CPP 54: Poster Session 3

Transport and Confinement, New Instruments and Methods, Charged Soft Matter, Physics of Food, (Active) Colloids and Complex Liquids, Gels and Elastomers, Nanoparticles and Composite Materials

Time: Thursday 15:00–19:00

 ${\rm CPP}~54.1 \quad {\rm Thu}~15{:}00 \quad {\rm P2}$

Properties of solvent mixture confined between silica slabs •XIANGYANG GUO, TOBIAS WATERMANN, CHRISTOPH ALLOLIO, and DANIEL SEBASTIANI — Institute of Chemistry, Martin Luther University Halle-Wittenberg, Von-Danckelmann-Platz 4, 06120 Halle (Saale) Firstly, we investigate the anomalous structure and hydrogen bond network of pure water confined between 2 silanol slabs through ab intio simulations. We compute the proton NMR chemical shifts of confined water as a measure for the strength of the hydrogen-bonding network based on a first principle approach. Our calculations illustrate both the modifications of the 1H NMR chemical shifts of the water with respect to bulk water and a considerable slowing down of water diffusion. Furthermore, we perform classical MD simulations on ethanolwater mixture under confinement using the same silica surface model. The diffusion coefficients of water and ethanol in the confined mixture are reported. The computed density profile shows that evident molecular segregation appears in the confined mixture. Ethanol molecules are more likely to form hydrogen-bonds with silica surface whereas most water exists as small hydrogen-bonded clusters at the center of the pore. This observation is corroborated by the wall-solvents radial distribution functions.

CPP 54.2 Thu 15:00 P2

Simulation of polymer melts in confined geometries — •ANDRE GALUSCHKO, MARCO WERNER, MICHAEL LANG, and JENS-UWE SOM-MER — Leibniz-Institut für Polymerforschung Dresden, Hohe Strasse 6, 01069 Dresden, Deutschland

Polymers in their disordered liquid state show unique viscoelastic properties when the chains start to entangle. The topological constrains created by interchain excluded volume and uncrossability, lead for a probing chain to move within a tube. We employ the Bond Fluctuation Model to simulate the diffusion dynamics of long polymer chains at melt conditions. When the melt becomes confinement between two ideal walls, the bulk limit is reobtained, when walls seperation becomes large compared the free chain extension. With increasing confinement the diffusion accelerates due to change of entanglement density and chain overlap density.

CPP 54.3 Thu 15:00 P2

Fluorescence correlation spectroscopy at reflecting substrates for investigation of vertical sample modulations — •DANIELA TÄUBER, KATHRIN RADSCHEIT, MICHAEL SCHULZ, and CHRISTIAN VON BORCZYSKOWSKI — Institut für Physik, TU Chemnitz, Germany

Fluorescence correlation spectroscopy (FCS) is widely used for characterization of dynamic material properties [1]. The usually employed confocal laser profiles render a vertical resolution of 1 micron. Reflecting substrates create interference patterns which allow for a vertical modulation of the fluorescence signal [2] in the range of 100-200 nm. Employment of spacer layers [2] and proper choice of excitation wavelength and fluorescent dyes or material properties, therefore, allows for tailored investigation of the vertical modulation of physical properties accessible by FCS. Here we present a modified correlation function for translational diffusion in thin films on reflecting substrates. Boundary effects and long range interactions affect the dynamics of materials and tracer molecules [3], in particular, within highly structured materials such as liquid crystals films [4] and liquid crystalline biomaterials. We apply the presented correlation function to investigate the dynamics of perylenediimides in thin liquid crystal films on silicon wafers with and without a 100 nm thick silica spacer layer.

 E.P. Petrov, P. Schwille, Springer Series on Fluorescence.
Springer, 2008, 145-197. [2] A. Lambacher, P. Fromherz, J. Phys.
Chem. B 105 (2001) 343. [3] D. Täuber, I. Trenkmann, and C. von Borczyskowski, Langmuir 29 (2013) 3583. [4] B. Schulz, D. Täuber, C. von Borczyskowski et al., Soft Matter 7 (2011) 7431.

CPP 54.4 Thu 15:00 P2 Diffusive mechanism of linear and branched molecules translocation through the "hairy" microchannels — \bullet IRINA NERATOVA^{1,2}, TORSTEN KREER¹, and JENS-UWE SOMMER^{1,2} — Location: P2

 1 Leibniz-Institut für Polymerforschung Dresden e.V., Hohe Straße 6, D-01069, Dresden, Germany — 2 Technische Universität Dresden, Institut für Theoretische Physik, Zellescher Weg 17, D-01069, Dresden, Germany

Polymer brush-covered or "hairy" channels have attracted a lot of attention in recent years for both engineering and biomedical applications. In recent years interest to polymer brush-covered nanochannels is based mostly on microfluidic processes which are intrinsic to living organisms. Many works have been done to understand the processes of opening and closing of the nanochannels. In our project we raise the question about the transport of the molecules through the "hairy" channels. By means of Molecular Dynamics simulations we study the flow dynamics in a microchannel. In particular we investigated the influence of the architecture of macromolecules with the same molecular weight on their ability to pass through a brush-covered channel driven by Poisseuille flow. The simulations indicate that flow conditions cause the speeding up of the transport of molecules with linear architecture through the nanochannel making their velocity comparable with fast but non-draining 30-arms stars. The simulation results reveal that stretching-collapse mechanism of linear molecules in the flow helps to diffuse freely through the pore while the large molecules like 5-, 10-, 15-arms stars are trapped in the channel.

CPP 54.5 Thu 15:00 P2

Segmental Mobilities in Polymer Films — •DIDDO DIDDENS¹, ANDREAS HEUER², JÖRG BASCHNAGEL¹, and HENDRIK MEYER¹ — ¹Institut Charles Sadron, Université de Strasbourg, 23 Rue du Loess, 67034 Strasbourg, France — ²Institut für physikalische Chemie, Universität Münster, Corrensstraße 28/30, 48149 Münster, Germany

The dynamical properties of polymer chains in thin films as compared to their counterparts in the bulk are of special interest for both practical applications as well as theoretical considerations. Here, we study the local segmental motion in polymer films on the basis of MD simulation data. In particular, we focus on the mobility of a given segment in dependence of its position within the film (i.e. in the center or close to the interface). This is done by our recently developed method [1], which utilizes the Langevin equation to interpret specific averages of the segmental motion in order to yield an effective mobility. Since this approach is purely local, it also allows the extraction of segmental mobilities for polymer chains in confined geometries, thus contrasting the non-local Rouse mode analysis. Additional emphasis is put on the effect of the interface (either a solid wall or vacuum) on the segmental motion.

[1] D. Diddens, M. Brodeck, A. Heuer, EPL 91 (2010) 66005

CPP 54.6 Thu 15:00 P2

Thermotropic Orientational Order of Discotics in Nanochannels: An Optical Polarimetry Study and Landau-de Gennes Analysis – •Mark Busch¹, Sylwia Calus², Carole V. Cerclier³, RONAN LEFORT³, DENIS MORINEAU³, BERNHARD FRICK⁴, KRISTINA KRAUSE⁵, ANDREAS SCHÖNHALS⁵, ERIC GRELET⁶, DANIEL RAU⁷, AN-DRIY V. KITYK², and PATRICK HUBER^{1,7} — ¹Materials Physics and Technology, Hamburg University of Technology, D-21073 Hamburg, - ²Faculty of Electrical Engineering, Czestochowa Uni-Germany versity of Technology, 42-200 Czestochowa, Poland — ³Institut de Physique de Rennes, CNRS UMR 6251, UniversiteÏ de Rennes 1, 35042 Rennes, France — ⁴Institut Laue-Langevin, BP 156, 38042 Grenoble Cedex 9, France — ⁵BAM Bundesanstalt für Materialforschung und prüfung, 12205 Berlin, Germany — ⁶Centre de Recherche Paul-Pascal, CNRS UPR 8641, Université de Bordeaux 1, 33600 Pessac, France -⁷Experimental Physics, Saarland University, 66041 Saarbrücken, Germany

Optical polarimetry measurements of the orientational order of a discotic liquid crystal (Py4CEH) confined in parallel-aligned nanochannels of monolithic, mesoporous alumina, silica, and silicon as a function of temperature, channel radius (3 - 22 nm) and surface chemistry reveal a competition of radial and axial columnar order. The evolution of the thermotropic nematic order parameter of the confined systems is continuous, in contrast to the discontinuous transition in the bulk. This behaviour is analyzed by Landau-De Gennes models for discotic order in nanoconfinement.

CPP 54.7 Thu 15:00 P2 Structure and Dynamics of Water in a Porous Silicate: Confinement from First Principles — •CHRISTOPH ALLOLIO¹, FELIX KLAMETH², and DANIEL SEBASTIANI¹ — ¹Institute for theoretical chemistry, Martin Luther University Halle-Wittenberg, Von-Danckelmann-Platz 4, 06120 Halle (Saale) — ²Institute for solid state physics, Technical University Darmstadt, Hochschulstr. 6-8, 64289 Darmstadt

Geometric confinement has a strong effect on water, making it quite different from the bulk.[1] To understand e.g. protein agglomeration, and folding, it is necessary to develop a better understanding of water under confinement. In order to realistically describe the confinement effects of an amorphous silica pore, we have constructed a fully atomistic model of a such a system using ab-initio molecular dynamics. Pressure and temperature effects on the water structure and thermodynamics, as well as local effects on water mobility have been investigated using both classical and first principles molecular dynamics. We find a considerable slowing down of water diffusion at a water silica interface, accompanied by a change in tetrahedral ordering and weakening of the H-Bond network. Results are in good agreement with predictions from a model interface.[2]

1. N. Giovambattista, P. J. Rossky, P. G. Debenedetti, Annu. Rev. Phys. Chem. 63 (**2012**), 179.

X. Y. Guo, T. Watermann, S. Keane, C. Allolio, D. Sebastiani,
Z. Phys. Chem. 226 (2012), 1415.

CPP 54.8 Thu 15:00 P2

Mechanical Characterization of single sub-micron Diameter Fibers via AFM — •BENEDIKT NEUGIRG¹, DANIEL KLUGE¹, JULIA SINGER², HANS-WERNER SCHMIDT², and ANDREAS FERY¹ — ¹Department of Physical Chemistry II, University of Bayreuth, 95440 Bayreuth, Germany — ²Department of Macromolecular Chemistry I, University of Bayreuth, 95440 Bayreuth, Germany

Many biological and artificial materials are composites with submicron diameter fibers as principal building unit. Mechanical characterization on the single fiber level requires advanced probing techniques beyond the standard methods. We utilize the AFM to do nanoscale bending which is applicable to a wide variety of systems. Generally, fibers are deposited on structured glass substrates and investigated in a combined AFM/optical microscope setup. In our contribution we will show results of fiber bending perpendicular and parallel to the substrate plane. We will discuss the advantages of these two bending modes, for example validation of boundary conditions, direct integration of optical methods and the detailed investigation of the mechanical properties beyond linear elastic deformations. Our study focuses on supramolecular fibrillar assemblies of benzenetrisamides. Although the main intermolecular interaction are hydrogen bonds (in contrast to covalent bonds in classical polymers), these structures show Young's moduli in the GPa range. By varying the molecular structure, stiffness and fiber diameter can be tailored. Besides self-assembly, electrospinning is a complementary preparation route which makes the material accessible via a "Top-down" as well as a "Bottom-up" approach.

CPP 54.9 Thu 15:00 P2

New Developments in Laboratory SAXS Instruments — •BASTIAN ARLT — Anton Paar Germany GmbH, Ostfildern, Germany

Surfactants, dispersions, polymer or protein solutions and (micro-) emulsions are intensively investigated systems in current science. Consequently, an essential point is the careful characterization of these systems in-situ. The small angle X-ray scattering (SAXS) technique offers precise and fast measurements to investigate parameters such as size, shape, interaction effects of particles in solution. Thus, SAXS is a complementary method to TEM, AFM, or NMR techniques. SAXS measurements are performed at synchrotron facilities or, thanks to recent developments, using laboratory instruments which have become an excellent alternative.

We are going to present the latest developments and trends in the field of laboratory SAXS instruments. Thanks to high-flux X-ray sources, short exposure times are possible. Additionally, Anton Paar has explored novel techniques in sample positioning which are commonly known from synchrotron measuring stations and allow extending the available detection range and to resolving smallest dimensions. CPP 54.10 Thu 15:00 P2

A high pressure cell for x-ray reflectivity measurements of liquid/solid interfaces and lipid layers — •PAUL SALMEN, JULIA NASE, BENEDIKT NOWAK, MICHAEL PAULUS, FLORIAN J. WIRKERT, and METIN TOLAN — Fakultät Physik/DELTA, Technische Universität Dortmund, 44221 Dortmund, Germany

We present a high pressure cell for in situ x-ray reflectivity (XRR) measurements[1]. By applying high hydrostatic pressures (HHP) up to 5 kbar, the liquid/solid interface can be studied. The cell consists of two separated parts, an outer cell to withstand the pressure and an inner cell with a separated volume containing the sample. As solid interface, silicon wafers, which can be covered by different coatings, are used.

