Chemical and Polymer Physics Division
Fachverband Chemische Physik und Polymerphysik (CPP)

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Overview of Invited Talks and Sessions

(Lecture Rooms C130, C264 and C230; Poster A (H 2.OG))

Invited and Prize Talks

CPP 1.1	Mon	9:30–10:00	C 130	**Multiple glassy states and mechanics of soft colloids** — •Dimitris Vlassopoulos
CPP 1.5	Mon	11:00–11:30	C 130	**Thermo-Rheological Properties of Fiber Networks** — •Christian Friedrich, Yasmin Korth, Martin Kühne
CPP 2.1	Mon	14:00–14:30	C 130	**Shear induced structures in lamellar systems: from layers to onions to onions and layers** — •Walter Richtering
CPP 2.5	Mon	15:30–16:00	C 130	**Structure and dynamics of magnetorheological fluids** — •Claus Gabriel, Hans Martin Laun
CPP 16.1	Tue	9:30–10:00	C 130	**Imaging the flow of concentrated colloidal suspensions** — •Wilson Poon, Lucio Isa, Rut Besseling
CPP 16.2	Tue	10:00–10:30	C 130	**Stochastic thermodynamics of driven soft matter** — •Udo Seifert
CPP 16.3	Tue	10:30–11:00	C 130	**Spatial cooperativity in soft glassy flows** — •Lydéric Bocquet
CPP 17.1	Tue	14:00–14:30	C 130	**Soft Matter under Flow** — •Gerhard Gompper
CPP 17.2	Tue	14:30–15:00	C 130	**Viscoelasticity of gels** — •Annette Zippelius, Peter Müller
CPP 18.1	Tue	16:30–17:00	C 130	**Bifurcations in complex fluids** — •Ingo Rehberg, DFG-Forschergruppe 608
CPP 26.1	Wed	14:00–14:30	C 264	**The Capillary Rise of Liquids in Nanopores** — •Patrick Huber
CPP 28.1	Thu	16:30–17:00	C 264	**Mixing in passive and active microflows** — •Arthur V. Straube
CPP 35.1	Fri	10:30–11:00	C 130	**Nonlinear light scattering: Bridging the gap between surface science & soft matter** — •Sylvie Roke

Invited talks of the joint symposium SYMP

See SYMP for the full program of the Symposium.

SYMP 1.1	Thu	9:30–10:00	H 0105	**Hydrodynamic cooperativity in active fluids** — •Ignacio Pagonabarraga
SYMP 1.2	Thu	10:00–10:30	H 0105	**Hydrodynamic Effects on Molecular Motion** — •Raymond Kapral
SYMP 1.5	Thu	11:15–11:45	H 0105	**Proton transport through water-filled narrow pores** — •Christoph Dellago
SYMP 1.6	Thu	11:45–12:15	H 0105	**Role of fluctuations in the selectivity mechanism for the KcsA potassium channel** — •Michael E. Paulaitis, Dilip Asthagiri, Lawrence R. Pratt
SYMP 2.1	Thu	14:00–14:30	H 0105	**DNA mechanics and dynamics** — •Richard Lavery
SYMP 2.2	Thu	14:30–15:00	H 0105	**Charge mobility of discotic mesophases of polyaromatic hydrocarbons: a multiscale quantum/classical study** — •Denis Andrienko
SYMP 2.4	Thu	15:30–16:00	H 0105	**Simulation of coarse-grained membrane models** — •Marcus Müller
SYMP 2.5	Thu	16:00–16:30	H 0105	**Fragments of a computational cell: mesoscopic simulations of soft matter** — •Julian C. Shillcock

Invited talks of the joint symposium SYSA

See SYSA for the full program of the Symposium.

SYSA 1.1	Tue	9:30–10:00	H 0105	**Level alignment at metal/organic interfaces** — •Fernando Flores
SYSA 2.1	Tue	10:45–11:15	H 0105	**Organic film growth and organic-metal interfaces** — •Norbert Koch
SYSA 2.5	Tue	12:00–12:30	H 0105	**Molecular n-doping of organic semiconductors** — •Antoine Kahn, Calvin Chan
SYSA 3.1	Tue	14:30–15:00	H 2013	**Charge transport and contact effects in organic semiconductors** — •Alberto Salleo, Leslie Jimison, Jonathan Rivnay, Ludwig Goris, Michael Toney
SYSA 4.1	Tue	16:30–17:00	H 2013	**Polymer electronics - Charge transport at organic-organic heterointerfaces** — •Henning Sirringhaus
SYSA 6.1	Wed	14:30–15:00	H 2013	**Organometallic Nanojunctions Probed by Different Chemistries: Thermo-, Photo, and Mechanochemistry** — •I. Stich, M. Konopka, R. Turansky, J. Reichert, N. L. Doltsinis, H. Fuchs, D. Marx
SYSA 7.1	Wed	17:45–18:15	H 2013	**Designing the nanostructure of the organic polymer - metal interface** — •Stephan V. Roth
SYSA 8.1	Thu	17:00–17:30	H 2032	**Nanostructure and transport in regioregular polythiophenes and their block copolymers** — Rui Zhang, Bo Li, Jessica R. Cooper, Mihaela Iovu, Genevevie Sauve, David N. Lambeth, Detlef-M. Smilgies, Richard D. McCullough, •Tomasz Kowalewski

Invited talks of the joint symposium SYSM

See SYSM for the full program of the Symposium.

SYSM 1.1	Tue	14:00–14:30	H 0105	**Two-Focus Fluorescence Correlation Spectroscopy: A versatile tool for precise measurements of molecular diffusion** — •Jörg Enderlein, Anastasia Loman, Thomas Dertinger, Iris von der Hocht, Bernd Müller, Victor Pacheco, Konstantin Komolov, Karl-Wilhelm Koch, Ingo Gregor
SYSM 1.2	Tue	14:30–15:00	H 0105	**Tracking and Manipulating Single Molecule Diffusion in Liquids** — •Frank Cichos
SYSM 1.3	Tue	15:00–15:30	H 0105	**Single Molecule Studies on Myosin Motors** — •Claudia Veigel
SYSM 1.4	Tue	16:00–16:30	H 0105	**Real-time observation of bacteriophage T4 gp41 helicase reveals unwinding mechanism** — M. Manosa, T. Lionnet, M. M. Spiering, S. J. Benkovic, D. Bensimon, •V. Croquette
SYSM 1.5	Tue	16:30–17:00	H 0105	**From valleys to ridges: Exploring the dynamic energy landscape of single membrane proteins** — •Daniel Müller

Sessions

CPP 1.1–1.8	Mon	9:30–12:15	C 130	**DRG-DPG SYMPOSIUM Rheology I**
CPP 2.1–2.8	Mon	14:00–16:45	C 130	**DRG-DPG SYMPOSIUM Rheology II**
CPP 3.1–3.9	Mon	10:00–12:30	C 264	**Liquid Crystals and Polar Fluids**
CPP 4.1–4.8	Mon	14:30–16:45	C 264	**Colloidal Fluids**
CPP 5.1–5.9	Mon	10:00–12:30	C 230	**New Materials**
CPP 6.1–6.10	Mon	14:00–16:45	C 230	**Electronic+Optical Properties**
CPP 7.1–7.26	Mon	16:45–19:00	Poster A	**POSTERS Rheology**
CPP 8.1–8.20	Mon	16:45–19:00	Poster A	**POSTERS Dynamics and Diffusion**
CPP 9.1–9.26	Mon	16:45–19:00	Poster A	**POSTERS Single Molecules, Biopolymers, Membranes**
CPP 10.1–10.12	Mon	16:45–19:00	Poster A	**POSTERS New Materials, Organic Semiconductors**
CPP 11.1–11.8	Tue	10:00–12:15	C 264	**DRG-DPG SYMPOSIUM Rheology III**
CPP 12.1–12.6	Tue	11:00–12:30	C 230	**Confined Fluids**
CPP 13.1–13.14	Tue	15:00–18:45	C 264	**Colloidal and Nanoparticles**
CPP 14.1–14.6	Tue	15:00–16:30	C 230	**Membranes**
CPP 15.1–15.8	Tue	17:00–19:00	C 230	**Single Molecules**
CPP 16.1–16.8	Tue	9:30–12:30	C 130	**SYMPOSIUM Driven Soft Matter I**
CPP 17.1–17.6	Tue	14:00–16:00	C 130	**SYMPOSIUM Driven Soft Matter II**
CPP 18.1–18.7	Tue	16:30–18:30	C 130	**SYMPOSIUM Driven Soft Matter III**
CPP 19.1–19.8	Wed	14:00–16:00	C 130	**SYMPOSIUM Driven Soft Matter IV**

CPP 20.1–20.37	Wed	16:00–18:30	Poster A	**POSTERS Driven Soft Matter**
CPP 21.1–21.29	Wed	16:00–18:30	Poster A	**POSTERS Colloids, Nanoparticles and Aggregates**
CPP 22.1–22.24	Wed	16:00–18:30	Poster A	**POSTERS Micro- and Nanofluidics**
CPP 23	Wed	14:00–17:15	C 243	**Single Molecules (joint session BP/CPP)**
CPP 24	Wed	17:30–19:30	PC 203	**Semiflexible Polymers and Networks (joint session BP/CPP)**
CPP 25.1–25.6	Wed	14:30–16:00	C 230	**Polyelectrolytes**
CPP 26.1–26.7	Wed	14:00–16:00	C 264	**Micro and Nano Fluidics I: Liquids at structured materials**
CPP 27.1–27.9	Thu	14:00–16:15	C 264	**Micro and Nano Fluidics II: Slipping + soft objects in flow**
CPP 28.1–28.7	Thu	16:30–18:30	C 264	**Micro and Nano Fluidics III: Migration and flow**
CPP 29.1–29.12	Thu	9:30–12:45	C 130	**Polymerphysics I**
CPP 30.1–30.11	Thu	14:00–17:00	C 130	**Polymerphysics II**
CPP 31.1–31.6	Thu	9:30–11:00	C 264	**Thin Films**
CPP 32.1–32.5	Thu	11:15–12:30	C 264	**Colloid Dynamics**
CPP 33.1–33.7	Thu	15:00–16:45	C 230	**Molecular Structure**
CPP 34.1–34.58	Thu	17:00–19:30	Poster A	**POSTERS Polymerphysics**
CPP 35.1–35.7	Fri	10:30–12:30	C 130	**Interfaces**
CPP 36.1–36.9	Fri	10:30–12:45	C 264	**Biopolymers and Biological Systems**
CPP 37.1–37.8	Fri	10:30–12:30	C 230	**Molecular Dynamics**

Annual General Meeting of the Chemical and Polymer Physics Division

Mittwoch 18:30–19:30 Raum C 264

- Begrüßung und Bericht
- Tagungsnachlese
- Stichwortkatalog, eingeladene Sprecher und Symposien für 2009
- Verschiedenes

CPP 1: DRG-DPG SYMPOSIUM Rheology I

Time: Monday 9:30–12:15 Location: C 130

Invited Talk CPP 1.1 Mon 9:30 C 130

Multiple glassy states and mechanics of soft colloids — •Dimitris Vlassopoulos — FORTH and Univ. of Crete, Hereklion, Greece

Colloidal glass transition and its manipulation represent a topic of ever increasing scientific interest. Hard sphere colloids and more recently their mixtures with linear non-adsorbing polymers has been the systems most frequently studied. Perhaps the most interesting recent observation is the melting of a (repulsive) glass upon adding polymer depletant, and the transition into a re-entrant different (attractive) glass upon further increasing the strength of depletion. Here, we are interested in changing the pair interaction potential. In particular, we use colloidal star polymers, a model system with ultrasoft interactions. We study their vitrification under different conditions: temperature-dependent solvent, mixtures with linear chains and binary asymmetric star mixtures. We find a wide range of glass transitions, which we try to rationalize by invoking the cage picture and with support from mode coupling theory. We demonstrate to power of rheology to act both as a sensitive detection tool and as a means of inducing structural changes. Concerning the former, the data are summarized in terms of kinetic state diagrams. For the latter, we present the phenomenology of yielding of the star glasses and suggest possible connections to aging. The main outcome is, we believe, an enhanced ability to tailor the flow of glassy suspensions of soft particles. In collaboration with E. Stiakakis, G. Petekidis, C. N .Likos, C. Mayer, E. Zaccarelli, F. Sciortino, M. Helgeson, N. J. Wagner, H. Iatrou, N. Hadjichristidis.

CPP 1.2 Mon 10:00 C 130

Shear stresses of colloidal dispersions at the glass transition in equilibrium and in flow — Jerome Crassous[1], Miriam Siebenbürger[1], •Matthias Ballauff[1], Markus Drechsler[2], David Hajnal[3], Oliver Henrich[3], and Matthias Fuchs[3] — [1]Physikalische Chemie I, Universität Bayreuth, 95440 Bayreuth — [2]Makromolekulare Chemie II, Universität Bayreuth, 95440 Bayreuth — [3]Fachbereich Physik, Universität Konstanz, 78457 Konstanz

We consider a model dense colloidal dispersion at the glass transition, and investigate the connection between equilibrium stress fluctuations, seen in linear shear moduli, and the shear stresses under strong flow conditions far from equilibrium, viz. flow curves for finite shear rates. To this purpose thermosensitive core-shell particles consisting of a polystyrene core and a crosslinked poly(N-isopropylacrylamide)(PNIPAM) shell were synthesized. Data over an extended range in shear rates and frequencies are compared to theoretical results from integrations through transients and mode coupling approaches. The connection between non-linear rheology and glass transition is clarified. While the theoretical models semi-quantitatively fit the data taken in fluid states and the predominant elastic response of glass, a yet unaccounted dissipative mechanism is identified in glassy states.

CPP 1.3 Mon 10:15 C 130

Optical Microrheology applied to different Soft Matter Systems and compared to Classical Bulk Rheology — Anna Kozina[1], •Pedro Diaz-Leyva[1,2], Christian Friedrich[2,3], and Eckhard Bartsch[1,2] — [1]Institut für Makromolekulare Chemie, Universität Freiburg, Germany — [2]Institut für Physikalische Chemie, Universität Freiburg, Germany — [3]Freiburger Materialforschungszentrum, Universität Freiburg, Germany

Over years it has been very important to understand how the macroscopic properties of soft materials are depending on their microstructure. Concerning mechanical properties such as viscosity and/or elasticity, they have been measured typically by Classical Bulk Rheology (CBR) which works at a macroscopic level. In this work we discuss a technique known as Optical Microrheology (OMR) which characterize the same mechanical properties, but using a microscopic approach. This method exhibits two important features: First, OMR is a non-invasive and non-destructive technique. Second, OMR is capable to reach high frequencies. We explore the capabilities of OMR studying several systems showing a clear viscoelastic behavior, but appreciably different in terms of microstructure. We use Dynamic Light Scattering in order to measure the dynamics exhibited in the materials, and consequently we can get the rheological moduli $G'(\omega)$ and $G''(\omega)$. We compare our results with those obtained by CBR applied on the same systems. Finally we discuss the possible origin of discrepancies between the results obtained with OMR and CBR respectively.

CPP 1.4 Mon 10:30 C 130

Macro- and micro- rheology of a soft colloidal suspension with tunable glassines — •Dirk van den Ende, Eko Purnomo, Siva Vanapalli, and Frieder Mugele — Physics of Complex Fluids, University of Twente, The Netherlands

We studied both the macro- and micro- rheology of soft thermosensitive microgel suspensions that can be tuned continuously and reversibly between the glassy state at low and the liquid state at high temperature. In the glassy state, the rheological properties (G', G'', and J) of the suspensions depend strongly on their age [1]. They can be described quantitatively by the soft glassy rheology (SGR) model. The underlying mechanism for the aging is the increase of the structural relaxation time τ_s as the system ages. However, τ_s is experimentally inaccessible by small amplitude frequency sweep experiments. Therefore we tested the recently introduced strain rate frequency superposition (SRFS) technique. The evolution of $\tau_s(t)$ as determined with SRFS is consistent with the predictions of the SGR model based on the linear measurements. Hence, no macroscopic inhomogeneities occur in the sample. The relaxation time τ_s is also determined from the mean square displacement (MSD) of probe particles, embedded in the system, using a Confocal Scanning Laser Microscope. This technique provides not only the MSD values but also the displacement distributions, which are indicative for heterogeneity of the suspension.

[1] E.H. Purnomo, D. van den Ende, J. Mellema, and F. Mugele, Europhys. Lett. 76, 74 (2006).

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Invited Talk CPP 1.5 Mon 11:00 C 130

Thermo-Rheological Properties of Fiber Networks — •Christian Friedrich, Yasmin Korth, and Martin Kühne — Freiburg Materials Reserch Center (FMF), University Freiburg, Stefan-Meier-Str. 21, 79104 Freiburg i. Brsg., Germany

The dispersion of fibers (nm-thick and mikrom-long fibers) in matrices, without bundling or aggregation, is of crucial importance for the beneficial combination of fiber properties with those of matrix fluids. For multi-walled carbon nanotubes (mwCNT) dispersed in ionic liquids (IL), we developed a technique enabling good dispersion of these fibers in the matrix fluid. Using different analytical tools (rheology, centrifugation) we were able to discriminate gel-forming varieties of CNT from those who do not gel. For those who give gels, we identified the concentration regions in which networking is dominant. While the temperature dependence of fibers modulus is crucial for the understanding of gels modulus temperature dependence, the module scaling with concentration depends on the fibers persistence length. In the last part of our presentation we deal with possibilities of its determination on the basis of morphological as well as rheological techniques. Although mwCNT-dispersions are highly polydisperse in persistence, an estimation of gels plateau modulus with the MacKintosh-Model is possible.

CPP 1.6 Mon 11:30 C 130

Nonlinear rheology of a glassy solution of semiflexible polymers — •Jens Glaser[1], Christian Hubert[1], and Klaus Kroy[1,2] — [1]Inst. f. Theoretische Physik, Universität Leipzig, PF 100920, 04009 Leipzig — [2]Hahn-Meitner-Institut, Glienicker Str. 100, 14109 Berlin,

Recent experimental studies on purified solutions of the semiflexible biopolymer F-actin show a pronounced transition from shear softening to shear stiffening behavior as a function of different physiological parameters. The results suggest a surprising invariance of the rheology of the F-actin solution with respect to the choice of the control parameter. We rationalize this property in terms of the recently introduced glassy wormlike chain (GWLC) model, where the nonlinear response is traced back to a strong stretching of the relaxation spectrum of an ordinary wormlike chain, quantified by a single stretching parameter which is the height of free energy barriers slowing down the relaxation of the polymer. Predictions for the maximum strain of the network, apparent power-law stiffening exponents and analytical results are given. The relation of the stretching parameter to changes in the physiological parameters is discussed.

