monitoring the fluorescence of the stable color centers during bleaching of the dye molecules.

### CPP 20.36   Mon 17:30   Poster A

**Simulation of lithium-ion model batteries: A lattice Monte Carlo approach** — •Alina Wettstein, Oliver Rubner, and Andreas Heuer — Institut für Physikalische Chemie, Münster

A great variety of theoretical approaches seeks to unravel the intrinsically multiscale and hence substantially complex behaviour of a battery cell. For the individual components such as electrolytes or electrodes atomistically resolved simulation techniques, e.g. molecular dynamics (MD) simulations, can be used. For the understanding of the whole cell continuum approaches have been developed. Here we present a lattice Monte Carlo (MC) model, which aims at simultaneous consideration of molecular-level properties and entire cell operation. Our MC model is designed as a modular system and includes the internal electrochemical processes as well as the particle motion given the relevant interactions and rates within a cell. We compute the experimentally accessible properties of a battery, such as voltage and capacity, for a minimum input of external parameters, i.e. diffusion coefficients that have been obtained from MD simulations. By means of this simplified, but yet highly flexible approach it is possible to further understand the basic principles of lithium-ion batteries.

### CPP 20.37   Mon 17:30   Poster A

**Incorporating chemical reactivity into classical molecular dynamics simulations** — •Myra Biedermann[1], Diddo Diddens[2], and Andreas Heuer[1,2] — [1]Institute of Physical Chemistry, University of Münster, Corrensstraße 28/30, 48149 Münster, Germany — [2]Helmholtz-Institut Münster (HI MS), Corrensstraße 46, 48149 Münster, Germany

We investigate the molecular transport and reaction processes at the interface between electrode and electrolyte in lithium ion batteries. More specifically, we are interested in the microscopic mechanisms which lead to the initial formation of the Solid Electrolyte Interphase (SEI) and the formation of dendrites in lithium ion batteries. For this purpose, we are working on incorporating chemical reactivity into classical molecular dynamics (MD) simulations by introducing reactive steps additionally to the MD steps. Our methodological approach is inspired by recent work of Takenaka et al. [1]. By doing so, we aim at developing a simulation method that incorporates chemical reactivity in a simple but realistic manner while retaining the time and length scales of standard MD simulations. The concepts are verified for a simple model system.

[1] N. Takenaka, Y. Suzuki, H. Sakai und M. Nagoaka, The Journal of Physical Chemistry C, pp. 10874-10882, 2014

### CPP 20.38   Mon 17:30   Poster A

**Finite-Size Effects in Molecular Dynamics Simulations of Ionic Liquids** — •Diddo Diddens[1], Volker Lesch[1], Andreas Heuer[1,2], and Jens Smiatek[1] — [1]Helmholtz-Institut Münster, Ionics in Energy Storage (IEK-12), Forschungszentrum Jülich GmbH, Corrensstraße 46, 48149 Münster, Germany — [2]Institut für physikalische Chemie, Westfälische Wilhelms-Universität Münster, Corrensstraße 28/30, 48149 Münster, Germany

Ionic liquids (ILs) have recently gained significant interest due to their potential application as electrolytes for batteries and supercapacitors or as solvents for catalysis or $CO_2$ capture. Due to the fact that the properties of a given IL strongly depend on the detailed chemical interactions between cations and anions, molecular dynamics (MD) simulations are frequently employed to gain deeper insights on the microscopic level. However, with this technique, one typically is limited to rather small (albeit periodic) systems, which significantly affects the ion transport properties [1]. While analytical finite-size corrections exist for the self-diffusion coefficient [1-3], the impact of the system size on the conductivity is more intricate. In this contribution, we utilize MD simulations in order to characterize the distance-dependent motional ion correlations contributing to the overall conductivity, and study how these correlations change with the system size. In addition, we rationalize our findings by analytical arguments.

[1] S. Gabl et al., J. Chem. Phys., **2012**, 137(9), 094501
[2] B. Dünweg, K. Kremer, J. Chem. Phys., **1993**, 99(9), 6983
[3] I.-C. Yeh, G. Hummer, J. Phys. Chem. B, **2004**, 108(40), 15873

### CPP 20.39   Mon 17:30   Poster A

**Tuning and Suppressing the Conduction of Ionic Liquids by Confinement in Nanoporous Metal-Organic Frameworks** — Anemar Bruno Kanj[1], Rupal Verma[1], •Modan Liu[2], Wolfgang Wenzel[2], and Lars Heinke[1] — [1]Karlsruhe Institute of Technology (KIT), Institute of Functional Interfaces (IFG) — [2]Karlsruhe Institute

of Technology (KIT), Institute of Nanotechnology (INT)

Ionic liquids (IL) are room-temperature molten organic salts and metal-organic frameworks (MOFs) are nanoporous functional-material platforms compound of metal ions and organic linkers. The composite of both IL and MOF is intriguing and has huge potentials for nanoscale electronic devices as batteries or sensors.