In the near future, we want to measure adsorption of proteins at lipid layers under HHP. Lipid capsules play a mayor role for example in food processing and drug delivery. To study a simplified system, we spin-coat layers of glycerol tristearate on silicon wafers. Here we present first XRR measurements

[1] F. J. Wirkert et al., Journal of Synchrotron Radiation 2014 (21) doi:10.1107/S1600577513021516

CPP 54.11 Thu 15:00 P2

Hybrid GRIN lense microresonator for sensing applications — •MICHAEL METZGER¹, ANDREAS HORRER², SABRINA RAU¹, GÜNTHER GAUGLITZ¹, DIETER KERN², MONIKA FLEISCHER², DAI ZHANG¹, ALFRED J. MEIXNER¹, and MARC BRECHT³ — ¹IPTC, University of Tübingen, Germany — ²Institute for Applied Physics, University of Tübingen, Germany — ³Zürcher Hochschule für Angewandte Wissenschaften, IAMP, Winterthur, Switzerland

An optical hybrid system consisting of a gradient-index lense (GRIN lense) and a Fabry-Pérot optical microresonator used as a sensitive and compact refractive index sensor is presented. GRIN lenses are miniaturized optical elements, which achieve their focusing effect by a gradient of the refractive index within the lens material. The GRIN lenses enable controlled positioning of the focal plane at one of their flat surfaces. Our microresonator consists of two opposing mirrors a silver coated GRIN lense and a curved mirror in close proximity $(\lambda/2$ -region). The transmission through the resonator shows a spectrally well-defined Newton ring pattern. The transmission wavelength depends on the mirror spacing and the intra cavity refractive index. The combination of a GRIN lense with a Fabry-Pérot optical microresonator gives us the opportunity to sense smallest changes of the intra cavity refractive index. The reflective layers can be supplemented with an antibody layer to conduct further analytical tests like detection of single macromolecules (e.g. antibody virus bonding) affecting the cavities' dielectric properties. This project was financed by Baden-Württemberg Stiftung.

CPP 54.12 Thu 15:00 P2

Spectroscopy of Dielectric Elastomer Actuators for the Application of Tunable Optical Elements — •IRMA SLOWIK¹, MARKUS FRANKE², MARKAS SUDZIUS¹, RENE KÖRBITZ², HARTMUT FRÖB¹, ANDREAS RICHTER², and KARL LEO¹ — ¹Institut für Angewandte Photophysik, Technische Universität Dresden, George-Bähr Str. 1, 01069 Dresden — ²Institut für Halbleiter- und Mikrosystemtechnik, Technische Universität Dresden, Nöthnitzer Straße 64 01187 Dresden

Dielectric elastomers are promising materials for electromechanical systems because of their high dielectric strength and their ability to deform under applied voltage up to very high strains > 300%. Dielectric elastomer actuators are used for artificial muscles, conformable displays, stretchable integrated circuits and biomedical electrode interfaces. Due to their high transparency and flexibility they show a high potential to build up tunable optical elements like tunable phase plates, cavities, or gratings.

We report on a dielectric elastomer film investigated by Fabry-Perot interferometry. The thin polymer film is sandwiched between two compliant ring electrodes. Under applied voltage, the electrostatic force squeezes the dielectric layer, which causes a deformation of the device. The thickness change in the actuator film can lead to a phase change up to several π . Additonally, dielectric elastomer actuator coated with a partly transparent mirror can act as a part of a tunable cavity. Due to the high resolution of the Fabry-Perot interferometer even small changes in the cavity length can be detected.

CPP 54.13 Thu 15:00 P2 Simultaneous Mapping of Long-range Attractive and Shortrange Repulsive Forces with MUSIC Mode Atomic Force Microscopy — •DIANA VOIGT, EIKE-CHRISTIAN SPITZNER, FABIAN SAMAD, and ROBERT MAGERLE — Chemische Physik, Fakultät für Naturwissenschaften, Technische Universität Chemnitz, D-09107 Chemnitz, Germany

Intermittent contact (IC) or tapping mode atomic force microscopy (AFM) usually focuses on the imaging of the surface morphology and the nanomechanical properties. Beyond that also long-range interactions, like electrostatic and magnetic forces, can be measured with AFM. Multi set-point intermittent contact (MUSIC) mode AFM is based on the point-wise measurement of amplitude and phase of an oscillating AFM tip as the tip-sample distance is reduced. It allows for the determination of the unperturbed height image as well as phase images for a wide variety of amplitude set-points from a single measurement run. Furthermore, the results are not affected from feedback-loop and tip-indentation artifacts. Here, we demonstrate the single-pass measurement of long-range attractive electrostatic and magnetic interactions in addition to the nanomechanical properties of the specimen. As model systems for mapping local differences in the hydrophilic/hydrophobic electrostatic interactions we use PS-b-PEO block copolymer thin films on a silicon substrate and collagen fibrils immobilized on PDMS. As a third example, the nanomechanical properties of a thin film of PS-b-PB block copolymer as well as the magnetic properties of an underlying CoPt thin film are measured in a single run.

CPP 54.14 Thu 15:00 P2

Modular fluidic System for Agglomeration Experiments — •DOMINIK GERSTNER and TOBIAS KRAUS — Leibniz-Institut für Neue Materialien (INM), Campus D2 2, D-66123 Saarbrücken

Nanoparticles (NP) are used in research and in an increasing number of applications. Agglomeration of their dispersion can occur in every processing step and is often regarded a nuisance. We exploit agglomeration to tune structure and properties of particle-containing nanocomposites [1]. To understand the structure-directing mechanisms, we systematically study the agglomeration of NP having different cores and surfaces. Here, we present a steady-state approach to NP agglomeration studies that uses fluidics and online analysis to improve precision, comparability and throughput. The setup lets us investigate shear effects in nanoparticle processing, too. We combine UV/Vis Spectroscopy and Small Angle X-ray scattering techniques to characterize agglomerates. We discuss experimental challenges that have to be overcome for such flow-based experiments. Proper reagent mixing is crucial, but limited by the laminar flows, and requires careful tuning of flow rates. Agglomerating particles tend to adsorb on the inner walls of the system. We develop strategies to avoid excessive fouling. This contribution shows first results on the tuning of agglomeration states under steady state conditions.

[1] P. Born and T. Kraus. Phys. Rev. E 87 (2013), 062313.

CPP 54.15 Thu 15:00 P2

Implementing a OPV slot dye coating device and determining the ramifications on morphology and device lifetimes •Sebastian M. Günther, Christoph J. Schaffer, and Peter MÜLLER-BUSCHBAUM — TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching, Germany Organic photovoltaics (OPV) represent a highly investigated technology with great advantages in comparison to current PV technologies. Even though recent organic PV devices are reaching efficiencies beyond 10%, there is still a substantial amount of research needed. That regards especially to analysis of morphology, which is a key parameter to efficient devices and also affects degradation as well as device lifetime. Therefore particularly the processing method is of interest as it is expected to have an extensive influence on the morphology. Currently investigated devices are generally processed via spin coating although this technique is not viable for large scale production. Thus the influence of a printing method on the structural characteristics will be investigated on the basis of samples produced by positive shim mask slot dye coating. This coating method for OPVs is a technique that allows for very thin film application provided that a very low viscosity solution (~1 mPas) is used. For further investigation a new printing device will be implemented. Thereby created films will be analyzed using X-ray reflectivity (XRR), optical and atomic force microscopy (OM, AFM) and UV/Visible light spectroscopy (UV/Vis). The morphology on a nanometer scale will be probed with grazing incidence wide and small angle scattering methods using X-rays and/or neutrons.

CPP 54.16 Thu 15:00 P2

High frequency laser modulated AC chip calorimeter -

•YEONG ZEN CHUA, EVGENI SHOIFET, and CHRISTOPH SCHICK — Institute of Physics, University of Rostock, Rostock 18051, Germany

Combination of different techniques for heat capacity spectroscopy and temperature-modulated calorimetry (TMDSC) allows the determination of complex heat capacity in a wide frequency range. TMDSC covers a limited frequency range from about 10^{-5} Hz to 0.1 Hz. An AC chip calorimeter gives the possibility to decrease the size of the measured sample, hence increases the sensitivity and frequency range. However, the investigation of the dynamic glass transition is still limited to the frequencies up to a few kHz. A new AC chip calorimeter with laser heating is capable of measuring the glass transition temperature of thin film samples in the frequency range up to 1 MHz. The dynamic glass transition of polystyrene and poly(methyl methacrylate) was studied in the frequency range of 10^{-5} Hz to 1 MHz with different calorimetric techniques.

CPP 54.17 Thu 15:00 P2 Block copolymer based membrane for lithium ion microbatteries — •MAJID RASOOL¹, EZZELDIN METWALLI¹, HANS BEYER², ANNA EBERLE², HUBERT A. GASTEIGER², and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching — ²TU München, Chemistry Department, LS Technische Elektrochemie, Lichtenbergstr. 4, 85748 Garching

In the light of an increasing demand on power sources for nanodevices, the nano-scaled lithium based membranes paves the way for new opportunities regarding design and application. The morphology of lithium ion-polymer hybrid films [1] based on P(S-b-EO) block copolymer (BC) electrolyte is investigated using small angle x-ray scattering (SAXS). Additionally, lithium containing BC films are sandwiched between two metal electrodes and the film conductivity at different temperatures and salt concentrations is measured using impedance spectroscopy. The current block copolymer electrolyte consists of both conductive lithium containing PEO domains as well as mechanically stable glassy polystyrene domains. Lithium ion incorporation is found to inhibit the crystallization of PEO block, enhance microphase separation and induce lamella-cylinder morphological transition at high lithium ion content. The correlation between the morphology and ionic conductivity of the current lithium ion-polymer hybrid BC films is employed to put an insight into the mechanisms responsible for the conduction of lithium ions in these systems. [1] E. Metwalli, et al., Macromol. Chem. Phys. 212, 1742 (2011).

CPP 54.18 Thu 15:00 P2 Aqueous suspensions of laponite discs under confinement — •MARTIN UHLIG and REGINE V. KLITZING — TU Berlin, Straße des 17. Juni 124 D-10623 Berlin, Germany

Laponite is a synthetic disc-shaped clay and mainly used as a nontoxic rheology modifier, e.g. in coatings, paints or personal care products [1]. In aqueous solution the diameter and thickness of a single disc is 25 nm and 1 nm, respectively. The disc's surface is negatively charged, while the rim is positively charged. The protonation of OH- groups, resulting in positive rim charges, can be tuned by pH. Laponite shows complex ageing behavior, as with time the disc's surfaces and rims approach each other and aggregate due to their opposite charges [1]. This contribution concentrates on the behaviour of Laponite discs in confinement. Nanometer scaled charged systems can show so called oscillatory forces in confinement. These forces are a result of electrostatic repulsion and were reported for silica particles [2] and polyelectrolytes [3]. Oscillatory forces indicate that one layer after the other of diluted charged particles is pushed out of the confinement. Both Thin Film Pressure Balance (TFPB) and Atomic Force Microscopy (AFM) are used to investigate if Laponite solutions under confinement show such a behavior. First results using the TFBP indicate oscillatory forces. Experiments studying the system with AFM and investigating the effect of pH as well as of ion concentration are in progress.

[1] Ruzicka, B. et al.; Soft Matter, 2011, 7, 1268-1286

[2] Klapp S. et al.; Phys. Rev. Lett., 2008, 100, 118303

[3] Üzüm, C. et al.; Macromolecules, 2011, 44, 7782-7791

of experimental physics, Ulm university, Ulm,Germany

CPP 54.19 Thu 15:00 P2 Self - Sensing Ionic Polymer Metal Composite — •PARISA BAKHTIARPOUR, MASOUD AMIRKHANI, and OTHMAR MARTI — Institue

Integration of sensor and actuating properties of Ionic Polymer Metal Composite (IPMC) have attracted a lot of interest in recent decades. The electrical response of IPMC to the bending can be used for selfsensing. However, using the self-sensing mechanism of patterned IPMC results into cross talk between sensing and actuating part, which even with shielding cannot be avoided entirely. Additionally, two sections are correlated in which the maximum efficiency on one part lead to the minimum efficiency on the other part. We solve these problems by using a high-frequency and a low-frequency voltage as sensing and actuating signal respectively, on an unpatterned sample. IPMC in the high-frequency can be considered as a variable resistance and in the low-frequency works like an actuator.

CPP 54.20 Thu 15:00 P2

Characteristics of the Hydrogen Bond Network of Water — •MIRIAM JAHN and STEPHAN GEKLE — Biofluid Simulation and Modeling, Universität Bayreuth

The special properties of liquid water originate from its hydrogen bond network. Using molecular dynamics simulations of bulk water we confirm the significant influence of hydrogen bonding on the orientational correlation of the molecular dipoles. While the dielectric permittivity of water is known to depend on these collective orientations of the molecules, it is still unclear which geometric structures communicate such collective effects.

Possible candidates are the loops of bonded molecules that characterize the long-range structure of bulk water. Loops are closed paths of hydrogen bonds, composed of the shortest connections between all participating molecules. Our simulations reveal that most of the loops in bulk water consist of six or seven molecules. We further investigate the influence of interfaces on the water hydrogen bond network. This might be the key to the effect that interfaces have on the dielectric permittivity.

$CPP \ 54.21 \quad Thu \ 15:00 \quad P2$

Dielectric effects of sodium salts in aqueous solution — •KLAUS FRIEDRICH RINNE¹, STEPHAN GEKLE², and ROLAND NETZ¹ — ¹Fachbereich Physik, Freie Universität Berlin, 14195 Berlin — ²Nachwuchsgruppe Theoretische Physik, Universität Bayreuth, 95440 Bayreuth

We present dielectric spectra obtained from equilibrium molecular dynamics simulations of 1 molar aqueous solutions (SPC/E water) of NaF, NaCl, NaBr and NaI. The ion specific static and dynamic effects match experiments results. Additionally, sodium chloride is studied concentration dependently.

The dielectric contribution of the water-polarisation auto-correlation is decomposed into different groups depending on solvation shells and the pair state of the nearest ion. It is shown that even second and third solvation shell water is affected by dielectric saturation leading to a red shift of the spectra compared to bulk water.

Moreover, the contribution of the water-ion polarisation crosscorrelation is included leading to a reduction of total dielectric signal by 5-10%. A continuous trend of the cross-correlation with increasing anion size is observed. For the first time the ion pairs are grouped in different ion pair configurations showing that the static equivalent conductance of a contact ion pair is about 50% lower than for ion pairs with larger separation. Furthermore, we show the dynamic ion current auto-correlation contributes about one percent to the total static dielectric constant of the solution.