[1] Semmrich C, Storz T, Glaser J, Merkel R, Bausch, A. R, Kroy K, Proc Natl Acad Sci USA, In Press (2007)
[2] arXiv:0705.0490, arXiv:0711:2427

CPP 1.7 Mon 11:45 C 130

Dynamics of branch point withdrawal for pom-pom melt — •Manfred H. Wagner and Víctor H. Rolón-Garrido — Polymertechnik/Polymerphysik, TU Berlin

According to tube model ideas, chain stretch at deformation rates below the inverse Rouse time of the chain, is only possible for polymer topologies with two or more branch points. The basic topologies which embody this idea are the H-molecule with two side chains, and the pom-pom molecule with q>2 side chains at each end of the backbone. According to the pom-pom hypothesis, maximum chain stretch of the backbone is limited by branch point withdrawal, i.e. the side chains are drawn into the tube of the backbone as soon as the relative tension in the backbone reaches a value of q. This so far unproven hypothesis can now be tested by considering recent elongational experiments by Nielsen et al. [Macromolecules 39, (2006) 8844] on a nearly monodisperse polystyrene pom-pom melt with q=2.5. The material strain measure determined from the experiments is found to be consistent with a constant maximum stretch, independent of the elongation rate, which is, however, significantly larger than q. To achieve quantitative agreement between experiment and modelling, (1) dynamic dilution of the backbone, which increases the tube diameter of the backbone and reduces equilibrium tension, (2) finite extensibility effects, (3) transition from chain stretch to tube squeeze at lower strain rates, and (4) the dynamics of branch point withdrawal need to be considered. Integrating all of these features in a stretch evolution equation with multiple time scales, the fundamental pom-pom hypothesis is confirmed.

CPP 1.8 Mon 12:00 C 130

Deformation of Inclusions and Lamellae in Melt Extension of Blends of Polystyrene and a Styrene-Butadiene Block Copolymer — •Ulrich Alexander Handge[1], Matthias Buschnakowski[2], and Goerg Hannes Michler[2] — [1]Polymer Physics, Department of Materials, ETH Zürich, CH-8093 Zürich — [2]Department of Physics, Martin-Luther-University Halle-Wittenberg, D-06099 Halle/S.

The end-use properties of block copolymers depend on their composition and microstructure. Blending block copolymers with a homopolymer can lead to materials with specific end-use properties and reasonable costs. Here we studied the melt rheology of blends of a styrene-butadiene block copolymer (LN3) and polystyrene (PS 158K, BASF AG). Three blends of LN3 and PS 158K were prepared with $\Phi = 20, 40$ and $80\,$wt.% PS 158K. Linear viscoelastic shear oscillations and melt elongation tests were performed at 170 °C. The deformation of the blend morphology with strain was investigated using transmission electron microscopy. PS 158K and LN3 formed a two-phase blend with a PS 158K or a LN3 matrix. The block copolymer chains of LN3 were arranged in a lamellar phase. Our rheological experiments revealed that the complex modulus, the extensional viscosity and the recoverable deformation of the PS 158K/LN3 blends mainly resulted from a mixing effect of the properties of PS 158K and LN3. In melt elongation, the inclusions in the PS 158K resp. LN3 matrix were deformed into an elongated shape, and the alignment of the lamellae of the LN3 block copolymer matrix for $\Phi = 20\%$ and 40% increased with strain.

CPP 2: DRG-DPG SYMPOSIUM Rheology II

Time: Monday 14:00–16:45 Location: C 130

Invited Talk CPP 2.1 Mon 14:00 C 130

Shear induced structures in lamellar systems: from layers to onions to onions and layers — •Walter Richtering — Physikalische Chemie RWTH Aachen

The size growth of multilamellar vesicles (MLV, *Onions*) of a nonionic surfactant system composed of 40wt% C10E3 in D2O was investigated by shear quench experiments, i.e. when the shear rate is reduced. The structural changes were monitored with the help of Rheo-Small Angle Neutron Scattering (SANS), Rheo-Small Angle Light Scattering (SALS) and optical microscopy. Two different pathways were observed. A continuous growth of vesicle size was found when the shear rate was reduced within the stability region of monodisperse MLV (Region III). However, a discontinuous pathway was observed for shear quenches from the monodisperse into the polydisperse MLV region (Region II). A shear quench into the high shear rate part of region II leads to a formation of lamellar domains which themselves follow the pathway of MLV formation in coexistence to the initial MLV structure. A shear quench into the low shear rate part region II leads to the formation of lamellar macro-domains, which display a tumbling behaviour and grow with time until the MLV formation process starts.

CPP 2.2 Mon 14:30 C 130

Linear to branched micelles transition: a rheometry and diffusive wave spectroscopy (DWS) study — •Norbert Willenbacher and Claude Oelschlager — Institut für Mechanische Verfahrenstechnik und Mechanik, Universität Karlsruhe, 76128 Karlsruhe

The shear modulus G* of aqueous wormlike micellar solutions of cetylpyridinium chloride and the strongly binding counterion sodium salicylate has been measured as a function of temperature, surfactant and salt concentration by using DWS based tracer microrheology as well as mechanical techniques including rotational rheometry, oscillatory squeeze flow and torsional resonance. Good agreement between both approaches is found in the frequency range from 0.1 to 100.000 rad/s. Upon increasing the salt concentration, at fixed surfactant concentration, the solutions exhibit two maxima of the zero shear viscosity. The first one is attributed to a transition from linear to branched micelles. From G' and G" at low and intermediate frequencies we obtain the mesh size of the entanglement network and the scission energy E_0. The latter passes through a maximum upon the transition from linear to branched micelles. In the frequency range above 10.000 rad/s a omegaˆ3/4 scaling is observed for the loss modulus G" as expected for semiflexible objects. The persistence length lp is determined from the moduli in this frequency range. For the linear micelles lp decreases with increasing salt content as expected, but increases significantly upon the transition to the branched structure. The structural changes at the second viscosity maximum are not resolved so far, we will discuss the variation of lp and E_0 in this concentration range.

CPP 2.3 Mon 14:45 C 130

Thermorheological behaviour of polyethylene in dependence on molecular structure — •Ute Kessner, Joachim Kaschta, and Helmut Münstedt — Lehrstuhl für Polymerwerkstoffe, Universität Erlangen-Nürnberg, Martensstrasse 7, D-91058 Erlangen

The thermorheological behaviour of polyethylenes is strongly influenced by their molecular structure. In the literature, they are reported to be thermorheologically simple or complex. A clear distinction is not made, however, between the behaviour in the linear and nonlinear ranges of deformation. This paper systematically addresses this topic by presenting the activation energies of various polyethylenes determined in the linear and nonlinear range. Thermorheological simplicity was found for the linear ethylene homopolymers (HDPE) under all applied conditions. The LDPE investigated showed a thermorheologically simple behaviour in the linear range, but a thermorheologically complex behaviour in the nonlinear regime. The activation energy decreases with increasing stresses and approaches the value of the HDPE. Long-chain branched polyethylenes polymerised with metallocene catalysts do exhibit a thermorheological complexity in the linear and nonlinear range of deformation.

Various branching topographies lead to distinct differences in the thermorheological behaviour and result in different flow activation energies. Using these results it will be shown in which way the thermorheological behaviour of different polyethylenes can be used to get an insight into their branching architecture.

CPP 2.4 Mon 15:00 C 130

Non-equilibrium phenomena in sheared bottlebrush polymer solutions — •Silke Rathgeber[1], Hyung-il Lee[2], Krzysztof

Matyjaszewski[2], and Emanuela Di Cola[3] — [1]Max-Planck Institut für Polymerforschung, Polymer Physik, 55128 Mainz, Germany. — [2]Carnegie Mellon University, Department of Chemistry, Pittsburgh, Pennsylvania 15213, USA. — [3]European Synchrotron Radiation Facility, 38043 Grenoble Cedex, France.

Time-resolved small-angle x-ray scattering (SAXS) experiments were carried out on concentrated solutions of bottlebrush polymers exposed to an external shear flow.[1] The rheological response of the sample were recorded online. We followed the complex structural changes occurring in a, perpendicular to the flow direction pre-aligned sample during its reorientation into the flow direction. In the stress-controlled rheometer mode the reorientation is accompanied by a shear thinning process with a reduction in viscosity of two orders of magnitudes. In the strain controlled mode the rheological response of the bottlebrush polymer solution to the rotational shear shows oscillations with changes in viscosity of almost two orders of magnitude. The SAXS data reveal that this oscillatory response is due to a reentrant phase transition between a shear molten phase and a line hexatic phase. It is not due to shear induced phase separation leading to shear band formation. The insitu-rheological SAXS measurements allow a detailed description of the structural changes occurring in the sample during structural built-up and break-down. [1] S. Rathgeber et al., Macromolecules 40, 7680 (2007).

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Invited Talk CPP 2.5 Mon 15:30 C 130

Structure and dynamics of magnetorheological fluids

•Claus Gabriel and Hans Martin Laun — BASF AG, Ludwigshafen am Rhein, Germany

This presentation intends to give an overview of the rheological properties of magnetorheological fluids (MRF). MRF are used as force- or torque transmitting fluids in electronically controllable dampers and clutches.

Some fundamental structure-property relationships related to dynamic frequency sweeps will be discussed. The linear regime of deformation is the broader the higher the applied magnetic field is. In this regime MRF behave predominantly as elastic bodies and the dynamic moduli are essentially independent of the magnitude of the applied magnetic field. Outside the linear regime the internal structure of MRF breaks down. The MRF properties derived from dynamic experiments will be compared with those obtained from steady-shear experiments. Moreover, the dependence of rheological properties upon the composition of MRF will also be discussed.

An important precondition for a reliable determination of rheological properties of MRF is the homogeneity of the flux density in the shear gap. Depending on the type of MRF formulation a non-homogeneous flux density distribution may cause a significant segregation of the magnetisable particles within the MRF. An improved measurement design is proposed with which these segregation phenomena can be reduced to a minimum.

CPP 2.6 Mon 16:00 C 130

Shear-induced structures and viscoelastic effects in ferrofluids from nonequilibrium simulations

•Patrick Ilg — ETH Zürich, Polymer Physics, 8093 Zürich, Switzerland

Ferrofluids – suspensions of nano-sized magnetic colloids – have attracted considerable attention due to the possibility of manipulating their flow behaviour by external magnetic fields [1]. From extensive, nonequilibrium Brownian dynamics simulations of realistic model-ferrofluids [2], we obtain the flow- and field-dependence of viscosity coefficients and normal stress differences in planar shear flow. We also observe strong shear-induced structural changes and discuss their relation to rheological properties.

[1] M. Kröger, P. Ilg, S. Hess, J. Phys. Condens. Matter 14 (2003) S1503. [2] P. Ilg, E. Coquelle, S. Hess, J. Phys. Condens. Matter 18 (2006) S2757.

CPP 2.7 Mon 16:15 C 130

Shear-induced structural changes in nanoparticle aggregates: a time-resolved x-ray microscopy study

•Günter K. Auernhammer[1], Jinyu Zhao[1], Doris Vollmer[1], Markus Weigand[2], and Kai Fauth[2] — [1]MPI Polymerforschung, Mainz, Germany — [2]MPI Metallforschung, Stuttgart, Germany

X-ray microscopy is an imaging technique which allows for a spatial resolution below 35 nm. Can it also be used to investigate shear-induced structural dynamics? When studying response to mechanical (shear) stimuli, the challenge lies in applying the stimuli with precision comparable to spatial resolution. We accomplished this by inserting a piezo actuator-driven shear cell into the focal plane of the x-ray microscope. We demonstrate the possibilities of this novel device by an investigation of shear-induced reorganization of 50 nm sized magnetite particles embedded in a polymer melt. As x-ray microscopy proves suitable for studying structural change, new prospects open up in physics at small length scales.

CPP 2.8 Mon 16:30 C 130

Transient behavior of thioxtropic flow studied by smoothed particle hydrodynamics

•Andreas Wonisch, Torsten Kraft, Michael Moseler, and Hermann Riedel — Fraunhofer Institute for Mechanics of Materials, Woehlerstr. 11, 79108 Freiburg

Many complex fluids exhibit thixotropic behavior: Under shear viscosity gradually decreases with time, followed by a gradual increase if the shearing is stopped. This time and shear rate dependent rheological behavior can be linked to the breakdown and buildup of structure in the fluid. Here, we employ smoothed particle hydrodynamics (SPH) - a meshless, particle-based Lagrangian simulation method - to study thixotropic fluid flow in three dimensions. In our model the structure of each SPH particle is characterized by a scalar structure parameter which is related to viscosity. Thixotropy is introduced by specifying a constitutive equation for the time derivative of the structure parameter. Our numerical method is verified by several simple test cases which are in close agreement with analytical solutions. We then investigate the transient behavior of thixotropic flow at low Reynolds numbers numbers for an industrial impregnation and removal process which involves both solid wall and free surface boundary conditions. It is demonstrated that different wetting conditions (characterized by the contact angle) have a profound impact on the transient flow behavior.

CPP 3: Liquid Crystals and Polar Fluids

Time: Monday 10:00–12:30 Location: C 264

CPP 3.1 Mon 10:00 C 264

Controlling Size and Arrangement of Smectic Focal Conic Domains

Wei Guo, Yasutaka Iwashita, Stephan Herminghaus, and •Christian Bahr — MPI for Dynamics and Self-Organization, Bunsenstr. 10, 37073 Göttingen

Defect structures in liquid crystals are of interest from both fundamental and applied viewpoints. For instance, topological defects can lead to the self-assembly of two-dimensional nematic colloidal crystals [1].

The present study is concerned with defect structures in smectic liquid crystals, so-called focal conic domains, which consist of a complex arrangement of curved equidistant molecular smectic layers which are wrapped around two singular lines. We describe a method to generate almost arbitrary two-dimensional arrangements of focal conic domains in smectic films. The method is based on the patterning of a silicon substrate with a thin gold layer that is evaporated through a lithographic mask. In smectic films on such substrates, the generation of focal conic domains is confined to the masked areas so that both the size of individual domains and the overall arrangement of many domains can be controlled. We study the generated structures on linearly and circularly patterned substrates by optical, fluorescence confocal, and scanning force microscopy [2], and discuss the use of focal conic domains as matrices for self-assembling microsystems.

[1] I. Muševič, M. Škarabot, U. Tkalec, M. Ravnik, and S. Žumer, Science **313**, 954 (2006).

[2] V. Designolle, S. Herminghaus, T. Pfohl, and Ch. Bahr, Langmuir **22**, 363 (2006).

CPP 3.2 Mon 10:15 C 264

Dielectric relaxation behavior of nematic liquid crystals dispersed in a ferroelectric polymer

•Lakshmi Meena Ganesan,

Axel Mellinger, Peter Frübing, Werner Werges, and Reimund Gerhard — Department of Physics, University of Potsdam, Am Neuen Palais 10, 14469 Potsdam, Germany

Polymer-dispersed liquid crystals (PDLCs) are a class of materials that consists of micrometer-sized liquid-crystal (LC) droplets embedded in a polymer matrix. Here, ferroelectric poly(vinylidene fluoride-co-trifluoroethylene) (P(VDF-TrFE)) (65/35 mol%) was used as the matrix polymer, since the electric field generated by the piezo- or pyro-electric effect of the matrix material could potentially be used to switch the director of the LC. In the absence of an external electric field, the nematic molecules at the interface are oriented spontaneously at a specific angle. The phenomenon of orienting the LC molecules at an interface is called anchoring. By application of an electric field, the nematic molecules can be oriented along the field direction. If the perpendicular refractive index of the liquid crystal matches the refractive index of the polymer matrix, the optical transmission of the PDLC film increases. The anchoring effect can be studied using dielectric relaxation spectroscopy. Two dispersion regions are observed in the dielectric spectra of the pure P(VDF-TrFE) film. They are related to the glass transition and to a charge-carrier relaxation. In PDLC films containing 10 wt% of LC, an additional, bias-field-dependent relaxation peak is found that can be attributed to the motion of LC molecules.

CPP 3.3 Mon 10:30 C 264

Charge transport in discotic liquid crystals: effect of temperature and mesophase symmetry — •Denis Andrienko[1], Valentina Marcon[1], James Kirkpatrick[2], Jenny Nelson[2], and Kurt Kremer[1] — [1]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany — [2]Department of Physics, Imperial College London, Prince Consort Road, London SW7 2BW, United Kingdom

Charge mobilities of several derivatives of discotic liquid crystals have been determined by combining three methods into one scheme: (i) quantum chemical methods for the calculation of molecular electronic structures, reorganization energies, and energetic disorder (ii) molecular dynamics for simulation of the relative positions and orientations of molecules in a columnar mesophase, and (iii) kinetic Monte Carlo simulations and Master Equation approach to simulate charge transport. Applying this scheme to differently substituted hexabenzocoronene derivatives we reproduce the trends and magnitudes of mobilities as measured by PR-TRMC and connect mobility directly to the microscopic morphology of the columns. It is shown that in the herringbone mesophase transfer integrals are higher, but so is energetic disorder. Analysing the temperature dependence of the distributions of charge transport parameters helps to establish a link between the system morphology/mesophase symmetry and charge mobility.

CPP 3.4 Mon 10:45 C 264

AFM Study of Surface-Induced Ordering in Liquid Crystals: Impurity Enhanced Ordering — •Doris Vollmer, Li-Juan Zhang, Michael Kappl, and Günter K. Auernhammer — MPI Polymerforschung, Mainz, Germany

We experimentally investigate surface-induced smectic-like ordering close to the isotropic-nematic phase transition of thermotropic liquid crystals of the n-CB series. Homeotropic alignment has been induced by depositing a lipid monolayer onto the silica surface. As shown by AFM the smectic like ordering alignment vanishes for temperatures a few degree above the phase transition.

Surprisingly, addition of a few percent of alkane to the liquid crystal enhances the presmectic ordering. In case of 4′-n-cyano-4-octylbiphenyl (8-CB) and octane we found maximal ordering at 4 percent of octane. This enhanced ordering depends on the length of the alkane, C_i, compared to length of the carbon tail of the liquid crystal, n-CB.