IL embedded in MOFs is known to have properties deviating from bulk phase solution. Experiment shows molar conductivity of IL can see a drastic 3-orders-of-magnitude drop with respect to bulk phase conductivity when heavily loaded into the MOF, filling MOF pores.

Here, employing molecular dynamics (MD) simulations we investigate molar conductivity with various loading factors of [BMIM][NTf2] in HKUST-1. Result suggests dedicated and homogeneous flows of cation and anions are formed when bulk-phase solution is exposed external electric field, whereas, embedded in HKUST-1, cations and anions are forced to share channels inside MOF. Increasing loading of IL, mobility of ions becomes hindered as the aperture between MOF pores limits the flow. With higher loading, transient jamming and eventually a jammed layer of IL is formed, leading to the drastic drop in molar conductivity. Statistics of MD confirm measurements from experiment.

CPP 20.40   Mon 17:30   Poster A
**Multi-Phase Transition Behavior of Highly Conductive Polybromide Ionic Liquids** — •Falk Frenzel[1], Karsten Sonnenberg[2], Sebastian Hasenstab-Riedel[2], and Friedrich Kremer[1] — [1]Universität Leipzig, Leipzig, Germany — [2]Freie Universität Berlin, Berlin, Germany

Over the last three decades Ionic Liquids (ILs) have reached such a remarkable scientific interest that nowadays this class of materials comprise a million dollar market being commercially used in application areas like medicine, energy technology and synthetic chemistry. Even though most scientific questions for 'standard' ILs have been addressed and already answered the novel subclass of (poly) halogenide Ionic Liquids opens the window to unique properties like multiple phase transitions. In order to study them as well as the molecular dynamics and charge transport mechanism X-ray scattering, broadband dielectric spectroscopy (BDS) and differential scanning calorimetry (DSC) have been employed to six different samples consisting of asymmetrical ammonium cations in composition with tribromide respectively nonabromide anions. The current study unravels three molecular relaxation processes, whereat one is assigned to the dynamic glass transition (DGT) while the other both are secondary relaxations, as well as the primarily charge transport mechanism that is determined to be a DGT assisted hopping process. Furthermore, the at room temperature remarkably high DC-conductivity ( >10 mS/cm) is strongly dependent on the thermally history below 300K due to distinct hystereses of the phase transitions.

CPP 20.41   Mon 17:30   Poster A
**Inter- and Intramolecular Interactions in an Extraordinary Conductive Polymeric Ionic Liquid** — •Arthur Markus Anton, Falk Frenzel, and Friedrich Kremer — Peter Debye Institute for Soft Matter Physics, Leipzig University

Polymeric ionic liquids (PILs) combine the advantages of neat ionic liquids, such as electrochemical and thermal stability or high ion conductivity, with the benefits of polymers like well-controllable processing and structure formation conditions. Due to these advantages, PILs are of principal importance for applications like super-capacitors or battery media. Recently, it has been reported from a novel PIL which exhibits the highest dc-conductivity at temperatures below 100°C and –contrary to the common dogma– an intensified charge transport with *rising degree of polymerization* [1]. In order to shed light on the origin of the material's extraordinary performance, we examined temperature-dependent FTIR spectroscopy in combination with broadband dielectric spectroscopy. On the one hand the pure cation exhibits a lower dc-conductivity ($2 \cdot 10^{-9}$ vs. $2 \cdot 10^{-7}$ S/cm at $T_g + 50$ K) than the polymeric system, on the other hand an extensive H-bond network is established, which is characterized through a distinct hysteresis in cooling-heating cycles demonstrating the stabilization of the structure through intermolecular interactions. Thus, the interplay between polymer and cations leads to the enhanced dc-conductivity which is higher than that of a separated part of the system. [1] F. Frenzel, A. M. Anton, F. Kremer et al., Macromolecules 50 (2017) 4022-4029

CPP 20.42   Mon 17:30   Poster A

**1H and 19F PFG NMR of choline-based ionic liquids in bulk and in carbon fibers** — •Emmanouil Veroutis, Steffen Merz, Markus Gehring, Rüdiger Eichel, and Josef Granwehr — Forschungszentrum Jülich GmbH, Institute of Energy and Climate Research - Fundamental Electrochemistry (IEK-9), 52428 Jülich, Germany

In recent years great interest has been attracted by room temperature ionic liquids (RTILs) due to their potential as new media for organic, catalytic and electrochemical applications. Given their interesting properties, such as very low vapor pressure, non-flammability, high thermal stability and wide electrochemical window, ILs are proposed as electrolytes for batteries. Despite of this research attention, electrolyte ILs and their interactions with electrodes in battery systems still remain poorly characterized.