CPP 54.22 Thu 15:00 P2

Thermodynamic Description of the LCST of Charged Thermoresponsive Copolymers — •JAN HEYDA¹ and JOACHIM DZUBIELLA^{1,2} — ¹Soft Matter and Functional Materials, Helmholtz-Zentrum Berlin, Hahn-Meitner Platz 1, 14109 Berlin, Germany — ²Department of Physics, Humboldt-University Berlin, Newtonstr. 15, 12489 Berlin, Germany

The dependence of the lower critical solution temperature (LCST) of charged, thermosensitive copolymers on their charge fraction and the salt concentration is investigated by employing systematic cloud-point experiments and analytical theory. The latter is based on the concept of the Donnan equilibrium incorporated into a thermodynamic expansion of a two-state free energy around a charge-neutral reference homopolymer and should be applicable for weakly charged (or highly salted) polymer systems. Very good agreement is found between the theoretical description and the experiments for aqueous solutions of the responsive copolymer poly(NIPAM-co-EVImBr) for a wide range of salt concentrations and charge fractions up to 8%, using only two global, physical fitting parameters.

In addition, the prediction of salt-specific contribution to LCST

is presented in the framework of so called partitioning concept. Inserted into thermodynamic expansion, a novel interpretation of LCST, and cloud point measurements is revealed. In particular, salt effects on transition thermodynamics are obtained for established polymers; PNIPAM or elastine-like-polypeptides.

CPP 54.23 Thu 15:00 P2

Stimuli-responsive reversible hydrogels from triblock polyelectrolytes and polyampholytes — •MARGARITA DYAKONOVA¹, MARIA T. POPESCU², CONSTANTINOS TSITSILIANIS², KONSTANTINOS KYRIAKOS¹, SEBASTIAN JAKSCH³, and CHRISTINE M. PAPADAKIS¹ — ¹TU München, Physik-Department, Garching — ²University of Patras, Greece — ³JCNS at FRM II, Garching

We investigate the conformational properties of stimuli-responsive hydrogels from triblock polyelectrolytes PtBA-P2VP-PtBA (PtBA and P2VP are poly(tert-butylacrylate) and poly(2-vinylpyridine) and polyampholytes PAA-P2VP-PAA (PAA is poly(acrylic acid)) where the transitions are due to the neutralization of charged groups [1]. Hydrogels are formed at polymer concentrations as low as 0.4 wt%. The mechanical properties depend strongly on the pH value and the salt content [1].

We focus on the related structural changes of the hydrogels. SANS revealed a dependence of the hydrogel structure of the polyampholyte on charge asymmetry and revealed several transitions with increasing electrostatic interaction. Low charge asymmetry causes the collapse of the chain into a globule dominated by the fluctuation-induced attractions between oppositely charged moieties while at higher charge asymmetry, a network is formed. The latter has been confirmed for the polyelectrolyte system. These results demonstrate the origin of the strong changes in mechanical properties.

CPP 54.24 Thu 15:00 P2 Small differences with big impact: Reentrant phase behavior induced by multivalent cations in protein solutions — •MARCELL WOLF, FAJUN ZHANG, FELIX ROOSEN-RUNGE, and FRANK SCHREIBER — Institut für Angewandte Physik, Auf der Morgenstelle 10, 72076 Tübingen

Subtle difference between proteins can lead to remarkably big differences in their resulting phase behavior. Using a multivalent cation, Y^{3+} , a reentrant condensation (RC) with a liquid-liquid phase separation (LLPS) within the condensed regime has been established in a negatively charged protein system [1,2]. Here we compare the phase behavior of two serum albumins, BSA and HSA. They are highly similar in the primary structure but the comparison of the RC behavior shows a strong difference. The condensed regime and the LLPS region is much broader for a HSA system and the LLPS boundaries where also shifted to lower salt and protein concentrations (c_p) , observed by optical microscopy. The major contribution of this changes can be explained by existence of dimers in BSA solutions, observed by GPC and DLS experiments. Due to the dimers a higher c_p is necessary to achieve the same monomer concentration than without dimers. In addition these will be also interactions between monomer and dimers which will also influence the phase behavior. Using an ellipsoid sticky hard sphere potential for fitting the data, determined by SAXS, the effective interaction was calculated [3]. [1] F. Zhang et al., PRL 101, 2008, 148101; [2] F. Zhang et al., Soft Matter 8, 2012, 1313; [3] M. Wolf et al. J. Mol. Liq., submitted.

 $\label{eq:CPP-54.25} \begin{array}{ccc} Thu \ 15:00 & P2 \\ \mbox{Influence of Polycation Molecular Weight and Diffusion} \\ \mbox{Barriers on Interdiffusion in Polyelectrolyte Mulitlayers} & $-$ \end{tabular} \\ \bullet \mbox{Peter Nestler}^1, \mbox{Matte Passvogel}^1, \mbox{Olaf Soltwedel}^2, \mbox{Heiko} \\ \mbox{AHRENS}^1, \mbox{RalF K\"{O}Hlers}^3, \mbox{ and CHRISTIANE A. Helm}^1 & $-$ \mbox{Inst. f.} \\ \mbox{Physik, Uni Greifswald, 17487 Greifswald, Germany} & $-$ \mbox{2MPI fur Festk\"{o}rperforschung, 70569 Stuttgart, Germany} & $-$ \mbox{Matter and Functional Materials, HZB, Berlin, Germany} \\ \end{array}$

After introduction of the Layer-by-Layer technique (LbL) twenty years ago, surfaces were modified by covering them with thin films of different composition. A wide variety of potential applications for polyelectrolyte multilayers (PEM) is known, for example chemical reactors, or microcontainers. For these films, it is important to know how interdiffusion due to external stimuli changes the internal film structure.

PEMs are made from poly(diallyldimethylammonium) (PDADMA), poly(styrenesulfonate) (PSS), and deuterated PSS-d. Each film consists of a protonated and a deuterated compartment. The films are annealed in 1 M NaCl and investigated with neutron reflectivity. During annealing the internal interface between both departments broadens due to interdiffusion.

A branched polycation layer (PEI) in the film centre serves as a diffusion barrier, and the diffusion constant through the barrier decreases monotonically with PDADMA molecular weight. Without the PEI diffusion barrier, PSS diffuses one to two orders of magnitude faster.

CPP 54.26 Thu 15:00 P2

Synthesis and characterization of polyelectrolyte complexes — •CHRISTIAN KESSLER — Physikalische Chemie der Polymere, TU Dresden, Germany

Polyelectrolyte complexes formed by Poly(dimethyldiallylammonium chloride) (PolyDADMAC) and poly(maleic acid) with three different copolymers were studied and characterized via light scattering, AFM and viscosity measurements. By varying the ratio of polyanion and polycation as well as the copolymers it was possible to tune properties like surface charge, hydrophilicity, radius, molar mass and overlap concentration. By using different chain lengths of PolyDADMAC two distinct complex structures could be obtained. Oppositely charged polyelectrolytes of roughly the same size resulted in spherical structures, while a size ratio of 1:10 produced needle-like complexes. Removal of the needles revealed additional compact spheres which could be shown by light scattering and AFM measurements. The addition of NaCl resulted in a reduction of the molar mass, radius and the second virial coefficient. Above a salt concentration of 0.03 mol/L these properties increased rapidly.

CPP 54.27 Thu 15:00 P2

Dynamics of wet colloids under mechanical load studied by 3D confocal microscopy — JENNIFER WENZL¹, LAURENT GILSON², ULRICH BRÖCKEL², and •GÜNTER K. AUERNHAMMER¹ — ¹Max Planck Institute for Polymer Research, Mainz, Germany — ²FH Trier, Umwelt-Campus Birkenfeld, Birkenfeld, Germany

Wet colloids are prevalent in many industrial applications, e.g. food processing, or pharmaceuticals. Detailed information of the microscopic behavior of wet colloids is still an open field. The challenge is the 3D visualization on the micro scale of the particle structure and liquid distribution, especially under mechanical deformation.

We present a study on model wet colloids, which can be observed in 3D with confocal microscopy. For a high spatial resolution, the refractive index of all components has to be matched: Silica particles (diameter 7μ m), dispersed in a mixture of an aqueous salt solution, and an organic solvent. Partial hydrophobization of the colloid surface allows us to change the contact angle of liquid-liquid interface, i.e. the interaction of the colloids with the liquid interface. We follow the reorganization of this model wet colloids under mechanical load on a single colloid level and discuss the effects due to capillary bridging.

CPP 54.28 Thu 15:00 P2

Aggregation behaviour of doubly thermo-responsive poly(sulfobetaine-b-(N-isopropylmethacrylamide) diblock copolymers — \bullet NATALYA VISHNEVETSKAYA¹, VIET HOANG², ANDRE LASCHEWSKY², and CHRISTINE PAPADAKIS¹ — ¹TU München, Physikdepartment, Physik weicher Materie — ²Institute of Chemistry, University of Potsdam

Diblock copolymers consisting of a thermo-responsive poly(Nisopropylmethacrylamide) (P(NIPMAM) block) and a zwitterionic poly(sulfobetaine) (P(SB) block) feature both a lower and an upper critical solution temperature in aqueous solution. This is expected to result in transitions from micelles to unimers to reverse micelles as temperature is increased. The self-organization of the diblock copolymers (P(SPP-b-NIPMAM)) in water can be varied by the addition of an electrolyte, resulting in combined UCST-LCST transitions.

The dependence of the phase transition temperatures in aqueous solution on the electrolyte concentration is investigated by means of turbidimetry. The aggregation behavior in aqueous solution with dual stimuli (temperature and electrolyte concentration) is studied by temperature-resolved small-angle neutron scattering, dynamic light scattering (DLS) and fluorescence correlation spectroscopy (FCS).

CPP 54.29 Thu 15:00 P2 Liquid-liquid phase separation in protein - PEG mixture — SALIBA BARSAUME¹, •FAJUN ZHANG¹, MICHAEL SZTUCKI², ROLAND ROTH³, and FRANK SCHREIBER¹ — ¹Institut für Angewandte Physik, Universität Tübingen, Germany — ²ESRF, Grenoble, France — ³Institut für Theoretische Physik, Universität Tübingen, Germany

We present a combined experimental and theoretical study of the liquid-liquid phase separation (LLPS) in protein-PEG mixture. Bovine gamma-globulin solutions mixed with PEG above a critical volume fraction undergo a LLPS at constant temperature. The partitioning of both protein and PEG has been determined which gives the binodal of LLPS. The critical point of the system has been extrapolated from the tie lines. The critical volume fraction is about 6% which is significantly lower than the theoretical value (13-23%) for colloidal systems with isotropic interaction. The resulting phase boundary is compared with the free volume theory for arbitrary shape (Y-Shape) of protein with a radius of gyration of 6.3 nm and the size ratio of 0.3-0.8 between PEG and protein. Furthermore, small angle X-ray scattering has been employed to determine the effective protein-protein interactions approaching LLPS. The reduced second virial coefficient has been determined for samples at the binodal and near the critical point of LLPS, which is further compared and discussed with the value predicted from colloidal theory.

CPP 54.30 Thu 15:00 P2

Three-body effects for critical Casimir forces — •THIAGO MATTOS^{1,2}, LUDGER HARNAU^{1,2}, and DIETRICH SIEGFRIED^{1,2} — ¹Max Planck Institute for Intelligent Systems, Stuttgart, Germany — ²IV. Institute for Theoretical Physics, Stuttgart University, Germany

Within mean-field theory we calculate the scaling functions associated with critical Casimir forces for a system consisting of three spherical colloids immersed in a binary liquid mixture near its consolute point. For several geometrical arrangements and boundary conditions we analyze the effect on the critical Casimir force between a pair of colloids due to the presence of a third one. By subtracting the pairwise forces from the total force we are able to determine the many-body forces acting on one of the colloids. We have found that the many-body contribution to the total critical Casimir force is more pronounced for small colloid-colloid separations, as well as for temperatures close to criticality.

CPP 54.31 Thu 15:00 P2

Mesoscopic approach to colloidal suspensions — •APURVA SARKAR and MARCO G. MAZZA — Max Planck Institute for Dynamics and Self-Organisation, Göttingen, Germany

We study the dynamics of a quasi-2D system of colloids, dispersed in a simple background solvent. The dynamics of the surrounding fluid is simulated through Stochastic Rotation Dynamics, which consists of random rotations of particles in a predetermined cell, such that mass, momentum and energy are conserved. In between these discrete time solvent-solvent collisions, the dynamics of the heavier colloidal particles is solved through a classical MD simulation. The colloid-colloid as well as colloid-solvent interactions are modelled via Lennard-Jones potentials, with different sets of interaction radii.

Different transport properties of the system such as self-diffusion coefficient and intermediate scattering factor are obtained from this hybrid MD-SRD code. We study and characterize the phase transitions observed in the system.

CPP 54.32 Thu 15:00 P2

Self assembly of order micro pore structure prepared by water vapor condensation on evaporative polystyrene solution — •FARID FARAJOLLAHI, MASOUD AMIRKHANI, and OTHMAR MARTI — Institute of Experimental Physics, Ulm University, Ulm, Germany

The condensation of water vapor on the evaporative polymeric solution does produce micro-droplets of water (MDW), which leave their trace on the surface after evaporation of both solvent and water. In the proper condition, polymer and organic solvents can effectively reduce the coalescence rate of MDW and form a self assemble hexagonal structure. The polymeric solution consisted of polystyrene and chloroform mixed with different short-chain alcohols (methanol, ethanol and n-propanol) was studied. At a fixed polystyrene concentration, the order pattern formation initiates at specific concentration for each alcohol and reduced by increasing the length of hydrophobic chain alcohol. The pattern observed only within a certain range of alcohol concentrations, which is wider for methanol and become narrow for longer chain alcohols. For each alcohol, the required concentration for pattern formation has reverse relation to the polymer concentration of the solution. As the hydrophobic part of the alcohol chain becomes longer, higher polystyrene concentration is needed to achieve the micro pore pattern.