Probably impurity enhanced ordering is due to a combination of improved molecular packing and enhanced presmectic fluctuations, because addition of octane causes a decrease of the width of the nematic domain.

break

CPP 3.5 Mon 11:15 C 264

Gas-Liquid Phase Behavior of Dipolar Fluids — •Jörg Bartke and Reinhard Hentschke — Bergische Universität Wuppertal, Germany

The gas-isotropic liquid-nematic liquid phase behavior of the Stockmayer fluid is studied using Molecular Dynamics simulation over a wide range of dipole strengths. In our simulations we do not observe the disappearance of the isotropic gas-isotropic liquid coexistence at high dipole strength contrary to earlier findings based on Monte Carlo techniques. Even though the formation of reversible dipole chains strongly affects the location of the critical point, it does not lead to its disappearance. In addition to the simulation results we present a theory explaining the dependence of the gas-liquid critical point in the Stockmayer fluid on the dipole strength. The theory is based on the Flory-Huggins lattice description for polymer systems in conjunction with a transfer matrix model for isolated chains of reversibly assembled dipolar particles. We find that the shift of the critical point as function of dipole strength, also observed in computer simulation, strongly resembles the critical point shift as function of chain length in ordinary linear polymer systems. In particular the decrease of the critical density with increasing dipole strength is a consequence of the existence of reversible chains near criticality.

CPP 3.6 Mon 11:30 C 264

A new approach to the quantitative prediction of phase behaviour of quadrupolar fluids — •Bortolo M. Mognetti[1], Leonid Yelash[1], Peter Virnau[1], Wolfgang Paul[1], Kurt Binder[1], Marcus Mueller[2], and Luis G. MacDowell[3] — [1]Institut für Physik, Johannes Gutenberg–Universität, Staudinger Weg 7, 55099 Mainz, Germany — [2]Institut für Theoretische Physik, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [3]Dpto. de Quimica Fisica, Facultad de Cc. Qumicas, Universidad Complutense, 28040 Madrid, Spain

We investigate the phase behaviour of simple quadrupolar fluid and short alkane in quadrupolar solvents using Grand-Canonical Monte-Carlo simulations. First we carefully investigate Coarse-Grained models for solvents in which molecules are represented by single Lennard-Jones beads plus a quadrupolar moment. We show that these models perform well in predicting equilibria states, also if compared to more realistic (and computationally more expensive) atomistic models. Furthermore we investigate mixtures. Previous investigations have failed to predict the correct type of the binary phase behaviour without modifying the Lorentz-Berthelot mixing rules. We discuss how the new polar coarse grained model for the solvent improves the description of the mixture without any new phenomenological parameter. In order to elucidate the role of quadrupolar interactions we test also the Lorentz-Berthelot rules in some apolar mixtures.

CPP 3.7 Mon 11:45 C 264

Disappearance of ferromagnetic ordering in nanoconfined dipolar fluids — •Sabine H.L. Klapp[1,2] and R. Andreea Trasca[2] — [1]Institute of Theoretical Physics, TU Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Stranski-Laboratorium of Physical and Theoretical Chemistry, TU Berlin, Strasse des 17. Juni 135, 10623 Berlin, Germany

We present Monte-Carlo (MC) simulation results for dipolar fluid films under strongly coupled conditions where the bulk fluid [1] and films of mesoscopic thicknesses [2] display ferromagnetic ordering. We demonstrate that the ordering persists down to nanoscopic wall separations where the system consists of only four monolayers [3]. For smaller thicknesses we observe stripe-like defects (domains) and finally the breakdown of ferromagnetic ordering for systems close to the two-dimensional limit [3,4]. The results for the liquid phase are supported by MC calculations starting from quasi-crystalline soft-sphere configurations. Our findings are relevant for systems of magnetic colloids but also for the ordering behavior of thin solid-like magnetic films.

[1] D. Wei and G. N. Patey, Phys. Rev. Lett. **68**, 2043 (1992)
[2] S. H. L. Klapp and M. Schoen, J. Chem. Phys. **117**, 8050 (2002).
[3] R. A. Trasca and S. H. L. Klapp, in preparation.
[4] S. H. L. Klapp, Mol. Sim. **32**, 609 (2006).

CPP 3.8 Mon 12:00 C 264

Field–controlled layer formation in dipolar nanofilms — •Jelena Jordanovic[1] and Sabine H. L. Klapp[1,2] — [1]Stranski-Laboratorium, Technische Universität Berlin, Strasse des 17.Juni 135, 10623 Berlin — [2]Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstrasse 36, 10623 Berlin

Using molecular dynamic we investigate the equilibrium behaviour of a dipolar model fluid confined between two plane parallel walls, focussing on the influence of an additional homogeneous external electric or magnetic field. Structural properties are examined for field directions parallel and perpendicular with respect to the walls. Confinement alone induces already an in–plane orientation of the dipole moments [1] such that a parallel field easily polarizes the system. Moreover, the parallel field enhances the layer structure typical for confined fluids. Contrary to that a perpendicular field gives a new preferential direction which competes with the in–plane orientation observed without field. As a consequence very large fields are required to reach similar polarisation values as with parallel field. A particularly interesting effect is that high fields can generate a new layer in the system accompanied by structural rearrangements within the layer [2].

[1] V. A. Froltsov and S. H. L. Klapp, J. Chem. Phys. **124**, 134701 (2006); *ibid.* **126**, 114703 (2007).

[2] J. Jordanovic and S. H. L. Klapp, in preparation.

CPP 3.9 Mon 12:15 C 264

The impact of substrate-induced molecular orientation on dimerization in nanoreactors — •Randy Mathes and Martin Schoen — Stranski-Laboratorium, Technische Universität Berlin, Straße des 17. Juni 135, 10623 Berlin

We investigate the impact of substrate-induced molecular orientation on dimerization in nano-confinement. Equilibrium properties are examined for different substrates and bond lengths and are compared to a bulk system. The system under study is a reacting mixture of Lennard-Jones spheres and homonuclear Lennard-Jones diatomics. We use Gibbs ensemble Monte Carlo to examine the bulk phase diagram. Substrate and bond length effects in confinement are studied using grand canonical Monte Carlo. In bulk systems we generally find higher mole fractions of dimers at higher densities and lower temperatures. As expected we find higher mole fractions of dimers in non-orientating confinement compared to a bulk system at fixed chemical potential. We exploit the preferred in-plane orientation of dimers near walls to tune dimer rates in confinement by enforcing molecular orientation perpendicular to the walls. From adsorption calculations we also expect a strong dependence on bond length.

CPP 4: Colloidal Fluids

Time: Monday 14:30–16:45 Location: C 264

CPP 4.1 Mon 14:30 C 264

Lateral critical Casimir forces between colloids and chemically patterned substrates — •Florian Soyka, Christopher Hertlein, Laurent Helden, and Clemens Bechinger — Universität Stuttgart, 2. Physikalisches Institut, Pfaffenwaldring 57, 70569 Stuttgart

The confinement of critical fluctuations in binary liquid mixtures near the critical temperature leads to so-called critical Casimir forces. Depending on whether the adsorption preference of the confining walls for one of the two mixture's components is identical or not, the force between the walls is either attractive or repulsive. In our experiments, we investigate the interaction between colloidal particles and a flat wall in a critical water - 2,6 lutidine mixture. As substrates we used glass surfaces which were chemically patterned on a micron-scale leading to a laterally periodic modulation of the substrate's adsorption preference for water and lutidine. When approaching the critical temperature, we observe strong lateral forces acting on the colloidal particles above such substrates which are attributed to critical Casimir forces. Apart from the fundamental importance of such interactions, lateral critical Casimir forces may be also utilized to create ordered arrays of colloidal particles which are important e.g. in photonic applications.

CPP 4.2 Mon 14:45 C 264

Charged colloids at water interfaces — •Martin Oettel[1], Alvaro Dominguez[2], Derek Frydel[3], and Siegfried Dietrich[3] — [1]Mainz University, Germany — [2]University of Seville, Spain — [3]Max-Planck-Institute for Metals Research Stuttgart, Germany

The effective interactions of colloids trapped at fluid interfaces exhibit qualitatively new features when compared to the ones in colloidal bulk solutions. Electrostatic interactions which are exponentially screened in ionic solvents become longer–ranged and dipole–like at interfaces between water and a nonpolar medium (usually taken to be air or oil). We show (within Poisson-Boltzmann theory) that charge renormalization makes the effective electrostatic repulsion weakly dependent on the surface charge density on the water side and independent on the salt concentration in the high charge density limit [1]. This is in stark contrast to expectations from linear Debye-Hückel theory which has been used frequently to interpret experimental results. Furthermore, inhomogeneities of colloid surface charge or an anisotropic colloid shape affect the effective interaction only in subleading terms which asymptotically decay faster than the leading dipolar interaction which is isotropic in the interface plane [2].

[1] D. Frydel, S. Dietrich, and M. Oettel, Phys. Rev. Lett. **99**, 118302 (2007).

[2] A. Dominguez, D. Frydel, and M. Oettel, arxiv:0706.3977.

CPP 4.3 Mon 15:00 C 264

Computer Simulation of Colloidal Electrophoresis — •Burkhard Duenweg[1], Vladimir Lobaskin[1,2], Krishnan Seethalakshmy-Hariharan[1], and Christian Holm[1,3] — [1]Max-Planck-Institut fuer Polymerforschung Mainz — [2]Physik-Department, TU Muenchen — [3]FIAS Frankfurt

We study the motion of a charged colloidal sphere surrounded by solvent, counterions, and salt ions, under the influence of an external electric field. The ions are modeled as particles which interact dissipatively with a lattice Boltzmann background, such that hydrodynamic interactions are taken into account. Similarly, the colloid is modeled as a spherical array of such point particles. Finite concentration values are taken into account by simulating the system in a box with periodic boundary conditions. In terms of dimensionless reduced parameters, the results compare favorably with experimental data. As a complementary approach, we solve the electrokinetic equations by a finite element method.

CPP 4.4 Mon 15:15 C 264

Dynamical heterogeneities in attractive colloids — •Annalisa Fierro[1], Emanuela Del Gado[2], Antonio de Candia[1], and Antonio Coniglio[1] — [1]Dipartimento di Scienze Fisiche, Università di Napoli "Federico II", Italy — [2]Polymer Physics, ETH Zürich

Dynamical heterogeneities in glasses are explained in terms of the correlated motion of particles, but their possible connections to any structural feature are still unclear. We study dynamical heterogeneities in colloidal gelation, where a complex slowing down of the dynamics, directly related to the formation of persistent structures, is observed at different volume fractions. By means of Molecular Dynamics simulations of a model colloidal suspension, we have been able to show that, at low volume fractions, the dynamical heterogeneities are in fact dominated by the clusters of long living bonds[1]. This feature is rather similar to the one observed in irreversible gelation, where the presence of dynamical heterogeneities can be explicitly related to the growing mean cluster size [2]. At higher volume fraction, instead, where crowding of the particles starts to be relevant, dynamical heterogeneities show the typical pattern observed in glassy systems. Interestingly, such behavior can be here well described in terms of a suitable mean cluster size of clusters due to finite lifetime bonds [1].

[1] A. Fierro, E. Del Gado, A. de Candia and A. Coniglio, cond-mat/0707.4071. [2] T. Abete, A. de Candia, E. Del Gado, A.Fierro and A. Coniglio, Phys. Rev. Lett. 98, 088301 (2007).

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CPP 4.5 Mon 15:45 C 264

Scaling laws in the rheology of colloidal dispersions — •David Hajnal[1] and Matthias Fuchs[2] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz, Staudinger Weg 7, D-55099 Mainz, Germany — [2]Fachbereich Physik, Universität Konstanz, D-78457 Konstanz, Germany

We have analyzed the shear flow behavior of dense colloidal dispersions close to the glass transition in the framework of a schematic version of mode-coupling theory (MCT). The schematic model contains the universal aspects of MCT [1] and was successfully applied to describe experimental data for the flow behavior and the linear viscoelasticity of thermosensitive core-shell dispersions [2].

We have derived a universal analytic expression which describes the flow curves quantitatively for small shear rates. This analytic expression provides a deeper understanding of the shapes of the flow curves. For instance, the scaling of the yield stress, the zero-shear limit of the shear stress, and its singular behavior at the glass transition point can easily be obtained by studying special asymptotic limits.

[1] M. Fuchs and M. E. Cates, Schematic models for dynamic yielding of sheared colloidal glasses. Faraday Discuss. 123, 267-286 (2003).
[2] J. J. Crassous, M. Siebenbürger, M. Ballauf, M. Drechsler, D. Hajnal, O. Henrich and M. Fuchs, Shear stresses of colloidal dispersions at the glass transition in equilibrium and in flow. J. Chem. Phys., submitted.

CPP 4.6 Mon 16:00 C 264

Relating structure, dynamics and rheology of soft micellar glasses — •Jörg Stellbrink, Barbara Lonetti, Marco Laurati, Lutz Willner, and Dieter Richter — IFF, Forschungszentrum Jülich, D-52425 Jülich

Soft colloids are the link between colloids and polymers, showing some interesting features, which originate from their special hybrid character. Recently, regular star polymers and block copolymer micelles have been independently used to investigate structure, dynamics and rheology on approaching the glass phase as a function of softness.

For kinetically frozen (PEP_m-PEO_n) block copolymer micelles we have shown, that the architecture of the individual micelle can be adjusted between the limits compact sphere like (m≈n) and star-like (m≫n). At the same time the (repulsive) micellar interactions vary from hard sphere like to ultra soft. Micellar structure factors in equilibrium can be described starting from either the hard sphere or the ultrasoft pair potential without adjustable parameters. Therefore PEP-PEO micelles are an excellent model system for soft colloids. Special emphasis will be on non-equilibrium phenomena as i.) jamming transitions in concentrated micellar solutions as observed by dynamic light scattering, pfg-nmr and rheology and ii.) the structural response of ordered/disordered colloidal phases to applied external shear as resolved by in situ neutron scattering techniques (Rheo-SANS).

[1] M. Laurati et al., *Phys. Rev. Letters*, **94**, 195504, 2005.
[2] M. Laurati et al., *Phys. Rev. E*, **76**, 041503, 2007.

CPP 4.7 Mon 16:15 C 264

Structural Rearrangements of Colloidal Gels under Shear — •Laurati Marco[1], Petekidis George[2], Koumakis Nikos[2], and Egelhaaf Stefan[1] — [1]Soft Matter Laboratory, HHU Duesseldorf, 40225 Duesseldorf, Germany — [2]Polymer and Colloid Group, IESL, FORTH, 71110 Heraklion, Greece

The experimental system investigated in this work are short-ranged attractive colloids obtained from mixtures of PMMA colloidal spheres and PS chains dispersed in cis-decalin. The colloid volume fraction is 40%, the polymer concentration is increased from the fluid to the gel phase. Structural rearrangements of gels under oscillatory shear are investigated by non-linear Rheology and Echo-Diffusing Wave Spectroscopy (Echo-DWS). Rheology allowed us to estimate yield strains and stresses of the gels. Echo-DWS allowed us to determine the characteristic times of the rearrangements and the mean square displacement. The amount and characteristic times of structural rearrangements depend on strain, polymer concentration and frequency of oscillation in a fashion which can be rationalized on the basis of a recently proposed simple model of structural rearrangements driven by breaking of two-particles depletion bonds (Smith,PRE,2007). Additionally, rheological measurements indicate interesting connections with the yielding mechanisms of attractive glasses (Pham,EPL,2006). Two distinct yielding points are observed: one, at strains comparable to the range of the interaction potential, corresponds to the strain at which bonds between particles are broken; the second, at larger strains, corresponds to irreversible rearrangement of the gel structure.

CPP 4.8 Mon 16:30 C 264

A local structural mechanism for dynamic arrest — •Paddy Royall[1], Stephen Williams[2], Takehiro Ohtsuka[3], and Hajime Tanaka[3] — [1]School of Chemistry, University of Bristol, Bristol, BS8 1TS, UK — [2]Research School of Chemistry, The Australian National University, Canberra, ACT 0200, Australia. — [3]nstitute of Industrial Science, University of Tokyo, 4-6-1 Komaba, Meguro-ku, Tokyo 153-8505, Japan

The mechanism by which a liquid may become arrested, forming a glass or gel, is a long standing problem of materials science. While possible dynamic mechanisms have received considerable attention, direct experimental evidence of structural mechanisms has proved elusive. The connection between long-lived (energetically) locally favoured structures (LFS), whose geometry may prevent the system relaxing to its equilibrium state, and dynamical arrest dates back at least to F.C. Frank in the 1950s. In a similar spirit, we propose a much broader definition of LFS which we identify with a novel topological method and combine these with experiments at the single particle level on a colloidal liquid-gel transition. The population and lifetime of the LFS is a strong function of (effective) temperature in the ergodic liquid phase, rising sharply approaching dynamical arrest, and indeed the LFS form a percolating network which become the 'arms' of the gel. Due to the LFS, the gel is unable to reach equilibrium, crystal-gas coexistence. Our results form the first direct experimental observation of a link between local structure and dynamical arrest, and open a new perspective on a wide range of metastable materials.

CPP 5: New Materials

Time: Monday 10:00–12:30 Location: C 230

CPP 5.1 Mon 10:00 C 230

Shear stable colloidal crystals as pH- and pressure sensors. — Roy Goldberg and •Hans Joachim Schöpe — Johannes Gutenberg-Universität Mainz, Institut für Physik, Staudinger Weg 7, 55099 Mainz, Deutschland

Opaline hydrogels were produced as polycrystalline bulk material with bcc-structure by immobilization of self-ordered charged colloidal particles crystallized under equilibrium conditions in a poly(acrylamide) matrix. The final size of a polycrystalline sample is about 7 qcm, a single crystal is up to several mm in length. The crystal size is tunable by varying the amount of photoinitiator and the hydrogel volume-change due to swelling. The resulting photonic crystals are of high quality showing high order reflections. These hydrogels show a reversible shift of the diffraction Bragg-peak wavelength in dependence of external conditions due to swelling or shrinking as funczion of the pH and under applied mechanical stress. The wavelength of the photonic band gap can be shifted over the entire spectrum of visible light (500nm). Bulk material offers the possibility to shift the position of the main Bragg reflection to smaller and to larger wavelength simultaneously: under compression the wavelength of the (110)-reflection parallel to the direction of compression decreases while perpendicular to the direction of compression it increases.

CPP 5.2 Mon 10:15 C 230

Novel electro-optic multistage switching in a polar smectic material — •Stephan Stern, Alexey Eremin, Alexandru Nemes, and Ralf Stannarius — Otto-von-Guericke-Universität Magdeburg

We report a very unusual and totally unprecedented electro-optic behaviour in a polar smectic phase of a bent-core mesogen, which cannot be attributed to either conventional antiferro-, ferri- or ferroelectric structures. Although x-ray investigations have shown a tilted smectic phase without in-plane order, the switching properties are very distinctive from those of typical ferro- or antiferroelectric liquid crystals. In order to determine the spontaneous polarization in dependence of the electric field we applied a triangular wave across the liquid crystal cell and found five peaks per half period. This behaviour can be attributed to five switching processes and corresponds to a hysteresis curve containing four loops (four stages of discontinuous switching) at high voltages and one continuous switching at lower voltages. The results were confirmed by measurements of optical transmission, birefringence and Second-Harmonic-Generation activity in the distinct states of the switching process. Based on this experimental results, possible structural arrangements of the mesogens in these distinct states of this mesophase are discussed.