In this study we present 1H and 19F Pulsed Field Gradient (PFG) NMR measurements on choline-based ionic liquids in bulk as well as confined in electrospun carbon fibers. The self-diffusion coefficients of the cation and the anion have been measured and correlated with electrochemical parameters, such as molar conductivity, transference numbers and ionicity. Furthermore, the interactions of cation and anion, but also the interaction with the carbon fibers have been examined by means of Nuclear Overhauser Effect Spectroscopy (NOESY) NMR, which provides through-space correlations between nearby nuclei. Finally, the influence of water on the physicochemical parameters of the studied ionic liquids has also been addressed by NMR.

CPP 20.43   Mon 17:30   Poster A
**Static and Dynamic Properties of [C$_2$Mim][NTf$_2$] Ionic Liquid on Neutral Sapphire Surface** — •Nataša Vučemilović-Alagić[1,2], Daniel Berger[4], Jens Harting[4,5], Christian Wick[1,3], David M. Smith[1,2], and Ana-Sunčana Smith[1,2,3] — [1]EAM, Cluster of Excellence, FAU, Erlangen, Germany — [2]Ruđer Bošković Institute, Zagreb, Croatia — [3]Institute for Theoretical Physics I, FAU, Erlangen, Germany — [4]Forschungszentrum Jülich GmbH, Helmholtz-Institut Erlangen-Nürnberg for Renewable Energy — [5]Department of Applied Physics, Eindhoven University of Technology, Eindhoven, The Netherlands

In the last decades it has become a common practice to use ionic liquids films in the context of catalysis. A particular advantage of these systems is their low vapour pressure and powerful solvation . Understanding the solvent effects both in the context of interface wetting and chemical reactions is vitally important for the technological applications of ILs, however, the understanding of these processes is still not satisfactory. To address this problem, we employ atomistic molecular dynamics (MD) simulations and investigate the behaviour of the archetypical imidazolium-based IL [C$_2$Mim][NTf$_2$]. We systematically study the role of the IL model introduced through the force field, and determine their static and dynamic properties at interfaces with a hydroxylated sapphire or vacuum. We use this model to study the structuring of IL and the changes of its transport properties as a function of the distance from the interface of choice.

CPP 20.44   Mon 17:30   Poster A
**Strong Polyelectrolytes and Specific Counterion Condensation Effects: A Molecular Dynamics Simulation Study** — •anand narayanan krishnamoorthy[1], christian holm[1], and jens smiatek[2] — [1]Institute for Computational Physics - University of Stuttgart — [2]Institute of Energy and Climate Research (IEK) - Forschungszentrum Jülich

We study specific counterion condensation effects in aqueous solution for monovalent alkali and halide ions with model polyelectrolyte using atomistic Molecular Dynamics simulations. Our results reveal significant differences between the individual ion types distributions around a rigid artificial strong polyelectrolyte. The results of the simulations demonstrate that mean-field theories which disregard the molecular nature of the solvent are inappropriate to explain the observed deviations. Furthermore we studied specific counterion condensation effects in non aqueous solvents like DMAc and methanol which provides an insight into specific ion effects in non aqueous medium and helps in understanding hoffmeister effects in non aqueous systems. Our results validate the strong dependence of condensation properties on ion chemical details and solvent effects in addition to electrostatic interactions.

CPP 20.45   Mon 17:30   Poster A
**Roughness and Salt Annealing in a Polyelectrolyte Multilayer** — •Amir Azinfar[1], Sven Neuber[1], Jiri Vanecek[2], Maria Vancova[2], Viteslav Stranak[2], and Christiane A. Helm[1] —

[1]Inst. f. Physics, Greifswald University, Germany — [2]Fac. of Science, University of South Bohemia, Ceske Budejovice, Czech Republic

The surface roughness of polyelectrolyte multilayers made from poly(diallyldimethylammonium chloride) (PDADMA) and poly(styrene sulfonate) (PSS,10.6 kDa) increases with the number of deposition steps until the linear growth regime is reached; then it is constant. AFM and Electron microscopy show the formation of micrometer-sizes features. The wavelength of the roughness features is approximately proportional to film thickness, which supports a mechanism whereby roughness is generated by anisotropic shrinking due to dehydration. Due to the viscous response of polyelectrolyte complexes the surface features are possibly better described as *damped* creases, where a small amount of flow is allowed in the most stressed regions. Annealing in high salt decreases in the long term the roughness.