Depletion induced sphere-cylinder transition in C12E5 microemulsion: A Small-Angle X-ray Scattering study — •MASOUD AMIRKHANI¹, SOHEIL SHARIFI¹, SERGIO FUNARI², and OTH-MAR MARTI¹ — ¹Institut für Experimentelle Physik, Universität Ulm, Albert-Einstein-Allee 11 89081 Ulm — ²HASYLAB, Notkestrasse 85, D-22607 Hamburg, Germany

Small-angle X-ray scattering was used to study the mixture of C12E5 (pentaethylene glycolmonododecyl ether)/H2O/n-decane microemulsion and polyethylene glycol (PEG). The size, shape and the structure factor of the microemulsion were investigated by adding the polymer (PEG) to the mixture. Attractive depletion potential was induced between the microemulsion droplets by the non-adsorb polymer. The range and strength of the attractive potential were changed by varying the molecular weight and concentration of PEG. The forward scattering, S(0), of the spherical microemulsion, declined gradually as the polymer concentration decreased. For PEG with the molecular weight of Mn = 285-315, the microemulsion morphology remained spherical, but the main peak of the structure factor moved towards a bigger q. When PEG with molecular weights of Mn = 2200 and Mn = 6000 were used, a shape transition from spherical to cylindrical was induced in line with increasing polymer concentration.

CPP 54.34 Thu 15:00 P2

Structure and Conductivity of Liquid Crystals having Carbonate Segments — •ANDREAS EISELE¹, KONSTANTINOS KYRIAKOS², MARGARITA DYAKONOVA², CHRISTINE M. PAPADAKIS², and BERNHARD RIEGER¹ — ¹TU München, Department Chemie, Garching — ²TU München, Physik-Department, Garching

The development of lithium ion batteries with higher capacity and a sufficient safety performance is essential for electric vehicles. It is essential to develop non-volatile and nonflammable electrolytes with good ion conductivity. A new approach is the use of liquid crystalline compounds. Liquid crystals which have ion conducting segments can transport ions efficiently as segregation leads to the formation of nanoscale ion pathways.

We investigated liquid crystalline molecules with a perfluorinated aromatic ring as mesogenic core and a cyclic carbonate as ion conductive moiety. Small-angle X-ray scattering revealed that they form the smectic phase. Spontaneous macroscopic alignment was observed. The influence of lithium salt on the alignment of the molecules and the layer spacing was investigated. The findings were compared with anisotropic conductivity measurements in the smectic as well in the isotropic phase to get new insights into the conductivity mechanism.

CPP 54.35 Thu 15:00 P2

Soret diffusion in ternary organic liquid mixtures — •MATTHIAS GEBHARDT and WERNER KÖHLER — Physikalisches Institut, Universität Bayreuth, D-95440 Bayreuth, Germany

Soret diffusion or thermodiffusion describes the coupling of the local composition of a mixture to a prescribed inhomogeneous temperature field. While significant progress has been achieved over the last decades both on the theoretical and the experimental side, truly multicomponent systems have hardly been considered so far. It is only recently that the focus of interest has turned from binaries to ternaries, which show already a strongly increased complexity in their diffusion behaviour. We have investigated the system of dodecane, isobutylbenzene and 1,2,3,4-tetrahydronaphthalene by means of a two color optical beam deflection technique. For this system the binary edges are well known in literature and can be used as limiting reference. We have developed a fitting routine to evaluate our experimental data based on the idea of Haugen [1]. Now, we are presenting the first results of our ternary measurements over the entire concentration range.

[1] K. B. Haugen and A. Firoozabadi, J. Phys. Chem. B, 110, pp. 17678-17682 (2006)

$CPP \ 54.36 \quad Thu \ 15:00 \quad P2$

Dynamical properties of finite colloidal clusters — •ANDRÉ SCHELLA¹, ANDRÉ MELZER¹, CHRISTOPH JULY², and CLEMENS BECHINGER² — ¹Institut für Physik, EMAU Greifswald, 17489 Greifswald — ²2tes Physikalisches Institut, Universität Stuttgart, 70569 Stuttgart

Colloidal systems are often regarded as macroscopic atomic systems since they allow a direct access to study matter on the kinetic level by means of video microscopy. When the particle number is low, less than thousand say, the system is said to be finite. Deriving physical properties of finite systems is always challenging, since usually thermodynamic quantities fail in the limit of low particle numbers. Moreover, volume effects and surface effects are always competing in small ensembles. In our contribution, we study colloidal clusters interacting via tunable magnetic dipole forces. The mode properties of these finite ensembles are derived using an Instantaneous Normal Mode (INM) technique [1]. So far, the INM technique has been successfully applied to dusty plasma clusters [2]. To calculate modes of the system, only instant cluster configurations are needed, thus allowing to use this approach even in overdamped situations. The effect of differently shaped confinements on the cluster dynamics will be discussed. Funding via SFB TR-24 Project A3 and the International Helmholtz Graduate School for Plasma Physics (HEPP) is gratefully acknowledged.

 T. Keyes, J. Phys. Chem. A 101, 2921-2930 (1997) [2] A. Melzer et al., Phys. Rev. Letters 108, 225001 (2012)

CPP 54.37 Thu 15:00 P2

Diffusion of nanoparticles in red blood cell suspensions — •VERA FORSTER and STEPHAN GEKLE — Biofluid Simulation and Modeling, University Bayreuth, Germany

We investigate the diffusion of nanoparticles near highly deformable red blood cells in comparison with theoretical predictions for rigid walls. In our simulations we use a hybrid model which consists of three different parts. The fluid is modelled via the Lattice Boltzmann method, while molecular dynamics are used for nanoparticles with viscous coupling for fluid-particle interactions. The third part contains the deformation of cell-membranes, whose elastic forces are determined from continuum elasticity theory. The immersed boundary method couples fluid and membranes. We measure diffusion directly by employing the mean-square displacement and indirectly via the particle mobility determined by pulling the particle through the liquid.

CPP 54.38 Thu 15:00 P2

Structure and Phase Transitions in a Series of Triphenylene-Based Discotic Liquid Crystals in the Nanoconfined State — •CHRISTINA KRAUSE, FRANZISKA EMMERLING, and ANDREAS SCHÖNHALS — BAM Federal Institute for Materials Research and Testing, Berlin, Germany

The structure and phase behavior of a series of discotic liquid crystal based on the triphenylene core (Hexakis [nalkyloxy] triphenylene, HATn; n=5, 6, 10, 12) is studied by means of X-ray Scattering and Differential Scanning Calorimetry (DSC) in the bulk and when confined to self-ordered alumina oxide membranes with different pore sizes. The influence of chain length and confinement on the phase transition is discussed in more detail: In confinement the two phase transitions between plastic crystalline and hexagonal ordered phase at lower and from the latter to an isotropic state at higher temperatures are also observed, but different phase structures close to the wall and in the pore center are evidenced by additional peaks in the heat flow for smaller pore sizes. While the former peaks are independent of the pore size, the depression of the phase transition temperatures of the latter ones can be described by the Gibbs-Thomson-equation. With decreasing pore size for both phase transitions the transition enthalpies decrease. The critical pore size d_{cri} estimated for phase transformation from the pore size dependence of the transition enthalpies for each material increases with increasing chain length.

CPP 54.39 Thu 15:00 P2

Molecular Dynamics of a Discotic Liquid Crystals studied by Inelastic Neutron Scattering — •CHRISTINA KRAUSE¹, REINER ZORN², BERNHARD FRICK³, and ANDREAS SCHÖNHALS¹ — ¹BAM Federal Institute for Materials Research and Testing, Unter den Eichen 87, D-12205 Berlin — ²Forschungszentrum Jülich, Jülich Centre for Neutron Science (JCNS), D-52425 Jülich — ³Institut Max von Laue -Paul Langevin (ILL), B.P. 156, F-38042 Grenoble Cedex 9

Discotic liquid crystals (DLC) consist of a flat and rigid aromatic core and attached flexible aliphatic chains. DLCs are self-assembled materials. The disc-shaped molecules organize into columns that further assemble into two-dimensional arrays with a hexagonal mesophase. The alkyl chains fill the intercolumnar space giving rise to a nanophase separated state. Dielectric relaxation spectroscopy, quasielastic and inelastic neutron scattering are employed to investigate the molecular dynamics of a homologous series of discotic liquid crystal based on the triphenylene core (Hexakis [nalkyloxy] triphenylene, HATn; n=5, 6, 10, 12) with varying length of the side chain in the bulk state. All materials under study show a boson peak (BP). Therefore, the influence of the length of the alkyl chains on its position and shape is investigated. With increasing lengths n of the side chains the BP shifts to lower frequencies and gains in intensity. This can be discussed employing a self-organized confinement model, where the confinement is generated by the highly ordered columns to the intercolumnar space, where with increasing n the confinement is weakened.

CPP 54.40 Thu 15:00 P2 Analysis of Particle-Particle Interaction Potentials of Nanoscaled Systems in Aqueous Solutions — •JULIAN SCHULZE¹, JOHANNES MÖLLER¹, MICHAEL PAULUS¹, JULIA NASE¹, METIN TOLAN¹, and ROLAND WINTER² — ¹Fakultät Physik / DELTA, Technische Universität Dortmund, 44221Dortmund, Germany — ²Fakultät Chemie und Chemische Biologie, Technische Universität Dortmund, 44221 Dortmund, Germany

In previous studies, small-angle X-ray scattering (SAXS) was used to study the intermolecular interaction potential of proteins in aqueous solution under the influence of varying conditions such as pressure, temperature, ionic strength and cosolvents. A non-linear correlation between the strength J(p) of the attractive part of the protein-protein interaction and hydrostatic pressure was found with a minimum at ² kbar, which is probably related to changes in the water structure. Adding NaCl led to a linear increase of the attractive part of the interaction potential, while adding the osmolyte trimethylamine-N-oxid (TMAO) causes a shift of the minimum of J(p) to higher pressures. In the presented work, the pressure dependent structure factor of Ludox colloidal silica has been determined by SAXS. Spherical nanoparticles offer the advantages of an easy, pressure-independent inner structure and tunable surface properties. The results are compared to results found for the protein lysozyme, and differences and similarities will be discussed. Furthermore, the pressure dependent structure of the solvent itself has been explored by wide-angle X-ray scattering (WAXS).

CPP 54.41 Thu 15:00 P2

Dynamic density functional theory of hard sphere crystals and interfaces — •MOHAMMAD HOSSEIN YAMANI and MARTIN OET-TEL — Institut für Angewandte Physik, Eberhard Karls–Universität Tübingen, Tübingen, Germany

Colloidal hard spheres are an intensely studied model system for studying bulk crystals and crystal-liquid interfaces. Classical Density Functional Theory (DFT) is one of the core theoretical approaches of statistical physics of fluids and crystals, which is able to treat this important system successfully and accurately. Hard-sphere bulk crystals and crystal-liquid interface have been studied using both Monte Carlo simulation and DFT of fundamental measure type (FMT) [1,2]. Density profiles, free energies and crystal-liquid surface tensions compare well between these two approaches. We use dynamical density functional theory (DDFT) to evaluate bulk crystal density profiles and free energies as well as the dynamical behavior of the crystal-liquid interface and related surface tension and compare to available simulation data. In the DDFT approach, we compare the sophisticated FMT and the Ramakrishnan-Yussouff (RY) functional with regard to their numerical efficiency for future applications in describing nucleation processes.

[1] M. Oettel et al, Free energies, vacancy concentrations and density distribution anisotropies in hard-sphere crystals: A combined density functional and simulation study, Phys. Rev. E 82, 051404 (2010).

[2] A. Härtel et al, Tension and Stiffness of the Hard Sphere Crystal-Fluid Interface. PRL, 108, 226101 (2012).

$CPP \ 54.42 \quad Thu \ 15:00 \quad P2$

Pressure calculation for bidisperse magnetic fluids — •EKATERINA NOVAK¹, ELENA PYANZINA¹, ELENA MININA^{1,2}, and SOFIA KANTOROVICH^{1,3} — ¹Ural Federal University, Lenin av. 51, Ekaterinburg, 620000, Russia — ²Institute for Computational Physics, University of Stuttgart, Allmandring 3, 70569, Stuttgart, Germany (current place of work) — ³University of Vienna, Sensengasse 8, 1090, Wien, Austria

Magnetic fluids are the systems of magnetic dipolar particles suspended in nonmagnetic liquids. Being a liquid even under the influence of magnetic field, ferrofluids are attractive for theoretical and experimental investigations. Industrially synthesized ferrofluids usually have high degree of polydispersity, i.e. the particle size distribution is rather broad. In the work [C. Holm et al, J. Phys.: Cond. Mat. 18 (2006)] it was shown that polydispersity influences microscopic properties of ferrofluids dramatically. Even for bidisperse systems an extensive cluster formation was inhibited by the poisoning effect. Thus, the polydispersity should lead to a change of the macroscopic properties. The present study is devoted to elucidation of the question how polydispersity influences one of the experimentally measurable macroscopic properties such as pressure of the system. We consider bidisperse systems of magnetic dipolar soft or hard particles as the simplest models of polydisperse magnetic fluid. We employ MD simulations, using ESPResSo, in combination with theoretical calculations of pressure based on the method of diagram expansion. In this way we investigate the influence of polydispersity and dipolar interactions on the compressibility of the system.