CPP 5.3 Mon 10:30 C 230

PbTiO3/P(VDF-TrFE) nanocomposites for flexible skin — •Markus Krause[1], Norbert Gaar[1], Reinhard Schwödiauer[1], Simona Bauer-Gogonea[1], Siegfried Bauer[1], Bernd Ploss[2], Ingrid Graz[3], Stephanie P. Lacour[3], Martin Zirkl[4], Barbara Stadlober[4], Jian-Zhang Chen[5], and Sigurd Wagner[5] — [1]Soft Matter Physics, Johannes Kepler University, Linz, Austria — [2]SciTec, University of Applied Sciences, Jena, Germany — [3]Nanoscience Centre, University of Cambridge, U.K — [4]Institute of Nanostructured Materials and Photonics, Joanneum Research, Weiz, Austria — [5]Department of Electrical Engineering, Princeton University, Princeton NJ, USA

Flexible electronics is often inspired by nature, for example by the feasibility of skin to sense touch and temperature changes. Mimicking such features of living systems is a challenge in macroelectronics research. Here we show that composites of ferroelectric ceramics and copolymers can be tailored to exhibit exclusively piezoelectric or pyroelectric responses depending on the poling procedure applied. They are therefore suitable for the development of smart skin applications.

0-3 composites of 70/30 P(VDF-TrFE) and 30% PbTiO3 nanopowder inclusions have been prepared and polarized to exhibit either piezo- or pyroelectric functionalities. Such elements on a single foil have been combined with flexible electronic components based on amorphous silicon and organic field-effect transistors. The generated signals are used to alter the conductance of the drain-source channel of the field effect transistors, and enable the demonstration of pressure and temperature sensors, by way of design. Work partially supported by the FWF.

CPP 5.4 Mon 10:45 C 230

Dielectric barrier discharges in ferroelectrets: Spectroscopic characterization and pressure dependence — •Xunlin Qiu, Axel Mellinger, Werner Wirges, and Reimund Gerhard — Institute of Physics, University of Potsdam, 14469 Potsdam, Germany

In recent years, a number of cellular and voided polymer-ferroelectret materials were discovered to exhibit a strong piezoelectric response after proper charging [1]. Charging occurs via a series of dielectric barrier discharges (DBDs); this process is critical for rendering ferroelectrets piezoelectric. In the present work, the transient light emission from the DBDs in cellular polypropylene ferroelectrets subjected to high electric poling fields, and the influence of gas pressure and composition on the DBDs were spectroscopically studied. The spectrum measured in air shows strong emission from the second positive system ($C^3\Pi_u \rightarrow B^3\Pi_g$) of molecular nitrogen (N_2), and the first negative system ($B^2\Sigma_u^+ \rightarrow X^2\Sigma_g^+$) of N_2^+, consistent with a DBD in air. From the strength ratios of selected vibronic bands, the electric field in the discharge was determined and found to be in good agreement with the values predicted by the Townsend breakdown model. Simultaneously, the build-up of the effective polarization of ferroelectrets under suitable voltage waveforms was studied by acoustical measurements. A polarization-voltage (P-V) hysteresis loop was obtained by analyzing the data in the light of an existing electromechanical model [2].

[1] M. Wegener and S. Bauer, ChemPhysChem **6**, 1014 (2005).

[2] X. Qiu, A. Mellinger, M. Wegener, W. Wirges and R. Gerhard, J. Appl. Phys. **101**, 104112 (2007).

CPP 5.5 Mon 11:00 C 230

Nanopatterning of gold particles using a polymer template: in situ GISAXS study — •Ezzeldin Metwalli[1], Sebastian Couet[2], Kai Schlage[2], Ralf Röhlsberger[2], Volker Körstgens[1], Matthias Ruderer[1], Weinan Wang[1], Gunar Kaune[1], Stephan Roth[2], and Peter Müller-Buschbaum[1] — [1]Physikdepartment E13, Technische Universität München, James-Franck-Str. 1, 85747 Garching, Germany — [2]HASYLAB at DESY, Notkestr. 85, 22603 Hamburg, Germany

The organization of metal nanoparticles within self-assembled polymer template is important for developing functional hybrid materials. Microphase-separated structures of mixed diblock-triblock copolymer thin films are used for the incorporation of gold atoms inside the polymer matrix via sputtering of gold. Polystyrene nanospheres are arranged in a liquid-like type with a well defined nearest neighbor distance inside a polyisoprene matrix acting as a template for directing the gold atoms. Sputtering conditions are selected with a low rate and a high pressure of argon gas inside the sputter chamber to avoid clustering in the atmosphere and on the polymer film. Due to the mobility of the gold atoms and the selective interaction with the polystyrene domains of the microphase separation structure, gold is accumulated in the PS spheres as probed with in situ grazing incidence small-angle x-ray scattering. Our study introduces the concept that, without thermal annealing of the gold attached polymer film, the gold assembly is not limited to the flat two dimensional but also included in three dimensional structures.

break

CPP 5.6 Mon 11:30 C 230

Relaxation and cyclic deformation behaviour of multigraft copolymers — Ralf Schlegel[1], •Roland Weidisch[1], Ulrike Staudinger[1], and Jimmy W. Mays[2] — [1]Institute of Materials Science and Technology (IMT), Friedrich-Schiller-University Jena, Löbdergraben 32, D-07743 Jena, Germany — [2]Department of Chemistry, University of Tennessee, Knoxville, USA

Multigraft copolymers consisting of a polyisoprene (PI) backbone chain and several grafted polystyrene (PS) arms form microphase separated morphologies in which the hard phase (PS) is coupled directly by chemical bonds to the soft rubbery phase. As shown in recent work PI-PS multigraft copolymers exhibit higher strains at break as well as lower residual strains in comparison to commercial triblock thermoplastic elastomers [Zhu06]. In this study the materials have been characterized by cyclic deformation (hysteresis measurements) and relaxation tests. Stress strain curves of the materials have been characterized by applying models of rubber elasticity. It could be observed that the mechanical properties in relaxation and during the hysteresis are significantly influenced by the unctionality and the number of branch points β. In addition the morphology impacts the mechanical behaviour. At low PS-contents at about 16 - 19 wt.-% tetrafunctional multigraft copolymers exhibit a spherical morphology and the values for the modulus increase with β, whereas they decrease in multigrafts with a PS content of about 23 - 25 wt-% forming a cylindrical morphology.

[Zhu06] *Zhu, Y.; Burgaz, E.; Gido, S.P. *Macromolecules*, 2006, 39, 4428-4436

CPP 5.7 Mon 11:45 C 230

Astonishing change of the hypersonic behaviour in a commercial gel due to supercooling of the sol-gel transition — •Ulrich Müller[1], Martine Philipp[1], Jan Kristian Krüger[1], Roland Sanctuary[1], Bartosz Zielinski[1], Jörg Baller[1], Ravindrakumar Bactavatchalou[1], and Patrick Alnot[2] — [1]Université du Luxembourg, LPM, Campus Limpertsberg, L-1511 Luxembourg — [2]Université Henri Poincaré - Nancy I, Nancy, France

The sol-gel transition in the commercial gel Kaisers glycerol gelatine (MERCK), composed of water, glycerol and gelatine is based on the formation of percolated physical network of the gelatine molecules. The measurements are performed by Brillouin spectroscopy for the determination of the hypersonic properties, polarimetry for the investigation of the network formation and refractometry. It will be shown that the hypersonic properties of that gel strongly depends on the thermal history of the material on one hand but that no special acoustic anomaly is found in the vicinity of the temperature of gelation on the other. Although differently supercooled gel states are clearly in thermodynamic non-equilibrium they did not show relaxations towards their equilibrium state. In agreement with that result different glass forming behaviour was observed.

CPP 5.8 Mon 12:00 C 230

Phases Sequences of a Gelatine Based Physical Gel at Low Temperatures — •Martine Philipp[1], Ulrich Müller[1], Claude Lecomte[2], Emmanuel Wenger[2], Roland Sanctuary[1], Jörg Baller[1], Bartosz Zielinski[1], Patrick Alnot[2], Didier Rouxel[2], and Jan Krüger[1] — [1]LPM, Université du Luxembourg, Luxembourg — [2]Université Nancy, Nancy, France

Only little is known about the low temperature properties of physical gels like gelatines dissolved in glycerol/water. Because of the inherent disorder of the gelatine molecules, depending on the cooling scenario different equilibrium and non-equilibrium low temperature states can be created. Taking Kaisers glycerol gelatine (Merck) as a model substance we will demonstrate that the low temperature behaviour of this gel is very interesting. Different stable glassy states have been found including that of a glass-ceramic. The latter is usually created by thermo diffusion (Soret effect) and grows in form of ball-like structures. Brillouin spectroscopy, X-ray scattering and optical microscopy are used to identify the different low temperature phases. An interpretation for the growth of the ball-like ceramic objects based on the Soret effect is proposed. The results are compared with the low temperature properties obtained for pure glycerol/water mixtures. In addition, the influence of inorganic nanoparticles on the phase formations within Kaisers glycerol gelatine is discussed.

CPP 5.9 Mon 12:15 C 230

The isopod cuticle: A model to study the influence of the structure and chemical composition on the mechanical properties of a biological composite material — •Sabine Hild[1], Andreas Ziegler[1], and Othmar Marti[2] — [1]Central Facility for Electron Microscopy; University of Ulm, Germany — [2]Experimental Physics; University of Ulm, Germany

The mineralized exoskeleton (cuticle) of crustaceans is an excellent model to study biological nano-composites. The cuticle consists of an organic matrix composed of chitin-protein fibers associated with various amounts of crystalline and amorphous calcium carbonate (ACC). Although this structural principle is ubiquitous for the cuticle of crustaceans, their mechanical properties are well adapted to their various habitats and escape strategies. To show possible adaptations of the mechanical performance of the exoskeleton to its biological requirements the chemical and structural composition of different isopod species were analyzed. Using confocal micro-Raman microscopy, SEM and SFM it was shown that for all investigated species the mineral phase is arranged in distinct layers. Calcite is restricted to the outer area of the cuticle, whereas ACC is localized in the middle having only little overlap with the calcite layer. Nano-indentation tests performed on the cross sections of the cuticle of different isopods reveals higher mechanical strength for the crystalline than for the ACC-rich phase. Our results suggest that variations in the thickness of the calcite containing layers as well as the amount of organic material leads to variations in exoskeleton hardness and flexibility.

CPP 6: Electronic+Optical Properties

Time: Monday 14:00–16:45 Location: C 230

CPP 6.1 Mon 14:00 C 230

Degradation mechanisms due to shading effects on organic solar cell modules — •Roland Steim[1,2], Pavel Schilinsky[1], Stelios A. Choulis[1,3], and Christoph J. Brabec[4] — [1]Konarka Technologies GmbH, Landgrabenstrasse 94, D-90443 Nürnberg, Germany — [2]Department of Electrical Engineering, University of Karlsruhe, D-76131 Karlsruhe, Germany — [3]Cyprus University of Technology, Department of Mechanical Engineering & Materials Science and Engineering, 3603 Lemesos, Cyprus — [4]Konarka Technologies, Altenbergerstrasse 69, A-4040 Linz, Austria

Organic solar cells based on Polymer:Fullerene blends have an open-circuit voltage in the range of 0.6V. Higher voltages that are needed for efficient sunlight to electrical energy conversion can be achieved by a serial connection of solar cells to modules. The voltage of each cell is added to the module voltage. The single solar cells within the module are dependent from each other and the failing of one solar cell can damage the whole module. We present data based on our investigations on module shading effects on organic solar cells. When shading one cell of a module, the shaded cell acts as load and is driven by the non-shaded ones. The shaded cell is under stress due to the applied reverse voltage and high current. Thus the shaded cell can be degraded as a function of shading time. We have investigated the failing mechanisms of reverse biased organic solar cells. We have identified, localized hot spots influence to the stability of organic solar cells under reverse bias stress. By device engineering modifications we have increased the stability of organic solar cell modules under shading.

CPP 6.2 Mon 14:15 C 230

Solution processable Cs-salt cathode structures for Polymer-LEDs — •Riikka Suhonen[1,2], Andreas Kanitz[1], Wiebke Sarfert[1], Ralph Pätzold[3], and Albrecht Winnacker[2] — [1]Siemens AG, CT MM1, Günther-Scharowsky-Str. 1, 91058 Erlangen, Germany — [2]Department of Material Science VI, University Erlangen-Nuremberg, Martensstraße 7, 91058 Erlangen, Germany — [3]OSRAM Opto Semiconductors GmbH, Leibnizstraße 4, 93055 Regensburg, Germany

The thin layers between the cathode and the polymer in polymer light emitting diodes (PLEDs) have been shown to have a big impact on the final device performance. Usually, in PLEDs low work function metals like Ba, Mg or Ca are used to reduce the energy barrier height between the cathode and the polymer thus providing a better electron injection from the cathode. Due to the high reactivity and quenching properties of these metals, search for electron injecting materials to replace them is ongoing. Recently, several alkali salts like LiF, CsF and Cs2CO3 have been shown to efficiently work as an electron injection layer. From these materials especially Cs2CO3 has proven to work very efficiently both as an electron injection layer.

In this contribution, we compare the performance of two cesium salts, cesium carbonate (Cs2CO3) and cesium stearate (CsSt). Both of these salts can be deposited from solution and by vacuum evaporation. Additionally, both of the salts show comparable or even better performance in comparison to the standard Ba cathode. Also the long term stability of the salt-cathode structures has been investigated.

CPP 6.3 Mon 14:30 C 230

Magnetic field effects on charge carriers in OLEDs — •Ulrich Niedermeier[1,2], Wiebke Sarfert[1], and Heinz von Seggern[2] — [1]Siemens AG, CT MM 1, Günther-Scharowsky-Str. 1, 91058 Erlangen, Germany — [2]TU Darmstadt, Department of Materials Science, Petersenstr. 23, 64287 Darmstadt, Germany

Magnetic field effects in organic light emitting diodes (OLEDs) have attracted more and more attention in recent research activities. In an external magnetic field both the current flow through an OLED and the light emission from the device are increased. We present results from magnetoresistance measurements suggesting that the presence of triplet excitons within the device is linked to the appearance of the magnetoresistive effect. In fluorescent emitters the effect occurs at voltages above turn-on where both electrons and holes are injected and form excitons. Introducing phosphorescent emitters in a fluorescent matrix results in a decrease of the magnetoresistance effect since triplet excitons are effectively removed from the system by radiative decay. Using different cathode and emitter materials we furthermore show a dependence of the magnetoresistance on the charge carrier balance within the device. In photoluminescence measurements of fluorescent emitters a magnetic field has no influence since optical excitation creates only singlet excitons. Finally, we discuss our results in the framework of two recently proposed theories on the origin of the organic magnetoresistance effect.

CPP 6.4 Mon 14:45 C 230

Investigation of grating formation in thin layers of an azobenzene-containing diblock copolymer — •Rafael Meinhardt[1], Sven Macko[1], Ansgar Draude[1], Yue Zhao[2], and Hilmar Franke[1] — [1]Department of Applied Physics, University of Duisburg-Essen, Duisburg, Germany — [2]Département de chimie, Université de Sherbrooke, Sherbrooke, Québec, Canada

A diblock copolymer composed of poly{(ethylene oxide)45} and poly{[6-[4-(4-cynophenylazo)phenoxy]ethyl methacrylate]55} has been synthesized. Thin films (< 800nm) have been prepared from solutions in trichlormethane by gravity settling. Film thickness and changes of the refractive index anisotropy after homogeneous exposure were measured by m-line-spectroscopy and metal film enhanced leaky mode spectroscopy. In a conventional two beam holographic setup gratings with a lateral periodicity of 2000 nm have been generated using an argon ion laser (488nm). An exposure time of a few seconds was sufficient to obtain a grating with first order diffractions exceeding the transmitted 0th order. Different experiments with different polarization configurations have been performed with in situ measurements of the diffraction efficiencies which lead to diffraction efficiencies in the range of 40%. We will demonstrate the formation of a refractive index grating and a surface relief grating with different time constants and quantify their ratio. The formation of surface relief gratings particularly in the initial state has been investigated by performing AFM measurements. Applications for grating coupling, optical switching and tuneable gratings will be presented.

CPP 6.5 Mon 15:00 C 230

Temperature dependent analysis of grating formation on

azobenzene polymer films. — •Padmanabh Veer[1], Ullrich Pietsch[1], Paul Rochon[2], and Marina Saphiannikova[3] — [1]Department of Solid State Physics, University of Siegen, ENC, 57068, Siegen, Germany — [2]Department of Physics, Royal Military College, Kingston, Ontario, Canada K7K5L0 — [3]Leibniz Institute of Polymer Research, 01069, Dresden, Germany

The temperature dependence of surface relief grating formation was studied using continuous and pulse like exposure. Surface relief gratings were inscribed on amorphous azobenzene polymer thin films using a holographic pattern of circularly polarized light at wavelength equal to 514 nm in a vacuum chamber to avoid the hot air turbulence and probed using a He-Ne laser of wavelength 633 nm by monitoring the first order diffraction peak (I1) as well as the specular reflected intensity (Is). Under continuous exposure permanent grating formation was observed up to a temperature of about 100 °C only. The same was found under pulse like exposure but grating still exists as long as the actinic light is on. Above 100 °C it relaxes entirely after switching the light off. Our findings can be interpreted by the competition between light-induced ordering of azobenzene side chains and temperature induced disorder. Because the accumulated stress within the polymer decreases with temperature, permanent grating formation can only be observed when the light-induced stress is above the yield stress. (Reference-Accepted Paper-P. veer1, U. Pietsch1, P. Rochon2, and M. Saphiannikova3 Molecular crystal and liquid crystal.)

break

CPP 6.6 Mon 15:30 C 230

Furan-bridged fullerenes - a new class of organic semiconductors? — •Markus Reinmöller, Uwe Ritter, and Wichard J. D. Beenken — Technische Universität Ilmenau, Institut für Physik

We performed quantum-chemical calculations of different oxygen-bridged C60-dimers. The calculations on relaxed structures have shown that a furan-like linkage is prefered. For this structure we found an anti-binding - insulating HOMO, whereas the LUMO may be conducting for a delocalized binding orbital between the two fullerenes. Unexpectedly, this orbital is not related to the oxygen but located on the opposite side - quasi free-hanging outside the furan-bridge. This result engaged us to investigate longer chains of several furan-bridged fullerenes, which may turn out as new organic semiconductor.