CPP 20.46   Mon 17:30   Poster A

**Electrostatic bending response of a helical chain of charges** — •Alexandra Zampetaki[1], Jan Stockhofe[1], and Peter Schmelcher[1,2] — [1]Zentrum für Optische Quantentechnologien, Universität Hamburg, Luruper Chaussee 149, 22761 Hamburg, Germany — [2]The Hamburg Centre for Ultrafast Imaging, Luruper Chaussee 149, 22761 Hamburg, Germany

We explore the electrostatic contribution to the bending response of a chain of identical charged particles confined on a finite helical filament. We analyse how the energy difference $\Delta E$ between the bent and the unbent helical chain scales with the length of the helical segment and the radius of curvature and identify features that are not captured by the standard notion of the bending rigidity, normally used as a measure of bending tendency in the linear response regime. Using instead $\Delta E$ to characterize the bending response of the helical chain for low values of the radius-to-pitch ratio we find that it exhibits interesting oscillations with the number of particles, encountered for commensurate fillings. These oscillations yield length-dependent oscillations in the preferred bending direction of the helical chain of charges. We show that the origin of such oscillations is the non-uniformity of the charge distribution caused by the long-range character of the Coulomb interactions and the finite length of the chain.

CPP 20.47   Mon 17:30   Poster A

**Interactions among Spherical Polyelectrolyte Brushes in Concentrated Aqueous Solutions** — •Yunwei Wang[1,2], Regine von Klitzing[1], and Xuhong Guo[2] — [1]Technische Universität Darmstadt,Darmstadt,Germany — [2]East China University of Science and Technology,Shanghai,China

Interactions among annealed spherical polyelectrolyte brushes (SPB) in concentrated aqueous dispersion are studied by rheology measurements, small angle X-ray scattering (SAXS) and wide X-ray scattering (WAXS). The SPBs consist of a solid poly(styrene) core and a shell of poly(acrylic acid) (PAA). The effect of SPB concentration; pH; salt concentration have been explored. At 12 wt-%, SAXS spectra show a new peak which is assumed to be caused by overlapping polyelectrolyte chains. They are associated and form locally ordered structures which reflects the enhanced interactions among SPB. The locally ordered structures of brushes are proved by WAXS. For further validation of the interaction between the PAA chains and its influence on the emulsion rheological properties, the concentration of 12wt% brushes of the different pH and salt concentration were studied.

CPP 20.48   Mon 17:30   Poster A

**Silica Coating for Stabilization of Tubular J-aggregates** — •Katherine Herman, Stefan Kirstein, and Jürgen P. Rabe — Humboldt Universität zu Berlin Institut für Physik, Berlin, Germany

Cyanine dyes are remarkable for their ability to form supramolecular aggregates with both diverse morphologies as well as the signature narrow absorbance and emission bands of J- or H- aggregates. Cyanine dyes that form one dimensional nanostructures are of particular interest not only for their potential as light harvesting and energy transport structures, but also as systems for fundamental linear and non-linear spectroscopic studies. However, several powerful methods for investigating optical and energy transfer properties require that the sample be stable under dry and low pressure conditions. A possible means of stabilization is inorganic coating of the water soluble aggregates. Here we present an approach for a silica coating to stabilize tubular aggregate of amphiphilic cyanine dyes for dry and low pressure investigations. An initial monolayer of silica is formed by ionic self assembly of a functionalized organosilane on the aggregate surface. Further shell growth is achieved by gradual addition of a second organosilane under basic conditions. Evidence for silica shell growth on the aggregate comes from fluorescence spectroscopy and atomic force microscopy.

CPP 20.49   Mon 17:30   Poster A

**Growth Kinetics and Molecular Mobility of Irreversibly Adsorbed Layers in Thin Polymer Films** — •Marcel Gawek and Andreas Schönhals — Bundesanstalt für Materialforschung und -prüfung, Unter den Eichen 87, 12205 Berlin

In well-annealed thin polymer films, with non-repulsive polymer/substrate interactions, an irreversibly adsorbed layer is expected to form. These adsorbed layers have shown great potential for technological applications. However, due to the hard accessibility of these buried layers in thin films, their growth kinetics and molecular dynamics are still not fully understood. Here, the irreversibly adsorbed layers of homopolymer thin films are revealed by solvent-leaching experiments. First, the growth kinetics of these layers is investigated as a function of original film thickness and annealing times. The thickness, topography and quality of the adsorbed layer is determined with Atomic Force Microscopy (AFM). Secondly, the molecular mobility of the adsorbed layer is investigated with Broadband Dielectric Spectroscopy (BDS) with high-resolution analyzers. A recently developed nanostructured capacitor (NSC) is employed to measure the adsorbed layers with a free surface layer. The results are quantitatively compared and discussed with respect to recently published work.