CPP 54.43 Thu 15:00 P2

Interferometric measurements of photothermally induced local temperature changes inside solutions of functional gold nanoparticles — •ALEXANDER NEDILKO¹, MALTE LINN¹, ANNE BUCHKREMER², MARCO SCHÜRINGS³, ULRICH SIMON², ALEXANDER BÖKER³, and GERO VON PLESSEN¹ — ¹Inst. of Physics (IA), RWTH Aachen — ²Inst. of Inorganic Chemistry, RWTH Aachen — ³Inst. of Physical Chemistry, RWTH Aachen

Metal-nanoparticle hybrid systems, such as DNA-gold nanoparticle (AuNP) networks and microgels with AuNP cores, have attracted great interest because of their unique optical properties and their versatile biomolecular and chemical functionalities. Since DNA dehybridization and microgel deswelling are temperature-sensitive, the AuNP hybrid systems can be switched between different states by photothermal heating via irradiation with cw laser light. In order to tailor these systems for possible future biomedical or nano-mechanical applications, it is crucial to investigate the laser induced thermal dynamics in the systems and in their vicinity. In this work, we measure the temperature increase inside different AuNP suspensions on a sub-millimeter length scale with a contact free, interferometric method, by exploiting the temperature dependent change of the refractive index of the solution. By spectrally separating the heating and the probing lasers, we are able to measure the photothermally induced temperature increase with ca. 30mK resolution, while simultaneously following the laser in- duced switching of the AuNP systems by monitoring the scattered probe laser light intensity.

CPP 54.44 Thu 15:00 P2

Buckling Instabilities of Liquid Crystal Filaments Under Compression Stress — •TANYA OSTAPENKO¹, SEYYED MUHAMMAD SALILI², ALEXEY EREMIN¹, ANTAL JÁKLI², and RALF STANNARIUS¹ — ¹Institute of Experimental Physics, Otto-von-Guericke-Universität, 39106 Magdeburg, Germany — ²Chemical Physics Interdisciplinary Program and Liquid Crystal Institute, Kent State University, Kent, OH 44242, USA

Elastic buckling of solid rods is a well-known phenomenon. However, liquid rods composed of viscous isotropic non-Newtonian fluids (e.g. silicone oil) will buckle only when the diameter-to-length ratio is less than 0.2 [1]. There have been no reports on how a quasi-onedimensional structured fluid may behave under compression stress, and to what extent the liquid crystal ordering is important in the resulting dynamics.

We report on the buckling behavior and relaxation dynamics for a variety of liquid crystal filaments under compression stress. The amount of off-axis deflection, or lack thereof, is dependent on both filament size and compression velocity. In contrast to other non-Newtonian fluids, liquid crystal filaments may buckle in multiple locations. Additionally, we observed a relaxation of the buckled material after compression. This indicates that there is some flow of material from the deflected segment into the menisci. We also discuss potential applications for this work.

[1] M. Le Merrer, D. Quéré, and C. Clanet, *Phys. Rev. Lett.* **109**, 064502 (2012).

CPP 54.45 Thu 15:00 P2 Meanfield approach to describe magnetic properties of anisotropic dipolar particles — •TAISIA PROKOPYEVA¹ and SOFIA KANTOROVICH^{1,2} — ¹Ural Federal University, Lenin av. 51, Ekaterinburg,620000, Russia — ²University of Vienna, Sensengasse 8, 1090, Wien, Austria

Various specially designed colloidal particles became accessible in experiment. The synthesis of such systems is still a challenge, and one needs reliable predictions for the relationship between the particle parameters (sizes, magnetic-nonmagnetic ratios, shape anisotropy) and the macro properties of large particle systems. Several types of magnetic colloids were synthesized, whose properties differed significantly from those of magnetic spherical single-domain nanoparticles in magnetic fluids. It is convenient to divide "non-standard" magnetic colloids into two groups according to their anisotropy. If the anisotropy is related to the particle shape, then for magnetic particles the dipoledipole interaction remains the same and the anisotropy only affects the steric interactions. Whereas, if the particles retain a spherical shape, however the dipole moment itself is shifted away from the particle centre of mass (anisotropic particles), the dipolar part of the Hamiltonian will change. Here, we focus our attention on the theoretical investigation of magnetic properties of recently introduced sd-particles [Kantorovich et al., Soft Mater, 2011] and magnetic Janus particles [Ruditskiy et al., Soft Mater, 2013]. We develop a first-order mean field approach to study the magnetization and susceptibility of these systems and verify our theory by comparing to the computer simulations.

CPP 54.46 Thu 15:00 P2

Non-additive resistance for the flow of colloids over two barriers — •URS ZIMMERMANN, MARCO HEINEN, and HARTMUT LÖWEN — Institut für Theoretische Physik II, Universität Düsseldorf, Universitätsstr. 1, 40225 Düssedorf, Germany

Ohm's law is one of the most central transport rules stating that the total resistance of sequential single resistances is additive. Using dynamical density functional theory we test additivity of sequential resistances on the scale of individual flowing particles by studying the transport of strongly interacting colloids over two barriers. If the barrier separation is getting comparable to the particle correlation length, the total resistance can be significantly larger or even smaller than the sum of the two individual resistances, depending on the barrier separation and the interaction strength between the particles. This allows to control and tune the total resistance with important applications in microfluidics.

CPP 54.47 Thu 15:00 P2

Active Brownian Motion in Crowded Environment — •PARMIDA SHABESTARI¹, FELIX KÜMMEL¹, IVO BUTTINONI², and CLEMENS BECHINGER^{1,3} — ¹2. Physikalisches Institut, Universität Stuttgart, Germany — ²Department of Materials, ISA, ETH Zürich, Switzerland — ³Max Planck Institute for Intelligent Systems, Stuttgart, Germany

Artificial active swimmers, i.e. Janus particles, suspended in a critical binary mixture, are capable of a self-diffusiophoretic motion upon illumination. In previous experiments, the dynamics of such swimmers close to walls and periodic arrays of rigid obstacles has been investigated [1]. Here, we investigate the dynamics of active swimmers in the presence of a bath of Brownian particles. Such crowded conditions closely resemble the situation of e.g. bacteria in their natural habitat and thus allows to understand how the interaction of active and passive particles affects the particle dynamics and their density distribution. Depending on the density of the Brownian background particles we observe the formation of metastable channels, whose shape and lifetime strongly depend on the densities of active and passive particles but also on the strength of the propulsion force.

[1] VOLPE G, BUTTINONI I, VOGT D, KÜMMERER H J AND BECHINGER C 2011 MICROSWIMMERS IN PATTERNED ENVI-RONMENTS SOFT MATTER 7 8810-5

CPP 54.48 Thu 15:00 P2

Cargo Transport with Active Brownian Particles — •JANNICK FISCHER¹, FELIX KÜMMEL¹, and CLEMENS BECHINGER^{1,2} — ¹2. Physikalisches Institut, Universität Stuttgart, Germany — ²Max Planck Insitute for Intelligent Systems, Stuttgart, Germany

Active Brownian particles are capable of taking up energy from their environment and converting it into directed motion; examples range from chemotactic cells and bacteria to artificial micro-swimmers [1]. One potential application of active Brownian particles is using them as shuttles to transport loads within liquid environments. The central issue is to accomplish effective loading and unloading schemes which are independent of specific interaction forces. Here we suggest a novel mechanism which only requires steric interactions and is based on a Ushaped swimmer which is fabricated by photolithography. By reversing the direction of motion, we expect that a load can be picked up and released easily. Apart from understanding the pickup and release on a microscopic scale, we also want to investigate how such swimmers can lead to the redistribution of passive particles depending on the choice of the applied swimming protocol.

Buttinoni, Ivo, et al. "Active Brownian Motion tunable by light."
2012 J. Phys.: Condens. Matter 24 284129

CPP 54.49 Thu 15:00 P2

Effective temperature of an active microrheological tracer in colloidal suspensions — •ROBERT WULFERT¹, BORIS LANDER¹, UDO SEIFERT¹, and THOMAS SPECK² — ¹II. Institut für Theoretische Physik, Universität Stuttgart, Germany — ²Institut für Physik, Johannes-Gutenberg-Universität Mainz, Germany

It remains an open issue which classes of non-equilibrium systems can be characterized by an effective temperature in a well-defined and meaningful way. A promising and rather generic approach is to consider the fluctuation-dissipation relation (FDR) for driven systems in a non-equilibrium steady state (NESS). We present numerical results obtained via simulation of colloidal suspensions, which are probed by pulling a single tracer particle with a constant force. For this active microrheological scenario, we determine conditions under which the velocity-force FDR becomes approximately time-independent. It can then be interpreted as an effective temperature, accounting for the tracer dynamics on all timescales with a unique value that is equal to the kinetic temperature. Furthermore, we discern in how far the effective temperature depends on the choice of observable by analyzing the anisotropic properties of the tensorial velocity-force FDR.

CPP 54.50 Thu 15:00 P2

Thermoresponsive switching behavior in thin films of cyclic and linear PNIPAM — •DAVID MAGERL¹, XING-PING QIU², FRANÇOISE M. WINNIK², and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching — ²Université de Montréal, Faculty of Pharmacy and Department of Chemistry, CP 6128 Succursale Centre Ville Montréal QC H3C 3J7, Canada

Stimuli-responsive hydrogels are a widely studied field of polymers with a huge potential of applications such as drug-delivery systems and sensors. Among this type of polymer PNIPAM is a well-known representative as a model system of a thermo-responsive polymer. It has been shown by comparative studies of linear and cyclic PNIPAM that a cyclic topography of the polymer greatly influences the switching behavior [1]. Within the scope of this study the properties of spin-coated thin films of linear and cyclic PNIPAM with well-defined molecular weights and different film thicknesses are investigated. Film swelling, when exposed to water vapor, and the switching behavior under a thermal stimulus is investigated. Due to the confinement by the substrate no uniform (3D) swelling but a 1D swelling that results in a thickness change of the films is observed by white-light interferometry and further analyzed.

[1] X.-P. Qiu, F. Tanaka, and F.M. Winnik, Macromolecules 2007, 40, 7069 - 7071

CPP 54.51 Thu 15:00 P2 Networks from amphiphilic star block copolymers — •XIAOHAN ZHANG¹, KONSTANTINOS KYRIAKOS¹, MARIA RIKKOU-KALOURKOTI², ELENI N. KITIRI², COSTAS PATRICKIOS², and CHRIS-TINE M. PAPADAKIS¹ — ¹TU München, Physik-Department, Garching — ²University of Cyprus, Nicosia, Cyprus

Amphiphilic conetworks comprise hydrophilic and hydrophobic chains which microphase-separate when swollen with water. This way, a large amount of internal interfaces is created which is of interest for, among others, tissue engineering. Using end-functionalized star block copolymers for their synthesis results in model networks with low defect density.

We investigate amphiphilic conetworks from various acrylic blocks which differ in composition, water solubility and mechanical properties. Their degree of swelling in water depends strongly on these characteristics. We study the structures of these conetworks using small-angle X-ray scattering which reveals information about the microphaseseparated morphology.

CPP 54.52 Thu 15:00 P2 Star-PEG-Heparin-Polyelectrolyte-Hydrogels - Rate Theory and Reaction Kinetics — •RON DOCKHORN^{1,2} 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

We are studying biohybrid hydrogels made of heparin, a rod-like highly charged glycosaminoglycan as a highly functionalized cross-linker, and non-charged, elastic 4-arm star-shaped-polyethylene glycol by using theory and simulations. We focus on the network structure and reaction kinetics by using the bond-fluctuation simulation method and determine the higher order defects at different initial conditions comparing to the rate theory. Also, we investigate the influence of the initial molar ratio, the variations of functionalized groups, and the concentration dependence of the reaction mixture on the reaction kinetics of the defects and on the percolation threshold of the gels. These findings are useful to optimize the mechanical properties of this biohybrid hydrogels for cell replacement-based therapies.

CPP 54.53 Thu 15:00 P2

Polyelectrolyte-4-Arm-Star-Shaped Hydrogels - Swelling Behavior in Different Solvent Conditions — •RON DOCKHORN^{1,2} 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 We are studying hydrogels made of charged 2/4-functional point-like cross-linker, and non-charged, elastic 4-arm-star-shaped polymer in solutions of various salt concentrations. We focus on the swelling behavior by using the bond-fluctuation simulation method with electrostatic interaction. We apply both the explicit Ewald summation and the Debye-Hückel-approximation. A mean-field type model is used which combines the effects of the gels and is compared to the simulation data.

CPP 54.54 Thu 15:00 P2

Laser Heated Nanoparticles in a Thermoresponsive PNI-PAM Polymer — •MICHAEL ORLISHAUSEN and WERNER KÖHLER — Physikalisches Institut, Universität Bayreuth, 95440 Bayreuth

Thermoresponsive polymers have gained wide attention in large areas of polymer physics and physical chemistry. We have investigated laser-heated gold nanoparticles (GNPs) in aqueous solutions of Poly-N-Isopropylacrylamide (PNIPAM) by means of optical microscopy. Gold colloids with radii of 125nm show high absorption around 532nm due to their plasmon resonance. Hence they can be used as effectively point-like heat sources, well below the diffraction limit. We have found that for small laser powers a circular two-phase region grows around the GNP, whose radius grows linearly with increasing power. Due to high surface temperatures well above 500K, a solvent-bubble, which is stabilized by Marangoni-convection, forms around the GNP. In our experiments, we have found that the estimated temperature on the surface of that bubble fits the calculated boiling point of water when taking the Laplace-pressure inside the bubble into account. At constant heating power the two-phase-region also shows a time evolution that can potentially be described on the basis of a demixing delay that depends on the local temperature difference to the critical temperature.

CPP 54.55 Thu 15:00 P2

Hybrid particle of gold nanoparticles embedded in thermoresponsive microgels — •MAREN LEHMANN, SARAH T. TURNER, LU-CAS KURTHS, and REGINE VON KLITZING — Stranki-Laboratory, Dept. of Chemistry, TU Berlin, Germany

For applications such as sensory and drug delivery systems, microgels with the ability to reversibly switch between a collapsed and expanded state in response to an external stimulus (pH, temperature), are attractive. Embedding metal nanoparticles into microgels can introduce new functionalities and enlarge the field of application to catalysis, medicine and nanoreactors [1] [2] [3]. There are different approaches to prepare hybrids of gold nanoparticles and microgels. Lu et al. demonstrated an in situ synthesis of Au-Pt nanorods in core-shell microgel particles by growing rods from gold seeds previously immobilized in the microgel network [4]. We embed gold nanospheres into PNIPAM microgel networks via various mixing routes in order to reach evenly loaded microgel particles. The differently prepared hybrid particles were compared regarding their zeta potential and volume phase transition depending on the temperature. Transmission electron microscopy images were used to evaluate the distribution and loading. The microgel particles were synthesized in a semi-batch method and with positively and negatively charged initiator molecules.