CPP 6.7 Mon 15:45 C 230

Localized Charge Transfer in a Molecularly Doped Conducting Polymer — •Emad F. Aziz[1], Antje Vollmer[1], Stefan Eisebitt[1], Wolfgang Eberhardt[1], Patrick Pingel[2], Dieter Neher[2], and Norbert Koch[3] — [1]BESSY GmbH, Berlin, Germany — [2]Universität Potsdam, Potsdam, Germany — [3]Humboldt-Universität zu Berlin, Berlin, Germany

Upon doping conjugated polymers can become highly conductive and thus important for the further development of all-organic optoelectronic devices. However, very little is known about the nature of donor/acceptor charge transfer (CT) in molecularly doped conjugated polymers. We present evidence for localized CT complex formation between the prototypical organic donor poly(3-hexylthiophene) (P3HT) and the molecular acceptor tetrafluoro-tetracyano- quinodimethane (F4TCNQ) in thin films by combining X-ray absorption near edge structure (XANES) measurements with theoretical modeling using density functional theory (DFT). This CT leads to molecular distortions and self- localization of the new hybrid energy levels on short single polymer chain segments.

E. F. Aziz, A. Vollmer, S. Eisebitt, W. Eberhardt, P. Pingel, D. Neher, N. Koch, Adv. Mater. 2007, 19, 3257-3260

CPP 6.8 Mon 16:00 C 230

Characterization of optical active nanostructures on silicon — •Thomas Baumgärtel, Harald Graaf, and Christian von Borczyskowski — Center of Nanostructured Materials and Analytics, TU Chemnitz, 09107 Chemnitz, Germany

It has been recently demonstrated, that nanostructures can be functionalized in a neat way through selective binding of dye molecules and nanoparticles [1]. Anchoring optically active molecules on nanostructured surfaces is a promising step towards building complex structures with variable properties and functions.

In our contribution we report on the characterization of nanostructures on silicon, that have been optically functionalized by binding of cationic dyes. The structures have been generated by local anodic oxidation of alkyl-terminated silicon via AFM. Due to the oxidation process, these silicon oxide structures are partially negatively charged. The cationic dyes rhodamine 6G and cresyl violet have been attached to the structures via electrostatic interactions and were studied using wide-field and confocal microscopy. A change in luminescence spectra of the dyes on the nanostructures, compared to the dyes in solution has been found. Furthermore, the bleaching behaviour of the dyes bound to the structure has been investigated.

[1] H. Graaf, M. Vieluf, and C. von Borczyskowski, Nanotechnology 18, 265306 (2007)

CPP 6.9 Mon 16:15 C 230

Spectroscopic and Electrochemical Investigation of Tubular J-Aggregates During Photo-Assisted Growth of Silver — •Dörthe M Eisele[1], Constans Weber[1], Jennifer Lyon[3], Hans v. Berlepsch[2], Stefan Kirstein[1], Christoph Böttcher[2], Keith J Stevenson[3], David A Vanden Bout[3], and Jürgen P Rabe[1] — [1]Humboldt University Berlin — [2]Free Universtiy Berlin — [3]University of Texas at Austin

Cyanine dye J-aggregates have been intensively investigated as sensitizers for photo induced electron transfer processes and are used in photographic films to form elementary silver specks in solid silver halide crystallites. Of particular interest are tubular J-aggregates formed by amphiphilic cyanine dye molecules upon self assembly aggregation in aqueous solution. A detailed understanding of their physicochemical properties is necessary for applications as spectral sensitizers in artificial light harvesting systems.

In this contribution, this light accelerated electron transfer from the tubular aggregates to noble metal ions such as silver is studied. This photo assisted charge transfer induces the growth of metallic nanoparticles that are located on the J-aggregate surface and does not disrupt the long-range tubular morphology. The reduction of the silver is observed by monitoring the oxidation of the J-aggregate using absorption and emission spectroscopy. Independent spectro-electrochemical investigations also show that the reduction of silver is associated with an oxidation of the cyanine dyes.

CPP 6.10 Mon 16:30 C 230

Photoinduced Formation of N2 Molecules in Ammonium Compounds — •Emad Flear Aziz[1], Johan Grasjo[2], Johan Forsberg[3], Egil Andersson[3], Johan Söderström[3], Laurent Duda[3], Wenhua Zhang[4], Jinglong Yang[5], Stefan Eisebitt[1], Christel Bergström[2], Yi Luo[4], Joseph Nordgren[3], Wolfgang Eberhardt[1], and Jan-Erik Rubensson[1] — [1]BESSY GmbH, Berlin, Germany — [2]Department of Pharmacy, Uppsala UniVersity, Sweden — [3]Department of Physics, Uppsala UniVersity, Sweden — [4]Theoretical Chemistry, Royal Institute of Technology, Stockholm, Sweden — [5]Hefei National Laboratory of Physical Sciences, at the Microscale, UniVersity of Science and Technology of China

Via fluorescence yield (FY) and resonant inelastic scattering spectroscopy in the soft X-ray range we find that soft X-rays induce formation of N2 molecules in solid NH4Cl and in related compounds. The nitrogen molecules form weak bonds in NH4Cl, so that a substantial fraction of the molecules remains in the sample. From measurements of the FY as a function of exposure and temperature, the rates for the photochemical processes are estimated. At elevated temperatures (363 K), several nitrogen atoms are removed from the sample per incoming photon. At lower temperatures (233 K), the rate is reduced to around 0.02 nitrogen atoms for each incoming photon. Virtually all these atoms form N2 molecules which are bound in the sample. The generality and implications of these results are briefly discussed.

Emad F. Aziz, et. al. J. Phys. Chem. A 111, 9662-9669 (2007)

CPP 7: POSTERS Rheology

Time: Monday 16:45–19:00 Location: Poster A

CPP 7.1 Mon 16:45 Poster A

Spatio-temporal behavior of dipolar nano-rods under shear — •Sebastian Heidenreich, Siegfried Hess, and Sabine H. L. Klapp — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergst. 36, D-10623

The flow properties of nano-rods are strongly affected by the dynamical behavior of molecular alignment. A theoretical description can be made by an relaxation equation [1] of the order parameter tensor. For plane Couette flow geometry the model leads to a rather complex orientational and flow behavior [2]. Depending on the model parameters and the boundary conditions various flows like shear banding flow can occur. To describe suspensions consisting of dipolar nano-rods that can form clusters with an effective polarization the relaxation equation has to be extended. In [4] the coupling of the orientation and the dipole moment was investigated for the bulk system. The additional dipole moment strongly affects the orientational dynamics. In this contribution we study a spatially inhomogeneous tensor model. In the plane Couette geometry structure emerges in the flow profile not known from the flow behavior of nano-rods without dipole moments. Furthermore, we present the effect of the dipole moment on the start up flow dynamics of shear bands.

[1] S. Hess, Z. Naturforsch. **30a**, 728, 1224 (1975)
[2] B. Chakrabarti, M. Das, C. Dasgupta, S. Ramaswamy, and A. K. Sood, Phys. Rev. Lett. **92**, 055501,(2004);
[3] S. Grandner, S. Heidenreich, P. Ilg S. H. L. Klapp, and S. Hess; S. Grandner, S. Heidenreich, S. Hess, and S. H. L. Klapp, EPJE in press

CPP 7.2 Mon 16:45 Poster A

Deviation from elongational flow in the capillary breakup of polyethylene oxide solutions — •Rainer Sattler and Christian Wagner — Campus, Gebäude E2 6 3.OG, 66041 Saarbrücken

The formation of the beads-on-a-string structure on a thinning thread of an elastic liquid is revisited. This structure occurs as previously shown in consequence of a linear instability. However, the evolution has been examined in more detail to evaluate existing iterative concepts and gain more insight into the processes involved. The reported formation of a solidified polymer thread during the final stages of the breakup could be deduced in-situ in an indirect way compared to the Scanning Electron Microscopy images previously presented. Two independent observations allow for a qualitative and quantitative prediction of it matching the known results.

More insight is given on the evaluation of the linear instability justifying the special Super-Resolution method. Singular occurrences of droplets on the fiber prior to the linear instability are discussed. Finally we put emphasis on the examination of the flow conditions within the liquid column from the formation of the cylindrical thread until the onset of the linear instability, falsifying the assumption of a purely elongational plug flow. We present its scope as well as the transition to a flow containing shear and even flow reversal between surface and core especially during the "breathing" instability of the fringe region presented elsewhere.

CPP 7.3 Mon 16:45 Poster A

Uncommon rheological effects during melting of dibenzylidene sorbitol fiber networks in poly (propylene oxide) — •Martin Kühne and Christian Friedrich — Freiburger Materialforschungszentrum, Stefan-Meier-Str. 21, 79104 Freiburg

Dibenzylidene sorbitol (DBS) is known to gel organic liquids as well as polymers such as poly (propylene oxide) (PPO) due to its capability of forming semiflexible fibers and corresponding networks. These networks are thermoreversible, which means they are melted by temperature increase and rebuild again during temperature decrease.

We investigated the melting process and related rheological effects of DBS fiber networks in PPO with special regard to temperature rate and deformation. At certain temperature rates and deformations an uncommon rheological behavior was found: Both G' and G" increase with increasing temperature. We found that this behavior is the result of a temperature gradient within the sample, which causes fragmentation of fibers. The temperature dependent balance between fragmentation and reorganization is responsible for the observed effects. As a consequence, at the lowest rates, the samples do not show such uncommon behavior and now G' depends on temperature with T^{-1}. This is in accordance to the predictions for the temperature dependence of plateau modulus of a network of semiflexible fibers.

CPP 7.4 Mon 16:45 Poster A

Shear induced brush deformation of soft colloids: Hybrid mesoscale simulations and Rheo-SANS experiments — •Jörg Stellbrink[1], Marisol Ripoll[1], Roland G. Winkler[1], Gerhard Gompper[1], Jan K.G. Dhont[1], Dieter Richter[1], Dimitris Vlassopoulos[2], and Peter Lindner[3] — [1]IFF, Forschungszentrum Jülich, D-52425 Jülich — [2]IESL-FORTH, Heraklion 71110 Crete, Greece — [3]Institute Laue-Langevin, F-38042 Grenoble, France

The deformation of a soft colloid by external shear fields crucially depends on its "degree of softness"and the applied Weissenberg number. ($Wi = \tau_c\dot{\gamma}$, with $\dot{\gamma}$ the applied external shear rate and τ_c the characteristic internal relaxation time of the deformable particle.)

Here we compare results obtained with multiparticle collision dynamics simulations (MPC) and Rheo-SANS experiments for dilute solutions of regular star polymers (the limiting *ultra-soft* colloid). To achieve large Weissenberg numbers we use high M_w polybutadiene (PB) star polymers dispersed in a PB oligomer matrix. We found excellent agreement between theory and experiment with respect to onset and amount of shear induced brush deformation for star polymers with varying functionality *f*.

Moreover, from MPC simulations we found that with increasing functionality star polymers exhibit a crossover in their flow properties from those of linear polymers to a novel behavior, which resembles the tank-treading motion of elastic capsules [1].

[1] M. Ripoll, R. G. Winkler, and G. Gompper, *Phys. Rev. Letters*, **96**, 188302, (2006).

CPP 7.5 Mon 16:45 Poster A

Interfacial Shear Rheology of Coffee Samples — •Jörg Läuger and Patrick Heyer — Anton Paar Germany, Ostfildern, Germany

Coffee is a complex dispersion, which for many coffee drinks is topped by a foam structure of tiny bubbles, e.g. the espresso foam. Interfacial rheology does not probe the foam itself, but measures the adsorption of the amphiphilic ingredients and their network formation at the liquid surface. Higher values of the interfacial properties and a faster film formation are expected to correlate with a better foam stability. Measurements on the film formation process and on the interfacial rheological properties of the final film of coffee samples are presented and discussed. Both oscillatory and rotational test have been performed on films with different coffee concentrations. Different techniques have been used to measure interfacial shear properties. Here we would like to focus on two geometries, which have been used in combination with standard types of rotational rheometers. One is the biconical geometry and the other the De Noüy ring. The aim of the paper is twofold: First, to show that interfacial rheology is a valuable tool to get information on the film formation and therefore the foam stability of coffee, and second, to compare the results obtained by a biconical disc geometry and a Du Nuöy ring.

CPP 7.6 Mon 16:45 Poster A

Wet sand flows better than dry sand — •Jorge Fiscina and Christian Wagner — Technische Physik, Saarland University, D-66123, Saarbruecken

We investigated the yield stress and the apparent viscosity of sand with and without small amounts of liquid. By pushing the sand through a tube with an enforced Poiseuille like profile we minimize the effect of avalanches and shear localization. We find that the system starts to flow when a critical shear of the order of one particle diameter is exceeded. In contrast to common believe, we observe that the resistance against the flow of wet sand is much smaller than that of dry sand. For the dissipative flow we propose a non-equilibrium state equation for granular fluids.

CPP 7.7 Mon 16:45 Poster A

In-situ investigation of the solid/liquid interface of a block copolymer solution under shear stress with μ-focus GISAXS — •Andreas Timmann[1], Stephan Volkher Roth[1], Steffen Fischer[2], and Stephan Förster[2] — [1]HASYLAB at DESY, Notkestr. 85, D-22603 Hamburg, Germany — [2]Inst. f. Phys. Chem., Uni HH, Grindelallee 117, D-20145 Hamburg, Germany

Block-copolymers are interesting for their ability to self organize in various structures. In dilute solution they form micelles, cylindrical micelles and vesicles. The length scales of these structures ranges from about 5 nm up to several hundred nanometers. Hence such structures are well suited for investigations using small-angle X-ray scattering.

The experiments were performed the beamline BW4 at HASYLAB, Hamburg [1] using the microfocus setup. We present the results of the investigation of a 13 *wt.*% solution of a poly-(isoprene-block-ethylene oxide) in water. The block degrees of polymerization of the isoprene and the polyethylene oxide were 55 and 170, respectively. The shear stress was applied by a stress-controlled Bohlin CVO rheometer in a plate-plate-geometry with a diameter of 20 *mm* and a gap of 1 *mm*. We investigated the interface layer of the solution with the rotor of the shear geometry at different temperatures. From the experiments it is clearly shown that the behavior of bulk and steel-liquid interface in a rheometric cell are quite different from each other.[2]

References:

[1] Roth et al., Rev. Sci. Instrum., 2006, 77, 085106
[2] Timmann et al., Appl. Phys. Lett., accepted

CPP 7.8 Mon 16:45 Poster A

Networks in polypropylene / carbon nanotube composites investigated by simultaneous rheological and electrical measurements — Nikolaos Katsikis[1], •Christian Triebel[1], Joachim Kaschta[1], Helmut Münstedt[1], Andreas Funk[2], and Walter Kaminsky[2] — [1]Lehrstuhl für Polymerwerkstoffe, Universität Erlangen-Nürnberg — [2]Institut für Technische und Makromolekulare Chemie, Universität Hamburg

Electrical conductivity of polymer composites filled with carbon nanotubes (CNT) can already be reached for concentrations far below 1 vol.%. To achieve such properties, a good distribution of the CNT is essential. This goal is very difficult to reach for polyolefins as their processing in the diluted state, necessary for a good distribution of nanoparticles, is complicated. Polypropylene/CNT composites were developed at the University of Hamburg by using metallocene catalysts. Materials of that kind were investigated by simultaneous measurements of rheological and electrical properties in order to get information on the formation of CNT - networks. For that purpose, a rheometer was equipped with heatable electrodes and a sensitive current measuring system. It was found that the distinct percolation threshold for the electrical conductivity is not reflected in rheological properties which show a more or less continuous change with the volume concentration. A model for an explanation of these findings is presented and discussed.

CPP 7.9 Mon 16:45 Poster A

Surface enrichment in statistical copolymer films — •Alexander Diethert, Ezzeldin Metwalli Ali, and Peter Müller-Buschbaum — TU München, Physik-Department LS E13, James-Franck-Str. 1, 85747 Garching

A prominent class of pressure sensitive adhesive (PSA) films is based on statistical copolymers. Typically two or three different monomers are combined to balance the different requests of the PSA films. In the presented work we focus on model systems and investigate the dependence on different monomers of the copolymer. With x-ray reflectivity the density profile perpendicular to the PSA surface is probed and enrichment layers are detected. From a model fit the type of monomer enriching at the surface and the thickness of the enrichment layer is detected.

This work is funded by the DFG in the project MU1487/4-2.

CPP 7.10 Mon 16:45 Poster A

Evolution of complex defects in cylinder phase of block copolymers: Experiment and Simulations — •Larisa Tsarkova[1], Andriana Horvat[1], Agur Sevink[2], and Andrey Zvelindovsky[3] — [1]Physikalische Chemie II, Universität Bayreuth, Germany — [2]Soft Condensed Matter Group,Leiden Institute of Chemistry, Leiden University, The Netherlands — [3]Centre for Materials Science, Department of Physics, Astronomy and Mathematics, University of Central Lancashire, Preston, United Kingdom

We study and classify typical and specific 2D defects which are repeatedly observed in thin films of cylinder-forming block copolymers upon long-term annealing as well as in simulations based on the dynamic self-consistent mean field theory (DSCFT). We demonstrate that pure topological arguments are not sufficient to characterize the stability and mobility of defects. Instead, specific features of block copolymer materials should be taken into account. In cylinder-forming block copolymers, representative defect configurations provide connectivity of the minority component and indicate the overall morphological evolution under given annealing conditions. The formation of specific non-topological neck-defects is tentatively similar to the initial stages of membranes/vesicles fusion. Lateral propagation velocity of a complex 3T-Junction was measured with in-situ SFM. Comparison with the DSCFT simulations suggests that lateral defect motion is diffusion-driven and indicates weak involvement of the bottom (wetting) layer in the lateral ordering of the structures at the free surface.

CPP 7.11 Mon 16:45 Poster A

Fluids in confinement: Dynamics of Foam Film Thinning — Silke Stöckle[1], •Rumen Krastev[1], Georgi Georgiev[2], and Helmuth Möhwald[1] — [1]Max Planck Institut für Kolloid- und Grenzflächenforschung, 14424 Potsdam/Golm, Deutschland — [2]University of Sofia, Deptment of Biochemistry, Sofia, Bulgaria

The thinning dynamics of foam films have become of interest and we are utilising this as a tool to study the behaviour of liquid in confinement. We show results on the dynamics of thinning of foam films stabilised by Dodecyl-D-Maltoside (C12G2) and by DMPG.