CPP 20.50   Mon 17:30   Poster A

**Phase Separation in Phthalocyanine-Fullerene Co-Deposited Thin Films** — •Berthold Reisz, Giuliano Duva, Valentina Belova, Clemens Zeiser, Santanu Maiti, Alexander Hinderhofer, Alexander Gerlach, and Frank Schreiber — Universität, Tübingen, Deutschland

Co-deposited blends of copper phthalocyanine (CuPc) and Buckminster fullerenes (C60) are well known phase separating donor-acceptor systems exhibiting (compared to successive deposition) a dramatic modification of the thin film architecture with improved solar cell performance [1,2]. Till today, neither the assignment of morphological features to distinct molecular phases nor the separation processes are known. We followed the growth of pure and blended thin films by in situ real-time X-ray reflectivity and found material dependent roughening during the growth. Post growth X-ray diffraction at two grazing angles of incidence revealed an accumulation of C60-molecules at the surface, which may correspond to the tall features seen from atomic force microscopy. Further experiments aiming at a deeper insight into the phase separation processes are planned.

[1] P. Sullivan et al., Appl. Phys. Lett. **84** (2004)
[2] S. Heutz et al., Sol. Energ. Mat. Sol. Cells **83** (2004)

CPP 20.51   Mon 17:30   Poster A

**Thin films of ultrahigh molecular weight diblock copolymers** — •Wei Cao[1], Senlin Xia[1], Michael Appold[2], Markus Gallei[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]TU Darmstadt, Ernst-Berl-Institute for Technical and Macromolecular Chemistry, 64287 Darmstadt

Block copolymer self-assembly has attracted considerable attention for many decades because it can yields ordered structures in a wide range of morphologies, including spheres, cylinders, bicontinuous structures, lamellae, vesicles, and many other complex or hierarchical assemblies. So far, most studies have used block copolymers with low or medium scale molecular weight. Due to scaling of the micro-phase separation structure with the molecular weight of the the block copolymers, large periods (about 100 nm) can be achieved with ultrahigh molecular weight (UHMW) block copolymers (Mn > 800 kg/mol). In thin film geometry this implies a confinement of the polymers. For polystyrene-block-polymethylmethacrylate UHMW diblock copolymers we prepare thin films. Different thermal and solvent post-treatments are studied to achieve highly ordered micro-phase separation structures. The film morphology is probed with atomic force microscopy (AFM), scanning electron microscopy (SEM) and grazing incence small angle x-ray scattering (GISAXS).

CPP 20.52   Mon 17:30   Poster A

**Printed low bandgap polymer films** — •Xinyu Jiang and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching

Printing of low bandgap polymer films is of interest in organic photovoltaics. Roll-to-roll processing and large-area processability on low cost together with flexible substrates make conjugated polymer-based organic solar cells extremely attractive as a cost-effective solution to today's energy-shortage problem. We study printed mixtures of the low-bandgap polymer PTB7 with the fullerene derivate PCBM with respect to optical absorption and electrical properties. The film structure and morphology is proved with atomic force microscopy (AFM), scanning electron microscopy (SEM) and grazing incidence small angle x-ray scattering (GISAXS).

### CPP 20.53   Mon 17:30   Poster A

**Investigation of the impact of antifoam agents on lipid membranes by XRR and BAM** — ●Mike Moron, Susanne Dogan, Julia Nase, Michael Paulus, and Metin Tolan — Fakultät Physik/DELTA, TU Dortmund, 44221 Dortmund, Germany

The control of foam by means of antifoam agents is of great importance in a number of applications. For example, the oral administration of simethicone is prescribed in the case of surfactant intoxication and also in order to prepare patients for coloscopy. In both cases, simethicone reduces the amount of foam. Other domains where antifoam agents play a role are for example the kraft pulp process, radioactive waste treatment, and machine detergents. While the macroscopic behaviour of liquid systems containing antifoam agents and lipids is well understood, the modes of action on the molecular scale are not. Various theories were established to describe the molecular mechanisms, but the actual behaviour showed up to be strongly dependent on the system under investigation. We present a surface pressure-dependent in-situ X-ray reflectometry and Brewster-angle microscopy study on Langmuir-Blodgett monolayers consisting of different lipids and simethicone. Both the X-ray reflectivities and the BAM-measurements were performed at the liquid-air interface. The reflectivities provide information on the vertical structure of the systems, whereas the BAM-measurements reveal the lateral structure. With this combined information, it is possible to analyse the different models.