K. Gawlitza et al. Phys.Chem.Chem.Phys.15, 37 (2013).
M. Karg et al. Curr. Opin. Colloid Interface Sci 14, 6 (2009).
H. Lange et al. Langmuir 28 (2012).
Y. Lu et al. ACS Nano 4, 12 (2012)

CPP 54.56 Thu 15:00 P2 molecular dynamics simulation of the LCST shifting of modified PNIPAM — •YONGBIAO YANG¹, GANESH BALASUBRAMANIAN², MICHAEL BÖHM¹, and FLORIAN MÜLLER-PLATHE¹ — ¹Alarich-Weiss-Str. 4 64287 Darmstadt — ²Iowa State University Ames, IA 50011, USA

The local conformation of chemical systems containing photoresponsive units such as spiropyran and merocyanine can be changed by light radiation of suitable wave length. Such photo-responsive units can be added to polymer chains which then become photo-responsive, too. As a result, the functionalized polymers can exhibit reversible functionalities. Poly(N-isopropylacrylamide) (PNIPAM) is a intensively used temperature-responsive polymer with the lower critical solution temperature (LCST) of 305 K. By grafting with merocyanine or spiropyran units, LCST of PNIPAM is expected to be changed. In our simulations, the temperature-responsive behaviour of modified PNIPAM is studied by using molecular dynamics simulations. Allatom models of modified PNIPAM in solution are built based on the parameters obtained from density functional calculations, and molecular dynamics simulations are performed for systems including a single polymer chain. The LCST of PNIPAM is found to be shifted after grafting photo-responsive units. But the influence of merocyanine and spiropyran units are very different. This originates from their different local structures according to our density functional calculations.

CPP 54.57 Thu 15:00 P2

Wetting induced structure formation in elastic porous media — •ZRINKA GATTIN, OHLE CLAUSSEN, STEPHAN HERMINGHAUS, and MARTIN BRINKMANN — Max Planck Institute for Dynamics and Self-Organization (MPIDS), Göttingen, Germany

When a deformable material is brought in contact with more than one fluid phase, the interplay between the elasticity and interfacial stresses can give rise to unexpected phenomena.

Motivated by experiments on the demixing of binary liquids in polymer gels we study the formation and interaction of liquid droplets in a 2D elastic medium. The phase separating liquids are represented with a lattice gas model, where the elastic matrix is introduced through a network of tethered particles having different affinities to the fluid phases. Our simulations show how the growth of the domains can be inhibited by the elastic medium, altering the dynamics and giving rise to characteristic patterns. The results are compared to predictions of a simple continuum model of the elastic matrix.

$CPP \ 54.58 \quad Thu \ 15:00 \quad P2$

Measurement of microviscosity in crosslinked polyacrylamideferrohydrogels by Mössbauer spectroscopy — •JOACHIM LANDERS¹, LISA ROEDER², ANNETTE SCHMIDT², and HEIKO WENDE¹ — ¹Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg -Essen, Germany — ²Department Chemie, Institut für Physikalische Chemie, Universität zu Köln, Germany

Several polyacrylamide (PAAm) hydrogels with different amounts of methylenbisacrylamide (MBA) crosslinker were prepared, containing acicular hematite (α -Fe₂O₃) nanoparticles. These were used as probes allowing us to examine the local dynamic properties by $^{57}\mathrm{Fe}\text{-M\"ossbauer}$ spectroscopy in systems with different degrees of cross-linkage. While static sextet spectra can be observed up to 265K, the width of the sextet lines increases dramatically near the water melting point in all samples, verifying movement of the nanoparticles when the hydrogel approaches the liquid state. This reveals that, contrary to expectations, embedded nanoparticles are not completely immobilized even in strong crosslinked hydrogel networks with us being able to quantify the effects of Brownian motion by Mössbauer spectroscopy. Theoretical calculations allow to estimate the temperature dependent microviscosity ν , which exceeds ν_{H2O} by far and is correlated to the amount of MBA crosslinker. (This work was supported by DFG WE2623/7-1, SPP1681)

$CPP \ 54.59 \quad Thu \ 15:00 \quad P2$

Smart surfaces from stimuli-responsive microgels via spin coating — •JOHANNES BOOKHOLD, BASTIAN WEDEL, and THOMAS HELLWEG — Universität Bielefeld, Universitätsstraße 25, Bielefeld, Germany

Stimuli-responsive nano- and microgels are in the focus of interest for a number of applications, such as sensors, drug-delivery and surface coatings. Among these colloidal particles temperature responsive microgels based on poly(n-isopropylacrylamide) (pNIPAm) are the most intensive studied systems. These microgels exhibit a reversible volume phase transition (VPT) at a temperature near the lower critical solution temperature (LCST) at about 305 K. For most applications a huge advantage of pNIPAm based microgels is that their properties and the external stimuli they respond to can be modified via copolymerization. The resulting properties of the particles can be predicted depending on the used comonomer. The production of coatings and thin films with tailor-made properties from microgels is especially interesting for applications in medical and biological research.

A general, reliable, fast and easy production process for thin films and surface coatings consisting of such microgels is a desirable goal. One already well established method in the field of surface coatings that can offer these features is spin coating. Therefore the access to a variety of microgel coatings and films showing different properties via spin coating is within the focus of this work. Manufactured coatings were characterized using ellipsometry, atomic force microscopy (AFM) and scanning electron microscopy (SEM).

CPP 54.60 Thu 15:00 P2

Characterizing the crosslinking process of PDMS with Rheometry — •RUDOLF HASSLACHER and SABINE HILD — Institute of Polymer Science, Johannes Kepler University of Linz, Altenberger Strasse 69, 4040 Linz, Austria

Depending on the desired features the wide variety of polydimethylsiloxanes (PDMS) types with different properties (viscosity, hardness, elongation modulus) and applications makes it necessary to select the used type properly. Additionally, knowledge about the crosslinking behavior of PDMS is very important for scientists dealing with it or its composites. During this work different types of PDMS were investigated to find a fully crosslinked PDMS with the desired properties. Therefore the crosslinking behavior was examined with Rheometry. The rheological measurements were carried out with an ANTON PAAR UDS 200 Rheometer. There are different ways of following the curing via Rheometry, namely strain-controlled time resolved frequency sweeps (= time-resolved mechanical spectroscopy = TRMS) and stress-controlled time tests. The TRMS measurements were done at a frequency range between 0.1 and 100 rads-1 (both at 25° C), the stress-controlled tests with constant stress = 75 Pa and constant frequency = 1 Hz. We found a reasonable accordance between these two ways. Through the rheological data we gain the parameters after which we can select the appropriate PDMS for our application.

CPP 54.61 Thu 15:00 P2

Vulcanized fiber studied by x-ray diffraction — •KARIN RÜSTER¹, DOMINIK DUMKE², MICHAEL PAULUS¹, CHRISTIAN STERNEMANN¹, JULIA NASE¹, JOHANNES MÖLLER¹, KOLJA MENDE¹, IRENA KIESEL¹, DOROTHEE WIECZOREK², and METIN TOLAN¹ — ¹Fakultät Physik / DELTA, Technische Universität Dortmund, D-44221 Dortmund, Germany — ²Fakultät Maschinenbau, Technische Universität Dortmund, D-44221 Dortmund, Germany

Vulcanized fiber is a material of various applications, for example it is used as an insulator in the electrical industry or in welding shields. As it is made from renewable resources, it gained increasing interest in recent years. There are two ways to produce vulcanized fiber: mercerisation and parchmentising. The raw paper is soaked with alkaline (mercerisation) or acidic solution (parchmentising) respectively, pressed to interconnect the layers, rested for a certain time, and washed out in steps of descending concentrations. During this process the material's properties change. The material becomes harder, stiffer, and thicker due to multiple layering and structural changes. The corresponding microscopic mechanisms are analysed by x-ray diffraction (XRD). The raw paper consists mostly of cellulose I_{α} and I_{β} , which transforms to cellulose II during the process of mercerisation. The structural changes during the process of parchmentising by zinc chloride were examined. The experiment was performed at beamline BL9 of the synchrotron light source Delta, Dortmund.

CPP 54.62 Thu 15:00 P2

Hydration and molecular interactions in PNIPAM films probed with FTIR spectroscopy — •ALFONS SCHULTE^{1,2}, MARTINE PHILIPP¹, CHRISTOPH SCHAFFER¹, and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching — ²Physics Department and College of Optics and Photonics, University of Central Florida, Orlando, FL 32816-2385, USA

The properties of bound water are of considerable interest for hydrogels and their LCST-type demixing transition. Poly(N-isopropyl acrylamide) (PNIPAM) is among the thermoresponsive polymers well studied in solution. In the present investigation we study molecular changes in PNIPAM films as a function of hydration employing FTIR spectroscopy. PNIPAM films with thickness over the range from 50 to 200 nm are prepared by spin coating on silicon substrates. The infrared spectrum in the CH, OH, and amide band regions provides details on the changes in conformation and hydrogen bonding. These are investigated during a heating-cooling cycle and the time evolution of water storage in the hydrogel films.

 $CPP \ 54.63 \quad Thu \ 15:00 \quad P2$

In Situ particle degradation of hyperbranched polyglycerol particles via Atomic Force Microscopy — •MARCEL RICHTER and REGINE VON KLITZING — TU Berlin, Straße des 17. Juni 124, 10623 Berlin

During the last decades hyperbranched polymers made of polyethylene glycerol (PEG) have attracted much interest in applications like drug delivery and sensors [1]. Due to their biocompability and multifunctionallity these particles afford the formation of efficient drug carriers [2]. The drug loading with these particles can be realised by the encapsulation during the particle synthesis. This guarantees a homogenous drug distribution with in the carrier. The drug release can be triggered by the particle degradation in response to biological stimuli such as changes in pH [3]. The particle degradation has been followed by atomic force microscopy (AFM) as a function of time. It has been found that particle erosion occurs with an exponential decay within the first minutes. Further progress in the degradation process leads to a slow down of the particle erosion. On the other hand, the particle degradation in bulk shows linear particle erosion. [1] *R. Haag, F. Kratz, Angew. Chem. Int. Ed. (2006), 45, 1198 [2] K. Knop et al., Chem. Int. Ed., (2010), 49, 6288 [3]*E. Fleige et al., Adv. Drug Deliv. Rev. (2012), 64, 866

CPP 54.64 Thu 15:00 P2 Using small angle neutron scattering and light scattering to investigate thermoresponsive copolymer microgels — •BASTIAN WEDEL, JOHANNES BOOKHOLD, and THOMAS HELLWEG — Universität Bielefeld, Universitätsstraße 25, Bielefeld, Germany

Temperature responsive microgels undergo a volume phase transition (VPT) at a certain temperature (VPTT). It is this specific property that makes such kind of structures interesting for various applications, such as sensors, nanoactuators or as drug delivery systems. An optimal performance of microgels requires a method for an adjustment of the application-specific properties. A suitable and easy method is constituted by the copolymerization of different monomers.

We present a study dealing with the investigation of the physical and structural properties of copolymer microgels based on different temperature responsive alkylacrylamide derivatives with consimilar structures. The used monomers are *N*-*n*-propylacrylamide (NNPAM), *N*-isopropylacrylamide (NIPAM) and *N*-isopropylmethacrylamide (NIP-MAM) with VPTTs of the homopolymer microgels of 22 °C, 32 °C and 43 °C respectively.

We analyzed the dependence of the feed composition and the surfactant concentration in the reaction solution at various temperatures to get an insight into the structural changes during the volume phase transition. Photon correlation spectroscopy and static light scattering were used to investigate the swelling behavior and the overall structure. Furthermore, we performed small angle neutron scattering experiments to clarify the structure on the lengthscale of the polymer network.

CPP 54.65 Thu 15:00 P2 Charge Storage in β -FeSi₂ Nanoparticles — •JENS THEIS¹, SE-BASTIAN KÜPPER¹, ROBERT BYWALEZ², HARTMUT WIGGERS², and AXEL LORKE¹ — ¹Fakultät für Physik and CENIDE, Universität Duisburg-Essen — ²Institut für Verbrennung und Gasdynamik and CENIDE, Universität Duisburg-Essen

The increasing use of mobile electronics creates a steady demand for new energy storages with very high capacitance. Here we report on the observation of a surprisingly high specific capacitance of β -FeSi₂ nanoparticle layers.

Lateral, interdigitated capacitor structures were fabricated on thermally grown silicon dioxide and covered by $FeSi_2$ particles by drop or spin casting. The $FeSi_2$ -nanoparticles, with sizes in the range of 10-30 nm, were fabricated by gas phase synthesis in a hot wall reactor. Compared to the bare electrodes, the nanoparticle-coated samples exhibit a 3-4 orders of magnitude increased capacitance. Time-resolved current voltage measurements show that for short times (seconds to minutes), the material is capable of storing up to 1 As/g at voltages of around 1 V. The devices are robust and exhibit long term stability under ambient conditions. The specific capacitance is highest for a relative humidity of 95%, while for a relative humidity below 40% the capacitance is almost indistinguishable from a nanoparticle-free reference sample.

The devices work without the need of a fluid phase, the charge storing material is abundant and cost effective, and the sample design is easy to fabricate.