The results show the strong influence of the C12G2 concentration on the film thinning.The films formed from solutions with low surfactant concentration reveal a high speed of film thinning which is much slower above a critical threshold surfactant concentration. The theoretical models describe the thinning process well only down to a certain thickness below which the film thins faster than theory predicts. The discrepancy could be explained by introducing an additional term to the classical DLVO theory which counts for the short range interactions or considering the properties of liquids in confined volumes.The films prepared from the lipid DMPG show complex thinning behaviour at different temperatures. The peculiarities complement well to the changes of the bulk properties of the lipid dispersions at the studied temperatures.

CPP 7.12 Mon 16:45 Poster A

Time evolution of surface relief structures in thin block copolymer films — •Andriana Horvat[1], Larisa Tsarkova[1], Agur Sevink[2], Andrey Zvelindovsky[3], Robert Magerle[4], and Armin Knoll[5] — [1]Physikalische Chemie II, Universität Bayreuth, Germany — [2]Soft Condensed Matter Group, Leiden Institute of Chemistry, Leiden University, The Netherlands — [3]Centre for Materials Science, Department of Physics, Astronomy and Mathematics, University of Central Lancashire, Preston, United Kingdom — [4]Chemische Physik, Technische Universität Chemnitz, Germany — [5]IBM Research GmbH, Sumerstrasse 4, Rüschlikon, Switzerland

The dynamics of early stage of terrace formation in thin supported films of cylinder forming triblock copolymers was studied both theoretically using self-consistent field theory (DSCFT) and experimentally by *in-situ* scanning force microscopy (SFM). In experiment, an initially flat film of incommensurable thickness was imaged continuously, and the evolution of vertical orientation of cylinders into parallel one, as well as the respective development of thickness gradient (terrace formation) was captured in detail. On the grounds of these experimental observations, the parameters of the computational model $A_3B_{12}A_3$ were determined to match the structures in experiment. Both systems show excellent agreement in details of structural phase transitions and in the dynamics of the step development, suggesting that the underlying transport mechanisms are governed by diffusion.

CPP 7.13 Mon 16:45 Poster A

Depth profilling of lamella-forming block copolymer films using SFM with quasi in-situ etching treatment — Eva Max, Markus Hund, and •Larisa Tsarkova — Physikalische Chemie II, Universität Bayreuth, Germany

State-of-the-art SPMs have limited in-situ sample treatment capabilities. Aggressive treatments like plasma etching or etching in aggressive liquids typically require to remove the sample from the microscope. In consequence, time consuming procedures are needed if the same spot of the sample has to be imaged after the step-wise treatment. We report a first prototype of an SPM setup with quasi in-situ sample treatment capabilities which utilizes a modified commercial SPM (Dimension 3100, Veeco Instruments Inc.) and present recent experiments using this approach. Thin lamella-forming block copolymer films have been subjected to consecutive plasma etching, and the structure depth profile has been reconstructed.

CPP 7.14 Mon 16:45 Poster A

Structure and dynamics within the length scale of the boundary layer — •Marco Walz[1], Nicole Voss[1], Max Wolff[2], Hartmut Zabel[2], and Andreas Magerl[1] — [1]Chair for Crystallography and Structural Physics, University of Erlangen-Nürnberg, Staudtstr. 3, 91058 Erlangen — [2]Chair for Condensed Matter Physics, Ruhr-University Bochum, Universitätsstr. 150, 44780 Bochum

Shear anomalies may manifest themselves by unusual solid-liquid interface properties. Structural issues can be studied by GISANS and reflectometry which can be tuned to be particularly surface sensitive. In earlier studies by GISANS slightly above the critical angle, we observed a crystalline ordering of micellar solutions depending on the chemical termination of the solid boundary. An extension to smaller angles implying an increased sensitivity to near surface structures shows that the local structure depends on the distance to the interface. In addition a first attempt to access the dynamics in the near surface region by grazing incidence neutron spin echo (GINSE) indicates that also the micellar dynamics in this region is responsive to the chemical potential of the boundary.

The authors gratefully acknowledge the financial support by the DFG grants MA801/12-1 and ZA161/18-1 within the priority program (SPP) 1164 and the BMBF grant ADAM 04ZAE8BO.

CPP 7.15 Mon 16:45 Poster A

Unusual growth exponent in liquid crystal foams — •Torsten Trittel, Victor Aksenov, and Ralf Stannarius — Otto-von-Guericke-Universität Magdeburg

We investigate foams made from pure thermotropic liquid crystals and observe a new type of scaling behaviour during foam coarsening. 2D foams are prepared in thin cells and studied by digital image anylysis. We calculate the temporal evolution of the mean bubble radius $\langle R(t)\rangle$ and find a scaling behaviour with $\langle R(t)\rangle \propto t^{\alpha}$. In ordinary soap foams, the growth exponents are $\alpha = 1/3$ (wet foams, circular bubbles) and $\alpha = 1/2$ (dry foams, polygonal bubbles), respectively. Our bubbles have a polygonal shape like in a dry foam, but we observe an anomalous growth exponent $\alpha \simeq 0.20$ in the smectic phase. This is not compatible with the classical theories of bubble growth in foams, neither for dry nor for wet foams. In the nematic phase, coalescense dominates the evolution and the foam collapses so fast that one can not determine a steady scaling growth exponent.

CPP 7.16 Mon 16:45 Poster A

Kinetic toy model for crystal plasticity — •Markus Hütter[1], Miroslav Grmela[2], and Hans Christian Öttinger[1] — [1]ETH Zürich, Department of Materials, Polymer Physics, CH-8093 Zürich, Switzerland — [2]Ecole Polytechnique de Montréal, Montréal, Quebec, Canada H3C 3A7

We propose a kinetic toy model to describe the dynamics of sliding layers as it occurs in the plastic deformation of single crystals, be it of polymeric, colloidal, or metallic nature. As its basic ingredient, the distribution function of relative strains between adjacent crystal layers is introduced with time evolution described by a diffusion equation with periodic boundary conditions. The model highlights the conceptual difference in the dynamics of the elastic and plastic strains, the latter being related to an average hopping rate that captures the evolving reference state. We illustrate the model by calculation of the stress response for both stationary and transient conditions. In order to discuss the physics behind the parameter that drives the plastic flow in the kinetic model, we use nonequilibrium thermodynamics to unify this model with a nonisothermal hydrodynamic description, which renders the set of evolution equations closed. Finally, we examine the relation of the kinetic toy model to macroscopic theories of elasto-viscoplasticity that employ the macroscopic deformation gradient as a fundamental variable.

CPP 7.17 Mon 16:45 Poster A

Single molecule probe diffusion in liquid crystalline films — •Benjamin Schulz, Jörg Schuster, and Christian von Borczyskowski — TU Chemnitz, Institut für Physik, 09107 Chemnitz

Liquid crystalline materials are widely used in modern displays. Image quality and switching speed of the display cells are critically influenced by details of the arrangement of the mesogenes at the interface. Thus, analytical techniques are required which are able to probe molecular orientation in liquid crystals on a nanoscale. We will present the first study on the use of single fluorescent dye probes which are especially tailored for the analysis of liquid crystalline materials on the single molecule level. Perylene dyes have been modified such, that the dyes align along the orientation of the mesogenes, and will thus, due to the orientation of their absorption and emission dipoles, probe the local orientation of the liquid crystal.

Diffusion trajectories of such dye probes in thin liquid crystalline films have been tracked by wide field microscopy techniques and analyzed following standard procedures [1]. The use of tailored probe molecules allows us to discriminate between homeotropic and homogeneous alignement of thin liquid crystalline films. By comparing diffusion properties of different dyes with variable alignment strength, details of the orientation of the films will be resolved in future. Here we present the comparison of the diffusion properties of two perylene derivatives, one strongly aligning and one not aligning.

[1] J. Schuster, F. Cichos, C. von Borczyskowski: Eur. Polymer J. 40 (2004), 993

CPP 7.18 Mon 16:45 Poster A

Rupture dynamics of smectic bubbles — •Frank Müller and Ralf Stannarius — Institut für Experimentelle Physik, Otto-von-Guericke Universität, 39106 Magdeburg, Germany

Equilibrium shapes of thin liquid membranes are well understood. On the other hand, when such films undergo fast transitions from a non-equilibrium to an equilibrium state like rupture, different dynamical mechanisms are involved which are in general poorly understood. We study such phenomena experimentally with a fast camera (up to 100.000 fps), using smectic liquid crystal bubbles as model membranes [1]. We observe several unexpected phenomena like 1. a global thickening of the film during rupture, 2. the propagation of mechanical waves, which result in light scattering, 3. an instability of the moving rim that separates the film from the hole and 4. the formation of a brim, which is due to the spherical shape of the film. All these phenomena are strongly dependent on film thickness.

[1] Müller F, Kornek U, and Stannarius R: Experimental study of the bursting of inviscid bubbles, Phys. Rev. E 75 065302(R), 2007

CPP 7.19 Mon 16:45 Poster A

Influences of Added Salt on the Drying Behavior of Polymer Dispersions - Simultaneous Use of Magnetic Resonance Profiling and Diffusing-Wave Spectroscopy — •Alexander König[1], Peter McDonald[2], Joseph Keddie[2], and Diethelm Johannsmann[1] — [1]Institute of Physical Chemistry, Clausthal University of Technology, Germany — [2]Department of Physics, University of Surrey, UK

Magnetic Resonance Profiling (MRP) was used to measure the non-uniform drying of charge-stabilized polymer dispersions. Drying is sometimes accompanied by packing of particles at the top of the film. In this case, the vertical distribution of free water, $\phi_{wat}(z)$, is strongly asymmetric. It is suspected - but not well investigated - that particle packing and coalescence create a skin. This process should be influenced by the interaction potential between particles (which can be influenced via addition of salt). As a measure of asymmetry, the skewness of the distribution $\phi_{wat}(z)$ was used. The skewness is defined as $m_3/m_2^{3/2}$, where m_i is the i-th moment of the distribution.

Diffusing-Wave Spectroscopy (DWS) probes the translational dynamics in concentrated dispersions. Both techniques were combined in-situ in order to correlate structure and dynamics.

The skewness, as determined with MRP, correlated well with the occurence of a static scattering component in DWS. Skin formation is stronger in the presence of salt, which is explained by a destabilizing effect of salt onto the interparticle membranes. Comparing different salts, we found that their relative influence onto interparticle coalescence followed the Hofmeister series.

CPP 7.20 Mon 16:45 Poster A

Competition of Phase Separation and Kinetic Arrest in a Binary Mixture with Depletion Attraction — •Anna Kozina[1], Pedro Diaz-Leyva[1,2], Christian Friedrich[1,3], and Eckhard Bartsch[1,2] — [1]Institute of Macromolecular Chemistry, Freiburg University, Germany — [2]Department of Physical Chemistry, Freiburg University, Germany — [3]Material Research Centre Freiburg, Freiburg University, Germany

Recently it has been shown that the introduction of short-range attractions by the addition of free polymer leads to such effects like melting of a colloidal glass and appearance of a reentrant glass transition [1] ('attractive' glass). The studied colloidal system consists of a binary colloidal mixture of 1:50 cross-linked polystyrene microgel particles in a good solvent. To introduce short-range attraction various amounts of linear polystyrene were added. A binary mixture was chosen to suppress crystallization and the size ratio Rg,polymer/Rcolloid ˜ 0.08 should exclude a fluid-fluid phase separation. Nevertheless, when driving the system into the attractive glass, a pronounced waiting time dependence of both density fluctuations and mechanical properties was observed. Using time resolved SLS we found evidence that this behavior is due to a micro phase separation of A and B particles with the concomitant formation of pure crystalline A and crystalline B micro domains. This phenomenon is reminiscent of the fractionation of polydisperse emulsion droplets via depletion attraction [2].

[1] T. Eckert and E. Bartsch, Phys. Rev. Lett. 89, 125701 (2002) [2] J. Bibette, J. Colloid Interf. Sci. 147, 474 (1991)

CPP 7.21 Mon 16:45 Poster A

Network induced relaxation dynamics in colloidal gels. — •Emanuela Del Gado — Polymer Physics, ETH Zürich

In contrast to other systems that show a slow relaxation, such as, e.g., glass-forming liquids, the structure of gels is given by a open network that is thought to be responsible for the unusual dynamical properties of these systems. It would be therefore essential to deeper understand this connection and to be able to tune the mechanical response via the structural features. We investigate the gel formation from the equilibrium sol phase in a simple model that has the characteristics of (colloidal) gel-forming systems at a finite temperature [1]. In the molecular dynamics simulations, at low volume fraction and low temperatures, particles are linked by long-living bonds and form an open percolating network. As a consequence, the dynamics show a non-trivial dependence on the wave-vector: At high wave vectors the relaxation is due to the fast cooperative motion of the branches of the gel network, whereas at low wave vectors the overall rearrangements of the heterogeneous structure produce the relaxation process. We study the lifetime of bonds and nodes of the gel network in order to relate these quantities to the complex relaxation dynamics observed. [1]E. Del Gado and W. Kob, Europhys. Lett. 71, 1032 (2005); Phys. Rev. Lett. 98, 028303 (2007); J. Non-Newt. Fluid Mech. 2007, in press.

CPP 7.22 Mon 16:45 Poster A

Ordnungsverhalten eines A-B Diblockcopolymers in einer (A/B/A-B) Polymermischung aus drei Komponenten — •Vitaliy Pipich, Lutz Willner und Dietmar Schwahn — Institut für Festkörperforschung des Helmholtz Forschungszentrum Jülich

Die Beimischung eines Diblockcopolymers zu einer binären Homopolymermischung führt zu einem komplexen Phasenverhalten [1]. Dies äußert sich in einem verbesserten Mischungsverhalten der beiden Homopolymere, zur Ausbildung einer Mikroemulsionsphase und schließlich zu einer geordneten lamellaren Phase[2]. Parallel beobachtet man in der homogenen Phase verstärkt das Auftreten thermischer Fluktuationen der Zusammensetzung [3]. In diesem Beitrag diskutieren wir den Strukturfaktor des Diblockcopolymers in solch einer A/B/A-B Polymermischung (A und B ist repräsentiert durch Polybutadien und Polystyrol). Solche Messungen sind mit der Neutronenkleinwinkelstreuung möglich, in dem nur ein Block des Diblockcopolymers durch entsprechende Deuterierung "sichtbar" gemacht ist. Theorien im Rahmen der Molekularfeldnäherung postulieren einen Strukturfaktor unabhängig von der Temperatur. Dieser Befund wird für kleine Diblockkonzentrationen bestätigt, stimmt aber nicht für Konzentrationen nahe und oberhalb der Lifschitzlinie. Es zeigt sich weiterhin, dass in diesem Konzentrationsbereich das Diblockcopolymer früher ordnet als das Homopolymer.

[1]*D. Schwahn, Advances in Polymer Science 183, 1 (2005). [2]*V. Pipich et al. J. Chem. Phys.123, 124904-1 (2005) [3]*V. Pipich et al. Phys. Rev. Lett. 94, 117801 (2005).

CPP 7.23 Mon 16:45 Poster A

Fluorescence correlation sprectroscopy for micro-rheological measurements — •Hubert Chevreau[1,2], Hans-Josef Beauvisage[1], and Silke Rathgeber[1] — [1]Max-Planck-Institute for Polymer Research, Polymer Physics, 55128 Mainz, Germany. — [2]Ecole Polytechnique Universitaire de Lille, 59655 Villeneuve D'Ascq Cedex, France.

To obtain information about the mechanical properties of the samples on microscopic length scales we exploited the capabilities of fluorescence correlation spectroscopy (FCS) to be used for micro-rheological measurements. Micro-rheology by means of FCS looks at the Brownian motion of a fluorescent μm tracer particle embedded in a matrix of which the rheological properties are to be determined. In principle with FCS micro-rheology the material response on micrometer length scales of a heterogeneous sample can be probed. We used fluorescent, carboxylate-modified colloidal spheres with a diameter of 0.1 μm as tracer particles. As a simple test system we have chosen polyethylene oxide (PEO) with varying molecular weights and different concentrations in water solutions in order to change the rheological response from viscous to viscoelastic. We followed different analysis methods to transfer the mean-square center-of-mass displacement to the shear moduli. Results are compared to results obtained from conventional rheological measurements.

CPP 7.24 Mon 16:45 Poster A

Supercooled Water Confined in Reverse Micelles - A Neutron Scattering Study — •Tinka Spehr[1,2], Bernhard Frick[2], Isabelle Grillo[2], and Bernd Stühn[1] — [1]TU Darmstadt, Deutschland — [2]Institut Laue Langevin, Grenoble, Frankreich

Water, the surfactant AOT and oil (toluene or decane) form a stable droplet phase microemulsion over a wide range of compositions. Spherical water droplets surrounded by a mono-layer of AOT are dispersed in oil. The size of the water pool can be varied by changing the molar ratio ω of water to surfactant: radii between a few Å and several nm can be obtained, which makes the droplets an attractive model system for the study of soft confined water. We used neutron time-of-flight (TOF), backscattering (BS) and small angle scattering (SANS) to study the system with a fixed droplet volume fraction $\phi = 0.2$ and ω ranging from 3 to 40. The phase behaviour of the microemulsion was investigated by SANS from 290 to 220 K. The droplet structure is stable down to temperatures T much below the freezing point of bulk water. The smaller the droplets (the smaller ω) the lower T down to which the droplet size is maintained. When reducing T below this phase transition the droplet size shrinks. Freezing of the confined water was observed by BS: the freezing temperature as a function of droplet size follows the same dependence as the phase transition temperature monitored[1]. Inelastic measurements (TOF, BS) show that the supercooled confined water is strongly slowed down compared to bulk water. Rotational and translational dynamics of the water are discussed.

[1]T Spehr, B Frick, I Grillo, B Stühn (2007), accepted by JPCM

CPP 7.25 Mon 16:45 Poster A

Statistics and dynamics of blends of linear and ring polymers. — •Michael Lang[1,2] and Michael Rubinstein[2] — [1]Leibniz-Institute for polymer Research, Hohe Str. 6, 01069 Dresden, Germany — [2]Department of Chemistry, University of North Carolina, 27599 Chapel Hill, N.C., USA

This work focuses on conformations and dynamics of blends of linear and ring polymers.

Rings in a melt of homo-polymer rings are compressed due to topology, if rings are significantly larger than the entanglement length. Dilute rings with degree of polymerization, N_r, immersed in a melt of linear polymers with degree of polymerization, N_l are almost ideal if $N_l > N_r^{1/2}$ and swell if $N_l < N_r^{1/2}$.