### CPP 20.54   Mon 17:30   Poster A

**Morphologies in liquid-liquid dewetting** — ●Roghayeh Shiri[1], Ralf Seemann[1], Dirk Peschka[2], and Barbara Wagner[2] — [1]Experimental physics, Saarland University, Saarbrucken, Germany — [2]Weierstrass Institute, Mohrenstr 39, Berlin, Germany

We study the dewetting of thin nanometric thin polystyrene (PS) films from liquid polymethyl-methacrylate (PMMA) substrates. In order to induce dewetting the PS/PMMA samples are heated above the glass transition temperature of both polymers. After a few minutes circular holes appear in the PS film and their radii grow with time and finally coalescence leading to a set of droplets on the substrate.

The considered mechanism leading to the symmetry breaking of the initially flat film is called spinodal dewetting, which is initiated due to the growth of thermally activated surface waves. The spinodal rupture of the liquid film results in a dewetting pattern of \*hills and gullies\* with a certain preferred wavelength $\lambda$ in both liquid/air and liquid/liquid interfaces leading eventually to the formation of holes after a certain time t. Interestingly, the deformation of the liquid/liquid interface is larger than that of the liquid/air interface due to the lower surface tension. According to theoretical predictions, can the deflection of both interfaces be in phase or antiphase which determines the dewetting pathway.

In this study we experimentally measured the preferred wavelength $\lambda$ and holes distance and we monitor deformation of interfaces by atomic Force Microscopy. Ultimately, the result of experimental observations will be compared with theoretical modelling.

### CPP 20.55   Mon 17:30   Poster A

**Structure formation of organic molecules on dielectric surfaces** — ●William Janke and Thomas Speck — Institut für Physik, Johannes Gutenberg-Universität Mainz, Germany

When buckminsterfullerenes ($C_{60}$) are deposited upon a substrate by means of molecular beam epitaxy, many different structures can form depending on the substrate in use and the experimental conditions. Calcium fluoride ($CaF_2$) as a substrate is particularly interesting since its interaction with $C_{60}$ is slightly weaker than the $C_{60}$-$C_{60}$ interaction, which leads to very interesting types of two-layered clusters. These clusters and other properties of the $C_{60}$-$CaF_2$ system have been observed in experiments [1]. To further the understanding of such deposition and diffusion systems, we study the diffusion and self-assembly of $C_{60}$ on $CaF_2$(111) by means of MD and KMC simulations as well

as theoretical considerations to build a comprehensive model for this system.

[1] Felix Loske, Jannis Lübbe, Jens Schütte, Michael Reichling, and Angelika Kühnle. Quantitative description of $C_{60}$ diffusion on an insulating surface. Phys. Rev. B, 82:155428, Oct 2010.

### CPP 20.56   Mon 17:30   Poster A

**Model-Free Thickness Determination of Nanoscale Foam Films using FTIR spectroscopy** — ●Eric Weissenborn and Björn Braunschweig — Institut für Physikalische Chemie, Westfälische Wilhelms-Universität Münster, Corrensstraße 28/30, 48149 Münster, Germany

The thin-film-pressure balance (TFPB) technique allows to determine intermolecular forces in free standing foam films. In order to calculate the surface potential of charged air/water/air interfaces, DLVO theory is applied where the correct size of the water core is extremely important. However, in the classical approach where the thickness is determined interferometrically, models of the adsorbate layer and its thickness have to be applied. In order to address the thickness of foam films, we have extended the abilities of a classical TFPB by combining interferometric UV/Vis spectroscopy and transmission IR spectroscopy in a single setup. Particularly, the coupling of a TFPB to a FTIR spectrometer allows to record IR spectra of foam films. From IR transmission spectra, we can not only accurately determine the foam film thickness as function of disjoining pressure by looking at the water O-H absorption bands, but can also determine their composition with the help of IR vibrational bands and their attribution to specific molecular vibrations. In order to demonstrate the proof of concept, we present disjoining pressure isotherms of cetyltrimethylammonium bromide ($C_{16}TAB$) foam films at 0.9 and 0.1 mM concentrations and compare the film thicknesses from both interferometric UV/Vis and infrared spectroscopy.