${\rm CPP}~54.66 \quad {\rm Thu}~15{:}00 \quad {\rm P2}$

In-Situ Observation of Wrinkle-Formation via UV/Ozone Oxidation — •BERNHARD GLATZ¹, MORITZ TEBBE¹, ANDREAS SCHEDL², and ANDREAS FERY¹ — ¹Department of Physical Chemistry 2, University of Bayreuth, Universitätsstraße 30, 95447 Bayreuth, Germany — ²Department of Macromolecular Chemistry 1, University of Bayreuth, Universitätsstraße 30, 95447 Bayreuth, Germany

Wrinkled surfaces are versatile tools on the micro- and nano-range, e.g. in their use as photonic crystals or for particle alignment. They can be formed by straining soft substrates that are coated with a thin hard film. The wavelength and amplitude of the resulting periodic surface deformations strongly depends on processing conditions, the thickness of the thin film and mechanical properties of film and substrate. Wavelengths between sub-micron and macroscopic range are accessible, however defect structures like cracks and wrinkle branches are inevitable side features in wrinkling processes and furthermore nonpredictable yet.

To better understand defect formation, we developed a setup, which allows observation an in-situ view of currently forming waves and their defect structures via Light Microscopy. We applied the system for investigation of defect formation in systems, which posses defined gradients in elastic constants [1]. We find that rather than appearing in a random fashion, branching defects become ordered and we discuss implications of this finding for the formation of hierarchical structures. [1] K. U. Claussen, M. Tebbe, R. Giesa, A. Schweikart, A. Fery and

H.-W. Schmidt, 2012, RSC Advances, 2 - 27, 10185 - 10188

CPP 54.67 Thu 15:00 P2

Response of gold nanorods in solution to external electric fields — •CHRISTINA LEDERLE¹, DANIEL SCHEID², MARKUS GALLEI², and BERND STÜHN¹ — ¹Experimental Condensed Matter Physics, TU Darmstadt, Germany — ²Ernst-Berl Institut für makromolekulare Chemie, TU Darmstadt, Germany

We study gold nanorods of defined length (60 nm) and diameter (20 nm) in different solvents. The nanorods are coated by a block copolymer layer (Polyisoprene-b-Polypropylensulfid) which enhances the miscibility of the rods in organic solvents (tetrahydrofuran, chloroform, hexane, toluene). We apply an external AC electric field up to 1000 V/mm while performing dynamic light scattering experiments (DLS) to yield in collective diffusion coefficients, relaxation times and stretching parameters. These parameters show a strong correlation with the strength of the electric field in solutions of gold nanorods in THF and chloroform. This is due to a strong dielectric response of the respective solvent which causes the nanorods to accelerate their diffusive dynamics. This effect is absent when hexane or toluene is used as solvent.

We present a detailed analysis of the dependency of the dynamical parameters on the applied electric field. The orientation of the gold nanorods depending on the electric field is investigated by small angle X-Ray scattering.

CPP 54.68 Thu 15:00 P2

maghemite nanoparticles embedded in thin block copolymer films — •YUAN YAO¹, EZZELDIN METWALLI¹, BO SU¹, VOLKER KÖRSTGENS¹, DANIEL MOSEGUI GONZALEZ¹, LIN SONG¹, GONZALO SANTORO², STEPHAN V. ROTH², MATTHIAS OPEL³, and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching — ²DESY, Notkestrasse, 85, 22603 Hamburg — ³Walther-Meissner-Institute, Walther-Meissner-Straße. 8, 85747 Garching

Maghemite nanoparticles embedded inside a polymer matrix mark a novel class of hybrid materials which have attracted high interest due to the potential for numerous applications such as sensors and high density magnetic storage devices. The control of the alignment of the maghemite nanoparticles within the polymer matrix is essential for producing well-aligned highly-oriented metal oxide-polymer nanocomposites. The alignment of maghemite nanoparticles in polystyrene-bpoly(N-isopropylacrylamide) P(S-b-NIPAM) diblock copolymer films is investigated. The thin hybrid films are prepared by spin coating. The structure of the resulting hybrid films is studied at different concentrations of maghemite nanoparticles using SEM, AFM, GISAXS and GIWAXS. The results indicate a morphological transition from lamella to hexagonal upon incorporation of maghemite nanoparticles into the diblock copolymer films. At high concentration of nanoparticles, large particles aggregates are formed on top of the polymer surface. The magnetic properties of the nanocomposite films at different temperatures are measured and compared with theoretical predictions.

CPP 54.69 Thu 15:00 P2

Whispering gallery modes in spherical copolymers — •DANIEL BRAAM¹, KENICHI TABATA², GÜNTHER M. PRINZ¹, YOHEI YAMAMOTO², and AXEL LORKE¹ — ¹Experimentalphysik und CENIDE, Universität Duisburg-Essen — ²Faculty of Pure and Applied Sciences, University of Tsukuba, Japan

Copolymers are promising candidates for use in optoelectronic devices because of their cost efficiency and superior optical properties.

By combining polymers to π -conjugated alternating copolymers (e.g. F8TMT2 with fluorene and tiophene in the repeating units [1]), isotropic microspheres can be fabricated. By adjusting the formation parameters, their size can be tuned from some hundred nanometers to several micrometers. Laser excitation of a single sphere leads to a broad photoluminescence spectrum with superimposed narrow peaks. The number of observed peaks is dependent on the sphere diameter and they are attributed to standing waves on the inside of the sphere, known as whispering gallery modes (WGMs). The measured peak positions are in good agreement with theoretical calculations of TMand TE-WGMs. This allows us to determine the copolymer's relative permittivity.

The investigated π -conjugated alternating polymer particles combine the properties of a dye, a dielectric and a resonator. This opens up the possibility to build photonic crystals by arranging spheres with a distinct and narrow size distribution to match and amplify certain WGMs, aiming for novel optoelectronic properties.

[1] Taeko Adachi et al., J. Am. Chem. Soc. 135, 870 (2013)

CPP 54.70 Thu 15:00 P2

How long is the interfacial length in a nanocomposite system? — •EVANGELOS VOYIATZIS, FLORIAN MÜLLER-PLATHE, and MICHAEL BÖHM — Eduard-Zintl-Institut für Anorganische und Physikalische Chemie and Center of Smart Interfaces, Technische Universität Darmstadt, Alarich-Weiss-Str. 4, D-64287 Darmstadt, Germany

The influence of fullerene inclusion on the structure of a polystyrene matrix as well as the spatial distribution of the atomic level stresses in the polymer and the cavity size distribution is studied by molecular dynamics simulations. The spatial deviations of the two latter quantities from their average bulk values are correlated with characteristic deviations of structural properties, such as the mass density distribution and segmental orientation of the polymer matrix. The structural properties of the polymer in the vicinity of the nanoparticle suggest the formation of two layers, a result that is in accordance with findings of previous studies. The inclusion of fullerenes enhances the stress anisotropies in their neighbourhood. This is pointed out by the magnitude of the spatial variations of both the average shear stress and the von Mises shear stress. The length of the interface formed between the fullerenes and the polystyrene matrix is estimated by monitoring the variations of the radial mass density and the radial atomic level stress distributions from their average bulk values. The two methods lead to significant differences in the estimated interfacial lengths. The values based on variations of the atomic level stresses are considerably shorter than the estimate obtained when using the variations of the mass density distribution.

CPP 54.71 Thu 15:00 P2

Work of Adhesion between Metals and Polymers on a Macroand Microscopic Scale — •MARIEKE FÜLLBRANDT, DIKRAN KESAL, and REGINE VON KLITZING — Stranski-Laboratorium für Physikalische und Theoretische Chemie, Technische Universität Berlin, Strasse des 17. Juni 124, 10623 Berlin

Polymer/metal hybrids are of high interest for example in lightweight constructions used in the automotive industry. They combine a high functional integration with a lower weight compared to pure metal parts. The joining of these dissimilar materials without using additional material is a central challenge. A fundamental understanding about the adhesion mechanisms at the polymer/metal interface is inevitable.

In this contribution the work of adhesion between different metal/polymer systems relevant for industrial applications is studied by atomic force microscopy (AFM) and contact angle (CA) measurements. AFM is used for the determination of the pull-off force between a metal substrate and a polymeric microsphere. Measurements are conducted in a dry nitrogen atmosphere at 30 °C. The measured adhesion forces are analyzed using theoretical models of contact mechanics. Different models are discussed and the effect of roughness is considered. With CA measurements the surface energy of the solids is determined. From that the interfacial energy between a given metal/polymer system can be determined and further be related to the work of adhesion. Results from AFM and CA measurements are compared and possible adhesion phenomena are discussed.

CPP 54.72 Thu 15:00 P2

Structure-Property relationships of Nanocomposites Based on Epoxy and Layered Double Hydroxides — •JING LENG¹, FRANZISKA EMMERLING¹, DE-YI WANG^{2,3}, and ANDREAS SCHÖNHALS¹ — ¹BAM Federal Institute for Materials Research and Testing, Unter den Eichen 87, 12205 Berlin, Germany — ²IMDEA Materials Institute, C/Eric Kandel 2, 28906 Getafe, Madrid, Spain — ³Center for Degradable and Flame-Retardant Polymeric Materials (ERCEPM-MoE), College of Chemistry, Sichuan University, Chengdu 610064, China

Two kinds of organically modified MgAl Layered Double Hydroxides (MgAl-LDH) were synthesized and reaction blended with an epoxy system (EP) to obtain polymerbased nanocomposites. The organic modification of the MgAl-LDHs were by sodium dodecylbenzene sulfonate (SDBS) modified and own synthesized SACC. The two kinds of nanocomposites were investigated by a combination of differential scanning calorimetry (DSC), small- and wide-angle X-ray scattering (SAXS and WAXS), and broadband dielectric spectroscopy (BDS) in dependence of the concentration of the nanofiller. The differences observed for the both kinds of nanoparticles are discussed in detail.

CPP 54.73 Thu 15:00 P2

Interactions between capped gold nanocrystals in vacuum: presence of three-body effects — \bullet NADEZDA GRIBOVA¹, GERNOT BAUER¹, CHRISTIAN HOLM², and JOACHIM GROSS¹ — ¹ITT, University of Stuttgart, Stuttgart, Germany — ²ICP, University of Stuttgart, Stuttgart, Germany

Self-assembly of capped nanocrystals became an active topic during the last years. Nanocrystals are currently used in many areas of engineering and life sciences or medicine. However, a full understanding of their mechanical and thermodynamical stability is still lacking. Nanocrystals are usually capped with some organic ligands, which prevent aggregation. These capping molecules play an important role in the self-assembly of the nanoparticles – the ratio between the ligand length and the diameter of the nanocrystal core determines the structure of the superlattice in which nanoparticles assemble.

In this study, we report the potential of mean force between gold nanocrystals capped with alkylthiols. We propose a simple but accurate temperature-scaling of this effective pair potential, based on a perturbation theory. Schapotschnikow and Vlugt [1] have shown that effective three-body interactions exist between capped nanocrystals. We analyze the dependence of the 3-body contribution on different ligand lengths and core sizes and show that the 3-body potential does not significantly depend on the temperature. We also propose a threebody potential that scales with the repulsive part of the effective pair potential.

[1] P. Schapotschnikow et al., Nano. Lett. 8, 2930, (2008)

CPP 54.74 Thu 15:00 P2

The effect of electric fields on CdSe-nanocrystals — •ROBERT NIEMÖLLER, DANIEL BRAAM, GÜNTHER M. PRINZ, MARTIN GELLER, and AXEL LORKE — Experimentalphysik und CENIDE, Universität Duisburg-Essen

Using a micro-photoluminescence (μ -PL) setup, we investigate fieldinduced spectral changes in the emission of CdSe/ZnS nanocrystals, pumped with a Nd:YVO₃ laser. We embed the nanocrystals between two layers of polymethylmethacrylat (PMMA) and place them inside a capacitor-like structure consisting of a doped silicon substrate and thin transparent metal electrodes. Thus, we are able to subject the crystals to a tunable electric field and record their PL simultaneously. Small agglomerates of crystals show different behavior in their PL when a voltage is applied, depending on the substrates used. The samples with p-doped substrates show a shift in their peak energy, which is proportional to the square of the applied voltage, caused by the quantum-confined Stark effect. From this dependency we can extract the polarizability of the nanocrystals which is in good agreement with values measured by other groups on a different sample structure. However, the samples prepared on n-doped substrates only show a shift when a negative voltage is applied to the metal electrode, leading to an asymmetric Stark shift. When cooled down to approximately 15 K, the structures on p-doped substrates exhibit a similar asymmetric dependence of the PL energy on the applied voltage.

CPP 54.75 Thu 15:00 P2

Unexpected low-frequency dynamics in $DGEBA/SiO_2$ — •RICK DANNERT¹, PATRICK ELENS¹, MATTHIEU THOMASSEY², JÖRG BALLER¹, and ROLAND SANCTUARY¹ — ¹Laboratory for the Physics of Advanced Materials, University of Luxembourg — ²G2IP / ICPEES CNRS UMR 7515 - ECPM / University of Strasbourg (France)

We investigate the complex rheological behaviour of nanocomposites based on low molecular weight epoxy resins. The resin consists of DGEBA (diglycidylether of Bisphenol-A) with different degrees of polymerization (monomers, dimers, trimers). The nanoparticles (diameter: 25 nm) consist of silica coated with a thin silane layer to achieve a good dispersion. In order to investigate the relaxation behaviour of the complex shear moduli, we exploit dynamic rheology at temperatures higher than the thermal glass transition temperature (258K). Measurements of the pure viscoelastic DGEBA system show powerlaw behaviour. The dynamic glass transition is shifted to lower frequencies by adding nanoparticles. In addition to the alpha process, the shear moduli show unexpected relaxations at much lower frequencies. These low-frequency relaxations are systematically investigated for different nanoparticle concentrations and by changing the relaxation dynamics of the matrix molecules. The latter is done by specifically modifying the length of the matrix molecules, e.g. by using dimers instead of monomers.