Dynamics of pure ring melts is enhanced as compared to pure linear melts. Thus, minority of linear chains immersed in ring melt experiences enhancement of diffusion and relaxation. On the other hand, minority of long entangled rings immersed in melt of long entangled linear chains gets temporarily trapped. This leads to a clear reduction in diffusion coefficient while keeping relaxation (as determined by half ring relaxation) almost unaffected.

CPP 7.26 Mon 16:45 Poster A

Micellar crystallization in salted solutions — •Nicole Voss[1], Marco Walz[1], Max Wolff[2], Hartmut Zabel[2], and Andreas Magerl[1] — [1]Chair for Crystallography and Structural Physics, University of Erlangen-Nürnberg, Staudtstr. 3, 91058 Erlangen — [2]Chair for Condensed Matter Physics, Ruhr-University Bochum, Universitätsstr. 150, 44780 Bochum

Micellar solutions of tri-block copolymers are an excellent model system for the study of crystallization in soft matter, since they have well-known and rich phase diagrams which may be identified through rheometry. The phases can be controlled by varying temperature or polymer concentration. Further, the aggregation and crystallization is highly sensitive to the presence of ions. Through the addition of salt the attraction between hydrocarbon chains and water can be tuned allowing a study of the macromolecule-solvent interaction.

We have studied the influence of CsCl with concentrations up to 1.5 mol/dm^3 on the phase diagram of the tri-block copolymer Pluronic

P123, consisting of a central part of 70 propylene oxide units terminated by two end groups of 20 ethylene oxide units (EO$_{20}$–PO$_{70}$–EO$_{20}$). The salient result of our investigation is a linear shift of all phase lines to lower temperatures under the addition of salt, whereas the fundamental structural properties of the phases are preserved.

The work was in part supported by the DFG priority program SPP 1164.

CPP 8: POSTERS Dynamics and Diffusion

Time: Monday 16:45–19:00 Location: Poster A

CPP 8.1 Mon 16:45 Poster A

dynamical and structural properties of sugar surfactant based bicontinuous microemulsions — •Stefan Wellert[1], Matthias Karg[1], Thomas Hellweg[1], Olaf Holderer[2], Hans-Juergen Altmann[3], and Andre Richardt[3] — [1]University Bayreuth, PC I, Universitaetsstrasse 30, D-95440 Bayreuth — [2]Juelich Centre for Neutron Science (JCNS), FZ. Juelich GmbH, Aussenstelle am FRM II, Lichtenbergstr. 1, D-85747 Garching — [3]Bundeswehr Scientific Institute (NBC-Protection), Humboldtstr., D-29633 Munster

Structural and dynamical properties of bicontiuous microemulsions developped for decontamination applications were studied by different scattering techniques. Microemulsion phases with a large internal surface like the bicontinuous region are of main interest for the application as soft and environmental compatible decontamination media for a variety of toxic compounds like pesticides or chemical warfare agents.

Based on APGs, RME, water and an additional alcohol we characterize the phase behavior of such systems as well as the microstructure, investigated using small angle neutron scattering (SANS), neutron spin echo spectroscopy (NSE) and dynamic light scattering.

Additionally, neutron spin echo measurements allow to gain insight into the dynamics of these films and to compare the data with theoretical descriptions like the approach of Zilman and Granek. Beside the undulations of the amphiphilic film also additional contributions due to collective motions are discussed.

CPP 8.2 Mon 16:45 Poster A

Raman spectroscopy of poly- and single-crystalline 12CaO·7Al$_2$O$_3$ (C12A7) at different temperatures — •Artur S. Seifert[1], Ilia Valov[2], Stefan G. Ebbinghaus[3], Peter J. Klar[1], and Juergen Janek[2] — [1]Institute of Experimental Physics I, Justus-Liebig-University, Heinrich-Buff-Ring 16, D-35392 Giessen. — [2]Institute of Physical Chemistry, Justus-Liebig-University, Heinrich-Buff-Ring 58, D-35392 Giessen. — [3]Solid State Chemistry, University of Augsburg, Universitätsstraße 1, D-86159 Augsburg.

Poly-crystalline 12CaO·7Al$_2$O$_3$ (mayenite) was synthesized by a solid reaction of Al$_2$O$_3$ and CaCO$_3$. Afterwards single-crystalline 12CaO·7Al$_2$O$_3$ of high purity was produced by a zone melt process. It has been recently suggested that reduced mayenite can be used as transparent conducting oxide (TCO) but this material is also known as an ion conducting solid electrolyte with fast oxygen transport. We study the variation of the vibrational modes of 12CaO·7Al$_2$O$_3$ as function of temperature in the range from 290 K to 900 K in different atmospheres, i.e. nitrogen, air and water. The vibration properties will be discussed with respect to ion storage and ion mobility within the material.

CPP 8.3 Mon 16:45 Poster A

Rectification in conical nanopores: a one-dimensional Poisson-Nernst-Planck modeling — •ilona kosinska[1,2], igor goychuk[1], marcin kostur[1], gerhard schmid[1], and peter hanggi[1] — [1]Institut fur Physik, Augsburg, Germany — [2]M. Smoluchowski Institute of Physics, Krakow, Poland

The ion current rectification is studied within a reduced 1D Poisson-Nernst-Planck (PNP) model of synthetic nanopores. A conical channel of a few nm to a few hundred of nm in diameter, and of few μm long is considered in the limit where the channel length exceeds much the Debye screening length. The rigid channel wall is assumed to be weakly charged. A one-dimensional reduction of the three-dimensional problem in terms of corresponding entropic effects is put forward.

The ion transport is described by the non-equilibrium steady-state solution of the 1D Poisson-Nernst-Planck system within a singular perturbation treatment. The analytic formula for the approximate rectification current in the lowest order perturbation theory is given.

The crucial importance of the asymmetry in the potential jumps at the pore ends on the rectification effect is demonstrated. This so constructed 1D theory is shown to describe well the experimental data in the regime of small-to-moderate electric currents.

CPP 8.4 Mon 16:45 Poster A

Diffusion of liquid medium-chain molecules investigated by QENS and PFG-NMR — •Christoph Smuda[1], Gerd Gemmecker[2], Sebastian Busch[1], and Tobias Unruh[1] — [1]Forschungsneutronenquelle Heinz Maier-Leibnitz and Physik Department E13, TU München, Garching, Germany — [2]Bayerisches NMR-Zentrum, Chemie Department, TU München, Garching, Germany

For the understanding of the functionality of colloidal drug delivery systems the molecule diffusibility inside the colloidal particles is an important parameter. In this contribution it is demonstrated that QENS is well suited for corresponding investigations. However, from measurements of the self-diffusion coefficients of the oligoisoprene derivative coenzyme Q$_{10}$ in nanosized droplets and in the bulk, respectively, at the time-of-flight spectrometer TOFTOF discrepancies to diffusion constants determined by PFG-NMR of more than one order of magnitude have been found. In order to find the origin of these deviations a systematical QENS study with a series of different medium chain n-alkanes was initiated. In accordance to the investigations on Q$_{10}$ it was found that in liquids of medium-chain molecules the diffusion mechanism changes on a nm length scale from a fast short range diffusion to a slower long range diffusion.

[1] T. Unruh, C. Smuda, G. Gemmecker, H. Bunjes, in Quasi-Elastic Neutron Scattering Conference 2006 (QENS2006), P.E. Sokol et al. (Eds.), Mater. Res. Soc. (2007) p. 137

CPP 8.5 Mon 16:45 Poster A

NMR surprizes with thin slices and strong gradients — •Achim Gädke[1], Benjamin Kresse[1], and Nikolaus Nestle[2] — [1]Institute of Condensed Matter Physics, Technische Universität Darmstadt — [2]present address: BASF AG Ludwigshafen GKP/P, G201

In the context of our work on diffusion-relaxation-coupling [1] in thin excited slices, we perform NMR experiments in static magnetic field gradients up to 200 T/m [2]. For slice thicknesses in the range of 10 μm, the frequency bandwidth of the excited slices becomes sufficiently narrow that free induction decays (FIDs) become observable despite the presence of the strong static gradient. The observed FIDs were also simulated using standard methods from MRI physics [3]. Possible effects of diffusion during the FID duration are still minor at this slice thickness in water but might become dominant for smaller slices or more diffusive media. Furthermore, the detailed excitation structure of the RF pulses was studied in profiling experiments over the edge of a plane liquid cell. Side lobe effects to the slices will be disucssed along with approaches to control them. The spatial resultion achieved in the profiling experiments furthermore allows the identification of thermal expansion phenomena in the NMR magnet. Measures to reduce the temperature drift problems are presented.

[1] A. Gädke, N. Nestle 2005 Diffusion Fundamentals 3 38.1-38.12
[2] I. Chang, F. Fujara, B. Geil, G. Hinze, H. Sillescu, A. Tölle, J. Non-Cryst. Sol. 172-174, (1994) 674-681
[3] T. H. Jochimsen, A. Schäfer, R. Bammer, M. E. Moseley, J. Mag. Res. 180 (2006), 29-38

CPP 8.6 Mon 16:45 Poster A

The short time self diffusion coefficient of a sphere in a suspension of rigid rods — •Jan Guzowski[1], Bogdan Cichocki[2], Eligiusz Wajnryb[2], and Gustavo Abade[2] — [1]Max Planck Institute fo Metals Research, Stuttgart — [2]Warsaw University

The short–time self diffusion coefficient of a sphere in a suspension of rigid rods is calculated in first order in the rod volume fraction ϕ. For low rod concentrations the correction to the Einstein diffusion constant of the sphere due to the presence of rods is a linear function of ϕ with the slope α proportional to the equilibrium averaged mobility diminution trace of the sphere interacting with a single freely translating and rotating rod. The two–body hydrodynamic interactions are calculated using the so–called bead model in which the rod of aspect ratio p is replaced by a stiff linear chain of touching spheres. The interactions between spheres are calculated using the multipole method with the accuracy controlled by a multipole truncation order and limited only by the computational power. A remarkable accuracy is obtained already for the lowest truncation order, which enables calculations for very long rods, up to $p=1000$. Additionally, the bead model is checked by filling the rod with smaller spheres. This procedure shows that for longer rods the basic model provides reasonable results varying less than 5% from the model with filling. An analytical expression for α as a function of p is derived in the limit of very long rods. The higher order corrections depending on the applied model are computed numerically. An approximate expression is provided, valid for a wide range of aspect ratios.

CPP 8.7 Mon 16:45 Poster A

Deuteron NMR studies on ice II — •Florian Löw[1], Marco Scheuermann[1], Burkhard Geil[2], and Franz Fujara[1] — [1]Institut für Festkörperphysik, TU Darmstadt, 64289 Darmstadt — [2]Experimentelle Physik III, TU Dortmund, 44221 Dortmund

Deuteron spin-lattice relaxation in high pressure ice II has been investigated at different temperatures.

Ice II, one of the high pressure polymorphs of ice, is a completely proton-ordered structure in which two crystallographicly distinguishable types of water molecules form a tetrahedrally linked network of hydrogen bonds.

Deuteron spin-lattice relaxation is sensitive to dynamics in the domain of the Larmor frequency at 46.7 MHz. Measurements at different temperatures of the deuteron spin-lattice relaxation time T_1 show that the magnetization recovery is unequivocally non-exponential which indicates a distribution of correlation times.

The samples (D_2O) have been prepared at appropriate pressures and temperatures. They can be recovered to ambient pressure at liquid nitrogen temperature where they remain metastable and can be studied. The sample quality is verified by x–ray diffraction. T_1–measurements have been performed while increasing the temperature stepwise. At a defined temperature a discontinuity in T_1 indicates a phase transition. The high pressure ice phase transforms to crystalline cubic ice I_c.

CPP 8.8 Mon 16:45 Poster A

Simulation of 3-Pulse Photon Echo with finite pulses — Wichard Beenken and •Ines Mynttinen — Technische Universität Ilmenau, Fachgebiet Theoretische Physik I

We performed computational simulations of the three-pulse photon echo experiments on Nile-blue as a reference. Our aim is to go beyond the impulsive limit and simulate the effect of a finite duration of the incoming laser pulses. As a first result we could show that the peak shift, i.e. the value of the first delay time where the photon echo is maximum, does not depend linearly on the pulse duration. This complicates the extrapolation of the peak shift to the impulsive limit, where it should theoretically resemble the two-point time correlation function for the fluctuating optical gap M(t). We will show how and up to which degree of time resolution from three-pulse photon echo experiment with finite pulse duration the correlation function M(t), which reflects the dissipative dynamics of the molecule in its environment, can be achieved by computational simulations of the signal dependence on the delay times. Furthermore we will discuss the sophisticated interplay between the intrinsic inhomogeneity of the molecule ensemble and the Fourier-limited spectral width of the incoming laser pulses in three-pulse photon echo experiments.

CPP 8.9 Mon 16:45 Poster A

Phase diagram of octylcyanobiphenyl confined to molecular sieves with hexagonal pore structure — Ligia Frunza[1], Stefan Frunza[1], Hendrik Kosslick[2], and •Andreas Schönhals[3] — [1]National Institute of Materials Physics, R-077125 Magurele, Romania — [2]Leibniz Institute for Catalysis at the University of Rostock, D-18059 Rostock, Germany — [3]Federal Institute for Materials Research and Testing (BAM), 12205 Berlin, Germany

The molecular dynamics of octylcyanobiphenyl (8CB) confined inside the pores of a series of AlMCM-41 samples with long range ordered structure, constant composition (Si/Al=14) but different pore sizes (between 2.3 and 4.6 nm diameter) was investigated by broadband dielectric spectroscopy (10 mHz to 1 GHz) in a large temperature interval. The filed molecular sieves show two relaxation processes: one has a bulk-like behavior and is due to the 8CB molecules in the pore centers. The second relaxation process is due to the dynamics of the molecules in a surface layer. The corresponding relaxation time is ca. two decades slower than that of the first one. Its temperature dependence obeys the Vogel/Fulcher/Tammann (VFT) characteristic for glassy dynamics. The characteristic parameters were obtained by the fit of the VFT-equation to the data and discussed as a function of pore diameter. It was found that the Vogel temperature decreases with increasing pore size.

CPP 8.10 Mon 16:45 Poster A

Gastdynamik im Tetrahydrofuran-Hydrat-Clathrat mit Hilfe der ^{2}H-NMR — •Andre Nowaczyk, Burkhard Geil und Roland Böhmer — Experimentelle Physik III, Universität Dortmund, 44221 Dortmund, Germany

Ziel unserer Arbeit ist die experimentelle Untersuchung der Gast-Dynamik in verschiedenen Clathrat-Systemen mit Hilfe der ^{2}H-NMR. Vorgestellt werden unsere bisherigen Ergebnisse bei der Untersuchung der Gastdynamik in einem Tetrahydrofuran-Hydrat-Clathrat. In diesem System findet ein Übergang von einer breiten, gaußartigen Linie bei Temperaturen über 40 K zu einem statischen Pake-Spektrum bei T¡15 K statt. Dieses Temperaturverhalten ist untypisch und wurde von uns mit Relaxationszeitmessungen untersucht, bei denen wir eine biexponentielle longitudinale Relaxation gefunden haben. Außerdem haben wir neben vollrelaxierten Festkörperechospektren in Abhängigkeit von Temperatur und Pulsabstand auch teilrelaxierte Spektren aufgenommen. Zusätzlich verwenden wir Messungen von Zwei- bzw. Vier-Zeit-Autokorrelationsfunktionen, um die Geometrie der molekularen Gastbewegung und eventuelle dynamische Heterogenitäten genauer zu untersuchen. Der untersuchte Temperaturbereich liegt zwischen 15 K und 45 K. Dort liegt die Dynamik in dem Zeitfenster, das mit unseren experimentellen Methoden zugänglich ist. Wir vergleichen unsere experimentellen Ergebnisse mit Simulationen verschiedener vorgegebener Bewegung.

CPP 8.11 Mon 16:45 Poster A

On the acoustic director interaction in the smectic A phase — •Josefina Perlo[1], Luis Aguirre[1], Jorge Revelli[2], and Esteban Anoardo[1] — [1]Universidad Nacional de Cordoba (FaMAF), Cordoba, Argentina — [2]Instituto de Fisica de Cantabria, Santander, Spain

It was shown that an acoustic field can be coupled to the collective dynamics of nematic and smectic-A specimens. Effects of ultrasound on the collective dynamics (order director fluctuations ODF) were observed through the study of the Larmour frequency dispersion of the spin-lattice nuclear magnetic relaxation time.

A fundamental task for the interpretation of the results was the understanding of the interaction mechanism between the acoustic field (a wave vector) and the mesophase director. First works on nematic showed that the acoustic field has an orienting action on the nematic director field.

The idea was extended to the smectic-A phase. The smectic nature of the problem was firstly simplified by considering a nematic in the limit of large anisotropy in the elastic constants. In this limit, the predicted behavior of the relaxation dispersion under sonication showed to be inconsistent. An improved result was obtained by considering the coupling between the smectic order and the ODF.

In this work we investigate details of the interaction between acoustic field and smectic-A phase through the inclusion of elemental features of this phase. We show that the acoustic director interaction can be enhanced if the external acoustic field matches an eigenmode of the smectic system.

CPP 8.12 Mon 16:45 Poster A

Moelcular dynamics in 2D confinement — •Ciprian Iacob, Anatoli Serghei, Rustem Valiullin, Alexey Khokhlov, Jörg Kärger, and Friedrich Kremer — Institute for Experimental Physics I, University of Leipzig, Leipzig, Germany

Broadband dielectric spectroscopy is employed to study the dynamic glass transition of several glass-forming liquids confined to nanoporous materials with pore sizes smaller than 10 nm. The nanopores are non-intersecting host systems which are prepared by electrochemical anodic etching of a highly doped p-type <100> oriented silicon substrate. The impact of interfacial interaction on the molecular dynamics in 2D confinement is analysed as well by coating the inner surface of the pores with diferent anorganic or organic surfactants.