### CPP 20.57   Mon 17:30   Poster A

**Real-time XRR study of protein adsorption at the solid-liquid interface guided by multivalent ions** — ●Simon Schönberg[1], Madeleine Fries[1], Alexander Hinderhofer[1], Fajun Zhang[1], Robert M. J. Jacobs[2], Maximilian W. A. Skoda[3], and Frank Schreiber[1] — [1]Institute for Applied Physics, University of Tübingen, 72076 Tübingen, Germany — [2]Department for Chemistry, Chemistry Research Laboratory, University of Oxford, OX1 3TA, United Kingdom — [3]Rutherford-Appleton Laboratory, ISIS Facility, Didcot

The unique influence of multivalent ions on the phase behaviour of protein solutions has been subject of past and current research [1]. Moreover, the influence of multivalent ions ($Y^{3+}$) on the adsorption behaviour of protein (BSA) at the solid-liquid interface and thus the connection of bulk and interface behaviour was recently established [2]. In this context, we designed a new liquid cell for measurements at the solid-liquid interface *via* X-ray reflectivity (XRR). This setup allows real-time measurements of protein adsorption through the use of a molybdenum source. We successfully established this new XRR setup, which enables us to reproduce previous outcomes of ellipsometry measurements on multivalent ion-tuned protein adsorption. Further it allows to study more parameters such as temperature dependency of our system, surface roughness and surface coverage/density and thus promotes a more detailed understanding of protein adsorption tuned by multivalent ions.

[1] Zhang, F. et al., Pure Appl. Chem (2014), 86, 191-202.
[2] Fries, M. R. et al., Phys. Rev. Lett. (2017), in print.

### CPP 20.58   Mon 17:30   Poster A

**Dynamics of nanoscopically confined PVME in thin films of an asymmetric PVME/PS blend** — ●Paulina Szymoniak, Sherif Madkour, and Andreas Schönhals — BAM Bundesanstalt für Materialforschung und -prüfung, Unter den Eichen 87, 12205 Berlin (Germany)

In recent years, substantial efforts have been devoted to investigating nanoscopic confinement of polymers, and its effect on glassy dynamics. Broadband Dielectric Spectroscopy (BDS) was used to study the dynamics of ultra-thin films of PVME/PS 50/50 wt% blend, employing a novel nano-structured capacitor sample arrangement. The investigated system shows a complex dynamic behavior. First, an $\alpha$-relaxation, related to a bulk-like layer was found. Second, an $\alpha$'-relaxation was observed, characteristic for dynamically asymmetric blends, where the out of equilibrium dynamics is attributed to weakly-cooperative PVME segments relaxing within a frozen environment of PS segments. Thirdly, for thinnest films, an Arrhenius-like process was

dominant in the dielectric spectra, indicating localized fluctuations of the segments. Relaxation rates of this process resembled that of the degenerated $\alpha$-relaxation of the adsorbed layer, found for pure PVME [1], thus it was assigned accordingly. For thinnest films, this process undergoes a further confinement, due to the topological constraints, introduced by PS. Such multiple confinement effect has not been reported for ultra-thin films of polymer blends, before this study [2]. [1] Madkour, S. et al. ACS Appl. Mater. Interfaces 2017, 9, 7535. [2] Madkour, S. et al. ACS Appl. Mater. Interfaces 2017, 9, 37289

CPP 20.59  Mon 17:30  Poster A

**Competition of mobilization and immobilization effects of segmental dynamics in epoxy/Boehmite nanocomposites** — •Paulina Szymoniak, Dorothee Silbernagl, Media Ghasem Zadeh Khorasani, Heinz Sturm, and Andreas Schönhals — BAM Bundesanstalt für Materialforschung und -prüfung, Unter den Eichen 87, 12205 Berlin (Germany)

The interphase between the inorganic filler and the polymer matrix is considered as one of the most important characteristics of inorganic/polymer nanocomposites. The segmental dynamics of this interphase is expected to be altered as compared to the pure matrix, which might percolate into the entire system. For instance, it was found that a so-called Rigid Amorphous Phase (RAF) is formed by adsorption of segments onto the nanoparticles, yielding in their immobilization. The RAF is available from the decrease of the specific heat capacity step $\Delta$Cp in the glass transition region of the nanocomposites. Here, precise Temperature Modulated DSC (TMDSC) was employed to study $\Delta$Cp of epoxy/Boehmite nanocomposites with different nanofiller concentrations. Surprisingly, the investigated system showed an increase of $\Delta$Cp with increasing filler concentration up to 10 wt%. This implies an increased fraction of mobile segments, and is in accordance with the found decreased value of the glass transition temperature Tg. Although for higher filler contents Tg further slightly decreases, $\Delta$Cp decreases in contrary, indicating a formation of RAF. This behavior was discussed as a competition of mobilization effects, due to an incomplete crosslinking reaction, and the formation of RAF.