CPP 54.76 Thu 15:00 P2 Characterization of the electronic and magnetic structure of multifunctional NaREF₄ (RE = rare earth) coreshell nanoparticles — •LILLI SCHNEIDER¹, THORBEN RINKEL², ARTUR CHROBAK³, MARKUS HAASE², and KARSTEN KÜPPER¹ — ¹Physics Department, University of Osnabrück, Germany — ² Institute of Chemistry, University of Osnabrück, Germany — ³Institute of Physics, University of Silesia, Poland

Rare earth (RE) based nanoparticles of type NaREF₄ have attracted lot of attention in the last few years due to their upconverting luminescence. Here, we want to concentrate on electronic and magnetic properties of NaREF₄/NaGdF₄ nanocrystals, since the magnetic behaviour of these fluorescent nanoparticles are of utmost importance from fundamental and applicative point of view as well. Hexagonal β -phase nanocrystals (3-22 nm) were prepared and characterized by X-ray powder diffraction (XRD) and transmission electron microscopy (TEM).

A detailed study of the electronic structure and magnetic coupling phenomena of the different core-shell nanoparticles is performed using X-ray photoelectron spectroscopy (XPS), magnetometry (SQUID) and X-ray magnetic circular dichroism (XMCD). First SQUID measurements of NaEuF₄/NaGdF₄ core-shell nanoparticles show butterfly shaped hysteresis loops at low temperature (2 K) in contrast to superparamagnetic behaviour observed for the corresponding "pure" NaEuF₄ and NaGdF₄ nanoparticles.

$CPP \ 54.77 \quad Thu \ 15:00 \quad P2$

Role of geometric parameters on nanoparticle-polymer brush composite systems — •MURIEL ROVIRA ESTEVA, STEFAN WELLERT, and REGINE VON KLITZING — Stranski-Laboratorium für Physikalische und Theoretische Chemie, Institut für Chemie, Technische Universität Berlin, Straße des 17. Juni 124, 10623 Berlin, Germany

Polymer brushes are polymers tethered to a surface or interface by one end, which at sufficiently high grafting densities show a stretched conformation away from the surface. Many of its applications involve interaction with particles of some kind, so understanding the interactions between nanoparticle and polymer brushes is of great importance.

A number of parameters may play a significant role on the structure as well as the dynamics of these systems (particle characteristics, brush morphology, polymer-nanoparticle interaction, solvent quality, etc.), but the extremely small sample volume and complexity of the system have rendered the experimental investigation of their influence a challenging task. Poly(2-(dimethylamino)ethyl methacrylate)) (PDMAEMA) brushes with embedded gold nanoparticles have been used as model systems in this work to explore the effect of the various parameters on the composites and obtain a global picture of their behaviour, particularly in their swollen state.

CPP 54.78 Thu 15:00 P2

Plasmonic nanoparticle assemblies with controllable plasmon resonance coupling — •TOBIAS HONOLD¹, MAREEN MÜLLER², AN-DREAS FERY², and MATTHIAS KARG¹ — ¹Physical Chemistry I, University of Bayreuth, Universitätsstr. 30, 95447 Bayreuth, Germany — ²Physical Chemistry II, University of Bayreuth, Universitätsstr. 30, 95447 Bayreuth, Germany

Surface plasmon resonances are collective oscillations of the electron gas at a metal surface which can be excited by electromagnetic radiation. These resonances become localized when the size of the metal object is reduced down to the nanoscale. The energy of this localized surface plasmon resonance (LSPR) depends strongly on the particle size, shape, the dielectric environment and on the metal itself. In addition, LSPRs are sensitive to the inter-particle distance. When two plasmonic nanoparticles approach each other coupling of the resonances occurs and the optical properties of the system can change significantly. In this contribution we show how we make use of this distance dependent coupling behavior in order to create plasmonic surfaces with tailored optical properties. In our approach we coat the plasmonic nanoparticles with polymer shells which then act as a steric spacer during particle assembly. These core-shell particles can nicely be assembled to form hexagonal close-packed monolayer or more complex structures such as linear assemblies realized through wrinkleassisted assembly. The inter-particle separation is controlled by the thickness of the polymer shell and hence plasmon resonance coupling becomes controllable

CPP 54.79 Thu 15:00 P2 Dendronized polymers replicated with graphene and graphene oxide — •SIMONE DELL'ELCE¹, VITALIJ SCENEV¹, BAOZHONG ZHANG², NIKOLAI SEVERIN¹, DIETER SCHLÜTER², and JÜRGEN P. RABE¹ — ¹Department of Physics, Humboldt-Universität zu Berlin, Newtonstr. 15, 12489 Berlin, Germany — ²Laboratory of Polymer Chemistry, Department of Materials, ETH Zürich, Wolfgang Pauli Strasse 10, HCI J541, 8093 Zürich, Switzerland

Graphene has been demonstrated to be highly bendable and stretchable to follow the topography of a solid surface with the precision down to single macromolecules (N. Severin et al., Nano Lett. 2011, 11, 2436). The question remains, inhowfar the locally strained graphene may have an impact on the conformation of the replicated macromolecules. Dendronized polymers (denpols) consist of a linear backbone surrounded by a dense cladding of structurally regular dendritic branches (dendrons), anchored to each repeating unit. Variation of the dendron generation allows to tune the properties of the denpols. We deposited denpols on an atomically flat mica substrate and covered them with either graphene or graphene oxide (GO) layers. Scanning force microscopy images reveal that the heights of the denpol replicas in GO match the heights of uncovered molecules. The heights of higher generation denpol replicas in graphene are substantially smaller as compared with the heights of the uncovered macromolecules. This may be attributed to graphene being stiffer than GO and more strongly interacting with the substrate, collapsing thereby to some extent the structure of the high generation denpols

CPP 54.80 Thu 15:00 P2

Controlled drug release using nanodiamonds as drug carriers — •TRAN MINH VU, ANDREA KURZ, ANNA ERMAKOVA, GOUTAM PRAMANIK, BORIS NAYDENOV, YUZHOU WU, TANJA WEIL, and FEDOR JELEZKO — University Ulm

We investigated the drug release of nanodiamond- Doxorubicin (ND-DOX) complexes in different pH. DOX is a chemotherapeutic against cancer cells, e.g. mammary or liver tumors. Using untreated DOX in order to kill cancer cells has two main problems: DOX also affects healthy cells and cancer cells can be resistant through drug efflux [1]. These problems can be overcome by using ND-DOX complexes [1]. Nanodiamonds are non- toxic [2], can move through membrane cells [2] and their surface can be functionalized making them able for drug delivery. Cancer cells have a lower pH environment compared to healthy cells, therefore we did a pH- sensitive experiment. We prepared a sample of ND-DOX in a solution at pH 7. With a standard confocal setup we performed fluorescence correlation spectroscopy (FCS) and determined the hydrodynamic radius r. We observed that by changing the pH of the ND-DOX solution from 7 to 5 the radius r=130 nm at pH=7 decreased to r=6 nm at pH=5. The fluorescence signal came from DOX (our NDs are non-fluorescent) thus indicated DOX release from the bigger ND-DOX complex. These measurements can be done time- dependent, respectively pH dependent leading to drug release time and the pH value which triggers the release. [1] Chow et al., Sci.Transl. Med. 3, 73ra21 [2] Chi-Cheng Fu et al., PNAS 104 (3) 727-732

CPP 54.81 Thu 15:00 P2

Resonance Energy Transfer Between Nanotubular J-Aggregates and Quantum Dots — •YAN QIAO¹, FRANK POLZER¹, SERGEI KÜHN², SEBASTIAN FRIEDE², STEFAN KIRSTEIN¹, and JÜRGEN RABE¹ — ¹Institut für Physik, Humboldt-Universität zu Berlin, Newtonstr. 15, 12489 Berlin, Germany — ²Max-Born-Institut für Nichtlineare Optik und Kurzzeitspektroskopie im Forschungsverbund Berlin e.V., Max-Born-Straße 2 A, 12489 Berlin, Germany

Resonance coupling between distinct excitons in organic / inorganic hybrid materials has become a promising approach towards the design of novel nano-structured opto-electronic devices [1,2]. Herein we report on the construction of colloidal nanohybrids built in aqueous solution from tubular J-aggregates of amphiphilic cyanine dyes and semi conducting quantum dots (QDs) of CdTe. QDs of different size were attached to the surface of the J-aggregates by electrostatic self-assembly. The close proximity between J-aggregates and QDs enables strong coupling between the dissimilar excitons with high energy transfer efficiencies. The direction of energy transfer is selected by the size of the QDs. FRET efficiency of 92% is achieved for transfer from QDs to the J-aggregates. For the opposite direction the J-aggregates act as light harvesting antennas and increase the effective absorption of the QDs by a factor of ten.

[1] B. J. Walker, V. Bulović, M. G. Bawendi, Nano Lett. 2010, 10, 3995.

[2] Q. Zhang, T. Atay, J. R. Tischler, M. S. Bradley, V. Bulović, A. V. Nurmikko, Nat. Nanotechnol. 2007, 2, 555.

CPP 54.82 Thu 15:00 P2

Long-term time-resolved photoluminescence studies of novel Ruthenocenyldecorated Sn/S cluster — \bullet NILS ROSEMANN¹, ELIZA LEUSMANN², MONA WAGNER², STEFANIE DEHNEN², and SANGAM CHATTERJEE¹ — ¹Fachbereich Physik Philipps-Universität Marburg, Marburg, Germany — ²Fachbereich Chemie Philipps-Universität Marburg, burg, Marburg, Germany

The use of ruthenium complexes opens a variety of applications, such as dye-sensitized solar cells and chromophores[1,2]. Single-crystals of novel core shell clusters with ruthenocene-ligand and inorganic Sn4S6 core were grown. As such crystals are known to be rather sensitive to irradiation; we perform long-term low-density photoluminescence measurements. To address individual single crystals, these are performed using a streak-camera setup with high spatial resolution in the μ m range. This way, the spectral information and ultra-fast carrier dynamics are investigated. Combining these information gives rise to any optical induced changes of the crystals.

[1] Angew. Chem. 123, 10870-10873, (2011)

[2] Inorg. Chem. 50, 5494-5508, (2011)

CPP 54.83 Thu 15:00 P2

Characterization of carbon nanotube containing polymer membranes — •TÖNJES KOSCHINE¹, KLAUS RÄTZKE¹, VOLKER ABETZ², THOMAS EMMLER², MUNTAZIM MUNIR KHAN², VOLKAN FILIZ², LUCA RAVELLI³, WERNER EGGER³, and FRANZ FAUPEL¹ — ¹CAU Kiel, Technische Fakultät, Institut für Materialwissenschaft, Kiel — ²Helmholtz-Zentrum Geesthacht, Zentrum für Material- und Küstenforschung GmbH, Geesthacht — ³Universität der Bundeswehr München, Fakultät für Luft- und Raumfahrttechnik, Neubiberg

Polymeric membranes are widely used for gas separation, where free volume is a key property for characterization. High free volume membranes, for instance PIM-1, are suitable candidates. Positron annihilation lifetime spectroscopy (PALS) is a well-established method for free volume measurements and has already been applied to these polymers [1]. In membrane applications the polymers have to be prepared as thin films and undergo aging, usually related to reduced free volume and resulting in reduced permeability. This has already been characterized by PALS [2]. In the present investigation we characterized thin films of PIM-1 and PIM-1 with 2 wt% of functionalized multiwall carbon nanotubes (f-MWCNT) on porous support (PAN). The typical thickness of the films was about 700 nm and therefore a moderated beam for positron lifetime analysis was used. All samples were measured in the as prepared state and after 300 days of aging. Results show, that incorporation of f-MWCNT into PIM results in reduced

aging.

[1]R. Lima de Miranda et al., Phys. Stat. Sol. RRL 1(5), 2007, 190ff

[2] S. Harms et al., Journal of Adhesion 88, 2012, 608-619

CPP 54.84 Thu 15:00 P2

Chain conformation of poly(butylene oxide) silica nanocomposites — •ADRIAN HAMM, WIM PYCKHOUT-HINTZEN, ANDREAS WISCHNEWSKI, JÜRGEN ALLGAIER, and DIETER RICHTER — Jülich Centre for Neutron Science JCNS and Institute for Complex Systems ICS, Jülich, Deutschland

Poly(butylene oxide) silica mixtures have proven to be a nanocomposite model system with many desirable features. As poly(butylene oxide) does not crystallize this opens up the possibility to investigate its behaviour with many different methods over a very broad temperature range. After preliminary small angle x-ray scattering experiments to prove good particle dispersion we used rheology and boradband dielectric spectroscopy experiments to gather information about the changes in sample behaviour that can be introduced by adding silica nanoparticles. As a next step we wanted to gain more microscopic insight and performed small angle neutron scattering experiments on our samples. We now want to present first results of these recent experiments on poly(butylene oxide) silica nanocomposites and show what we leared about the change in chain conformation introduced by the nanoparticles.

CPP 54.85 Thu 15:00 P2 **Upconversion Quantum Yields of Rare Earth Doped Nanoparticles dependent on dopant concentration** – •MARTIN KAISER¹, WÜRTH CHRISTIAN¹, HYPÄNNEN IKO², EMILIA PALO², SOUKKA TERO², and RESCH-GENGER UTE¹ – ¹BAM Bundesanstalt für Material- forschung und -prüfung, Richard-Willstätter-Str. 11, 12489 Berlin – ²Department of Biotechnology, University of Turku, Tykistökatu 6A, FI-20520 Turku, Finland

Hexagonal β -NaYF₄ doped with Er^{3+} and Yb^{3+} is currently the most efficient up-conversion (UC) or also called 'Anti-Stokes' phosphor which converts near-infrared (NIR) to green light. The design of efficient nm-sized UC particles requires reliable spectroscopic tools for the characterization of the signal-relevant optical properties of these materials like the up-conversion quantum yield (UC QY), which equals the ratio of high energy photons emitted to low energy photons absorbed. We present here a custom-designed integration sphere setup equipped with a high-power 980 nm-laser diode for spectrally resolved and power density-dependent measurements of UC QY. Power dependent UC QY and luminecence lifetime measurements of nm-sized β -NaYF₄:Er³⁺, Yb³⁺ with different dopant concentrations will be discussed.