CPP 20.60  Mon 17:30  Poster A

**Temperature Dependent Photoluminescence Studies on Zinc Phthalocyanine Thin Films** — •Gabriel Freiherr von Eyb[1], Maximilian Frank[1], Simon Wiegand[1], Sebastian Hammer[1], and Jens Pflaum[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Bavarian Center for Applied Energy Research (ZAE Bayern), 97074 Würzburg

In recent years, there has been many opto-electronic applications implementing zinc phthalocyanine (ZnPc) as active organic component [1]. For the performance of those devices the temperature dependent optical behaviour of ZnPc is of relevance but has not been investigated to a sufficient extent.

In this work we analyse the spectral photoluminescence (PL) of ZnPc thin films in a temperature range of 20 to 360 K. The films under study were prepared by vacuum sublimation on glass and SiO2 substrates. Optical excitation of excitons in the ZnPcs Q-band reveals two main emission components whose intensity varies with temperature. The high energy component experiences a decrease in intensity towards

lower temperatures, almost vanishing completely at 20K. The low energy emission decreases as well, but not at the same extent. Combining the temperature dependent PL data with (room temperature) life-time measurements, we will address the role of singlets and triplets in the radiative and non-radiative relaxation processes in ZnPc and discuss possible similarities with a thermally activated delayed fluorescence mechanism.

[1] M. Brendel, et al., Adv. Func. Mater. 25 (2015) 1565

CPP 20.61  Mon 17:30  Poster A

**Quantifying surface potentials at liquid-gas interfaces from vibrational SFG spectroscopy** — Eric Weissenborn, Felix Schulze-Zachau, Georgi Gochev, •Natalia García Rey, and Björn Braunschweig — Institute of Physical Chemistry, Westfälische Wilhelms-Universität Münster, Corrensstrasse 28/30, 48149 Münster, Germany

Knowing the double layer potential ($\psi_0$) of the liquid-gas surface is essential to analyze the mechanisms of foam stabilization. However, no straightforward method is available to measure $\psi_0$. The intrinsic negative charging of pure water surface is significantly modified by adsorbing ionic surfactants while non-ionic surfactants change only slightly the $\psi_0$-magnitude. Adsorption of cationic surfactants will first neutralize the surface negative charge and further will cause charge reversal. By mixing non-ionic and cationic surfactants, we can tune the negative/zero/positive $\psi_0$ at the air-water surface. On charged interfaces, the SFG intensity depends not only on the $2^{nd}$-order of susceptibility ($\chi^{(2)}$) but also on the $3^{rd}$-order ($\chi^{(3)}$) due to impact of $\psi_0$. SFG spectroscopy used to quantifying the $\psi_0$ requires first its calibration to untangle the $\chi^{(2)}$ and $\chi^{(3)}$ from the spectra. $\psi_0$ is estimated from theoretical (DLVO) analysis of the disjoining pressure isotherm for a foam film as measured with the thin-film pressure balance (TFPB) technique. These experiments will allow for validation of data form OH-SFG spectra taken for isolated surface that can be applied to extract $\psi_0$-values. This is the first study to our knowledge that combines TFPB and SFG experiments for studying soft interfaces.

CPP 20.62  Mon 17:30  Poster A

**Structure of ice/clay nanocomposites** — •Hailong Li[1], Rika Unkelbach[1,2], Julian Mars[1,2], Ann-Christin Dippel[3], Olof Gutowski[3], Veijo Honkimäki[4], and Markus Mezger[1,2] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz — [2]Max-Planck-Institut für Polymerforschung, Mainz — [3]Deutsches Elektronen-Synchrotron DESY, Hamburg — [4]ESRF-The European Synchrotron, Grenoble

Material properties of permafrost strongly depend on the texture of the confined crystalline ice and the properties the quasi-liquid premelting layer (qll) formed at ice/solid interfaces. The layered sheet silicates vermiculite and kaolin with high interface to volume ratios are ideal model systems to study interfacial melting in geologically relevant ice/clay composites. The crystalline ice fraction and its preferred orientation was determined by temperature dependent x-ray diffraction experiments. Well below the melting point of bulk water, the formation of a qll is observed. The temperature dependent thickness of this qll follows a logarithmic growth law. However, different coefficients are observed for the charged vermiculite and uncharged kaolin clays.