CPP 8.13 Mon 16:45 Poster A

TD-NMR studies on CuSO4 salt hydrates — •Nikolaus Nestle[1], Sebastian Kleinschmidt[2], Peter Magin[1], and Robert Wengeler[1] — [1]BASF Aktiengesellschaft, Ludwigshafen — [2]Universität Magdeburg, FB Chemie

Despite the high concentration of paramagnetic copper ions, solid CuSO4 hydrates exhibit surprizingly narrow NMR signals. This is known since the late 1940s [1]. Using TD-NMR methods established for polymer studies, the relaxation behaviour of CuSO4 preparations with different water content was studied at room temperature. For the water content of the pentahydrate and below, the NMR signal exhibits a pure solid-state-type magnetization decay behaviour. For slightly overstoichiometric moisture contents, a liquid-like signal is observed in addition to the solid signal. However, the relative amplitudes of the solid and the liquid signal do not mirror the stoichiometric composition of the pentahydrate and the excess water. Instead, the solid signal amplitude only accounts for four hydrate water molecules while the fifth water exhibits rapid exchange with the liquid phase and thus contributes to the liquid-type signal. This finding is in good agreement to results from investigations into the crystal structure of solid CuSO4 pentahydrate [2].

[1] N. Bloembergen, Physica 16, 95-112 (1950). [2] J.J. Rush, J.R. Ferraro, A. Walker, Inorganic Chemistry 6, 346-351 (1967).

CPP 8.14 Mon 16:45 Poster A

Adsorption Kinetics of Individual Dye Molecules on Semiconductor Nanocrystal Surfaces — •Mario Heidernätsch[1], Thomas Blaudeck[1,2], Jörg Schuster[1], and Christian von Borczyskowski[1] — [1]Optical Spectroscopy and Molecular Physics, TU Chemnitz, 09107 Chemnitz, Germany — [2]Print and Media Technology, TU Chemnitz, 09107 Chemnitz, Germany

Grafting of colloidal semiconductor quantum dots (QDs) with organic molecules is a common approach to adjust their optical, chemical, and electronic properties. In this respect, QD surfaces offer a certain yet finite number of binding sites to functionalization with molecules. With that, however, the common concepts of bimolecular reaction kinetics including their dissociation constants do not hold any more.

In our computational study, we employ numerical ab-initio techniques to separate the nanoaggregate formation process into the Brownian motion of an individual molecule in solution and its eventual adsorption and desorption in the potential of a particular binding site on the QD surface. Interestingly, the extrapolation of these elementary processes to an ensemble of QDs and molecules allows insights into the relationship between surface coverage and binding energies. Conclusions thereon are up to date impossible to draw solely by experimental methods. The comparison with previous results on the formation kinetics further backs the presence of a dynamic equilibrium.

CPP 8.15 Mon 16:45 Poster A

viscosity and structural alteration of a coarse-grained model of polystyrene under steady shear low studied by reverse nonequilibrium molecular dynamics — •paola carbone, xiaoyu chen, and florian müller-plathe — Eduard-Zintl-Institut für Anorganische und Physikalische Chemie, Technische Universität Darmstadt, Petersenstrasse20 D-64287 Darmstadt, Germany

The reverse nonequilibrium molecular dynamics (RNEMD) method is implemented to predict the viscosity of a coarse-grained model of short-chain polystyrene. The coarse-grained model has been derived to reproduce the structure of polystyrene. It is therefore not a generic model, but polymer-specific. The zero-shear viscosity from simulation result is linearly dependent on the molecular weight for short-chain systems, in agreement with experiments and the theoretical prediction of the Rouse model. The shear-thinning behaviour for all studied systems follows a power law. The exponent of the power law depends on the chain length and it increases with the molecular weight. The zero-shear viscosity is also compared with experimental data, where the pronounced difference found is originated mainly by the inherent dynamic properties of the coarse-grained model used. The structural changes under shear are quantitatively investigated, indicating that the process of chain alignment, in combination with chain stretching, leads to a macroscopic anisotropy of the material.

References

1.X. Chen, P. Carbone, W. Cavalcanti, G. Milano, F. Müller-Plathe, Macromolecules, 2007, 40, 8087-8095

CPP 8.16 Mon 16:45 Poster A

Soft spots of hard spheres — •Erik Lange — University of Konstanz

The influence of the potential shape on the structure and dynamics of a colloidal suspension has been of longstanding interest. We use simulations to tackle this question from a new angle.

Exploiting molecular dynamics simulations we find strong differences in the local structure for different potentials. Even a rescaling with respect to the distance from the freezing point does not reconcile this disagreement. However the structure factor

$$S_q = \frac{1}{N}\sum_{ij}\exp\left[i(\mathbf{q}\cdot(\mathbf{r}_i-\mathbf{r}_j))\right]$$

shows a remarkable indifference towards subtleties in the potential.

The fact that a number of different systems display the same structural property suggests a closer look at the structural relaxation. As a result our work provides a clear tool to predict where differences should be negligible.

Indeed the longtime diffusion coefficients coincide as well as the stress-stress correlation at intermediate to long times.

So this is an approach that makes it clearer where softness matters and where hard spheres have soft spots.

CPP 8.17 Mon 16:45 Poster A

A colloidal approach to unspecific protein adsorption of protein films — •Olaf Leidinger, Markus Bellion, and Ludger Santen — Fachrichtung theoretische Physik, Universität des Saarlandes, 66041 Saarbrücken

We investigate the unspecific adsorption of proteins, which are modelled as colloidal particles. The particle-particle interactions are described in the framework of the DLVO theory, which includes steric repulsion, electrostatic and van der Waals interactions. In addition to this, we introduce an internal degree of freedom representing different conformations of the model protein at the surface.

By means of extensive Monte Carlo simulations we reproduce the experimentally observed characteristics of the biofilm formation. The adsorption kinetics can be divided into three intervals: Initially the adsorption is limited by the flux of particles to the surface. In a second interval one observes domain formation of compactified proteins and finally the surface coverage reaches its stationary value. The robustness of this scenario is scrutinized for various model parameters.

CPP 8.18 Mon 16:45 Poster A

NMR studies of mobility on ferrocene adsorbed in MOF-5 — •Markus Wehring[1], Pieter C. M. M. Magusin[2], Saeed Amirjalayer[3], Rochus Schmidt[3], and Frank Stallmach[1] — [1]Faculty of Physics and Earth Sciences, University of Leipzig, Germany — [2]Chemical Engineering and Chemistry, Eindhoven University of Technology, Netherlands — [3]Faculty of Chemistry and Biochemistry, Ruhr-University Bochum, Germany

Metal-organic frameworks (short: MOF) are a relatively new class of crystalline materials with a nanoporous structure. MOFs consist of metal coordination centres and organic linkers forming a three dimensional pore system with prospective applications in heterogeneous catalysis, separation and gas processing. In this study we investigate the host-guest interaction of MOF-5 (Zn_{4}O(bdc)_{3}) loaded with ferrocene (FeC_{10}H_{10}) via two-dimensional MAS NMR and PFG NMR techniques. In agreement with computer simulations, we found that the adsorbed ferrocene molecules are located close to the carbon rings of the organic linkers of the MOF-5 lattice. Additional the self-diffusion-coefficient were measured and compared with results of MD simulations.

CPP 8.19 Mon 16:45 Poster A

Charging dynamics of carbon nanotube forest electrodes — •Lars Pastewka[1] and Michael Moseler[1,2] — [1]Fraunhofer Institut für Werkstoffmechanik, Wöhlerstraße 11, 79108 Freiburg, Germany — [2]Freiburger Materialforschnungszentrum, Stefan-Meier-Straße 21, 79104 Freiburg, Germany

Efficient energy harvesting requires devices which are able to store large amounts of electrical energy in short times. In this context, electrostatic double-layer capacitors with nanostructured electrodes have been discussed. Here, we exemplarily analyse ion transport into carbon nanotube forest electrodes in order to extract response times and capacities using a multiscale modeling approach. Starting from a quantum mechanical treatment of the capacitance of single tubes we construct a molecular dynamics model for ion transport into these electrodes. Finally, a continuum transport equation is derived which reproduces the molecular dynamics results and can be used for investigating systems with realistic forest heights and electrode separations.

CPP 8.20 Mon 16:45 Poster A

Travelling Fronts in an A+B -> 2A Reaction under Subdiffusion — •Daniela Froemberg and Igor M. Sokolov — Humboldt University, Berlin

Using the continuous time random walks approach, we derive the analog of the Fisher-Kolmogorov-Petrovskii-Piskunov equation for subdiffusion, having a form of an integro-differential equation. In contrast to the normal F-KPP equation, the reaction introduces a nonlinearity into the transport term which in addition contains a fractional derivative. We show that the subdiffusive F-KPP equation includes the normal equation as a limiting case. Linearizing the equation in the leading edge of the traveling front we obtain the velocity of the front and investigate its dependence on the subdiffusion parameter alpha, the generalized diffusion coefficient, and the local reaction rate coefficient.

CPP 9: POSTERS Single Molecules, Biopolymers, Membranes

Time: Monday 16:45–19:00 Location: Poster A

CPP 9.1 Mon 16:45 Poster A

Quantification of singlet-singlet annihilation in an acceptor-donor-acceptor compound at the single molecule level — •Burkhard Fückel[1], Gerald Hinze[1], Florian Diehl[1], Fabian Nolde[2], Klaus Müllen[2], and Thomas Basché[1] — [1]Institut für Physikalische Chemie, Johannes Gutenberg-Universität, Jakob-Welder-Weg 11, 55099 Mainz, Germany — [2]Max-Planck-Institut für Polymerforschung, Ackermannweg 10, 55128 Mainz, Germany

We have investigated a new multichromophoric compound consisting of a central perylendiimide donor (D) chromophore and two terrylendiimide acceptor (A) chromophores adjacent to it (A-D-A). After electronic excitation of the donor chromophore, energy is rapidly transferred to the acceptor chromophores. Time-resolved measurements by means of optical single molecule spectroscopy revealed that singlet-singlet annihilation (SSA) takes place upon excitation of both acceptor chromophores.

We quantitatively determined the rate of the SSA process at the single molecule level. Our approach combines the detection of photon arrival time coincidences with Monte Carlo simulations. On average the SSA rate is found to be two to three times faster than the fluorescence lifetime of terrylendiimide.

CPP 9.2 Mon 16:45 Poster A

Gold Nanoparticles Decorated with Oligo(ethylene glycol) Thiols: The Effect of Salt Nature on the Stability of Colloid-Protein Mixtures — •Fajun Zhang[1], Maximilian W. A. Skoda[1,2], Robert M. J. Jacobs[2], Stefan Zorn[1], Richard A. Martin[3], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen, Germany — [2]CRL, University of Oxford, UK — [3]Department of Physics, University of Bath, UK

The stability of mixtures of oligo(ethylene glycol) (OEG) thiol self-assembled monolayer protected gold colloids and globular proteins in solution, depends strongly on the nature of added salts. UV-vis spectroscopy was used to study the stability of the mixtures by monitoring the time dependence of the flocculation [1]. It was shown that the OEG-protected gold colloid solution is stable in the presence of NaCl, NaSCN, MgCl2, but loses its stability on addition of Na2SO4. In the mixtures of colloid and protein, the colloids lose their stability and form aggregates upon adding protein above a critical concentration, c*, due to the depletion effect [1]. Adding NaCl or Na2SO4 to the mixtures enhances the colloid aggregation; NaSCN stabilizes the solution, and MgCl2 results in a long induction time before aggregation. The observed salt nature effects follow the “Hofmeister series” and are discussed based on the salting-in or salting-out effect as well as the ion-absorption effect. The salt nature effect is planned to be further studied by SAXS. [1] F. Zhang, et al., J. Phys. Chem. B. 2007, 111, 251. J. Phys. Chem. A. 2007, DOI: 10.1021/jp074293v. Euro. Biophys. J. Submitted.

CPP 9.3 Mon 16:45 Poster A

Blinking induced bleaching and recovery of organic dyes in polymer materials — •Ines Trenkmann, Jörg Brabandt, Jörg Schuster, and Christian von Borczyskowski — TU Chemnitz, Institut für Physik, 09107 Chemnitz

Fluorescence intermittency, usually referred to as blinking, is a common feature of individual emitters embedded into or close to dielectric materials such as polymers or silicon oxides [1]. If the photoluminescence from ensembles of emitters is observed under conditions similar to single emitter studies, blinking processes lead to a reversible change of the intensity, which is in most cases a decrease of intensity [2]. Such reversible intensity decays and its recovery have been studied by us for ensembles of different dye/polymer systems. Our preliminary results show, that the kinetics of the fluorescence recovery is rather a function of the matrix than of the emitter. While fluroescence recovery of dyes in PVA occurs on a time scale of seconds it takes several hours to days in polystyrene. Based on those findings and recent publications [1] the model of blinking as a process of ejecting and trapping of charges in dielectric materials gains further evidence. In conclusion, we suggest to use blinking vive versa as a probe for charge trapping in dielectric properties. Our results show, that blinking phenomena can be studied easily on the ensemble level by bleaching and recovery experiments.

[1] F. Cichos, C. von Borczyskowski, M. Orrit: Curr. Op. Coll. Interf. Sc. 12 (2007), 272

[2] J. Brabandt, J. Schuster, C. von Borczyskowski: J. Luminescence 127 (2007),224

CPP 9.4 Mon 16:45 Poster A

New NIR fluorophores for single molecule microscopy — Georg M. Fischer, Martin Winterhalder, Magnus Isomäki-Krondahl, Andreas Zumbusch, and •M. Yavuz Yüce — Department Chemie, Universität Konstanz, Fach M722, D-78457 Konstanz

Excitation in the near infrared (NIR) geneally leads to lower background signal in single molecule experiments. For this reason, strongly fluorescent chromophores which absorb and emit in the NIR are highly desirable for such applications. According to the energy gap law, however, most fluorophores will only exhibit very weak NIR fluorescence emission. Here we present a new class of dyes based on diketopyrrolopyrroles. At absorption wavelengths of up to 800 nm, these dyes still exhibit fluorescence quantum yields of more than 50%. We have characterized a broad variety of derivatives both on the ensemble and on the single molecule level.

CPP 9.5 Mon 16:45 Poster A

Measuring distance fluctuations by single pairs of gold nanoparticles — •Miriam Wähnert[1], Romy Radünz[2], and Frank Cichos[3] — [1]Molecular Nanophotonics Group, University Leipzig, 04103 Leipzig — [2]Molecular Nanophotonics Group, University Leipzig, 04103 Leipzig — [3]Molecular Nanophotonics Group, University Leipzig, 04103 Leipzig

Single Molecule fluorescence resonance energy transfer (SMFRET) measures distance changes. This is heavily applied in biophysical studies. In combination with time resolved time tagged fluorescence detection it even allows the study of the dynamics of conformational fluctuations. However, the distance fluctuations accessible are limited to a range up to about 10 nm. Further, the technique suffers often from fluorescence blinking or bleaching of either donor or acceptor of the energy transfer dye couple.

We report on experiments, which employ the plasmon coupling between two gold nanoparticles to monitor distance fluctuations. The plasmon coupling of two gold particles is visible at distances up to a few 10 nm. Therefore it measures distance fluctuations on a much longer lengthscale than SMFRET. The interaction of the two plasmon oscillations shifts the extinction spectrum to longer wavelength. An optical signal off resonance of the single particle resonance is a measure for the particle distance. We use a photothermal detection technique to monitor the distance fluctuations between very small particles that are difficult to detect by optical scattering. First experimental results will be presented together with a numerical analysis of the technique.

CPP 9.6 Mon 16:45 Poster A

Investigations of single quantum dot (QD) blinking via Fluorescence Correlation Spectroscopy (FCS) — •Nicole Amecke and Frank Cichos — Molecular Nanophotonics Group, University of Leipzig, Linnéstraße 5, 04103 Leipzig

The intermittency of QD fluorescence (blinking) is a well known, intensively studied, but still not fully understood phenomenon. Control over this peculiarity is strongly desired for many applications of QDs as reliable light sources. This however remains still a fair wish and needs deeper understanding of the underlying processes. The observed dark states are supposed to result from ionization processes, where one charge is ejected from the QD into localized states of the surrounding medium. Auger processes, enabled by the remaining charge, will then inhibit photon emission until neutralization. The durations of dark (charged) as well as bright (neutral) periods are found to obey power law statistics, which can be understood to result from a tunneling process of the charge to and from a wide distribution of trap states in the matrix. This explanation holds for a solid matrix while deviations in liquid matrices can be expected. In ensemble investigations effects of blinking simply result in lower emission intensity. FCS, however, offers a method to investigate blinking of QDs in solution. When keeping the detection volume small via confocal spectroscopy, the diffusion of single emitters through the focus can be investigated, obtaining diffusion properties, but also blinking effects. We find that both, shape and contrast, of the correlation function depend on the excitation power. This leads to an apparent concentration change as deduced by FCS.

CPP 9.7 Mon 16:45 Poster A

Kinetics of TmHU binding to DNA as observed by optical tweezers — •Mathias Salomo, Carolin Wagner, Ulrich Keyser, and Friedrich Kremer — Linnéstraße 5, 04103 Leipzig

The kinetics of binding for the histone-like protein TmHU (from Thermotoga maritima) to DNA is analyzed on a single molecule level by use of optical tweezers. For the reaction rate a pronounced concentration-dependence is found with an "all or nothing-limit" which suggests the cooperative nature of the binding-reaction. By analyzing the statistics of mechanically induced dissociation- events of TmHU from DNA multiple reaction sites are observed to become more likely with increasing TmHU concentration. This is interpreted as a hint for a secondary organizational level of the TmHU/DNA complex. The reaction rate of TmHU binding to DNA is remarkably higher than that of the HU protein from Escherichia coli which will be discussed.

CPP 9.8 Mon 16:45 Poster A

Higher order laser modes as a tool to determine single-molecule orientation in an optical microresonator — •Raphael Gutbrod, Anna Chizhik, Dmitry Khoptyar, and Alfred Johann Meixner — University of Tübingen, Institute for Physical and Theoretical Chemistry, Auf der Morgenstelle 8, 72076 Tübingen (Germany)

Subwavelength optical microresonators show great potential as a platform for single-photon emitting sources and sensors on the nano-scale. Due to modification of the optical state density inside the microresonator the emission properties of single molecules can be strongly modified, which includes spectral and spatial redistribution of the spontaneous emission as well as enhancement and inhibition of the spontaneous emission rate due to the Purcell-effect [1].

A recently developed technique for determination of single-molecule orientation is based on excitation with azimuthally and radially polarized doughnut laser modes. Analysing the single molecular excitation patterns with confocal microscopy allows one to determine the orientation for many molecules from one scan image.

Using a novel microresonator designed in our group we investigate the excitation patterns of fluorescent beads with these laser modes aiming at a better understanding of the cavity electrodynamics. This is a crucial point for optimal cavity design which may open a perspective for new integrated nano-optical sensing.

[1] M. Steiner, F. Schleifenbaum, C. Stupperich, A. V. Failla, A. Hartschuh, A. J. Meixner . ChemPhysChem 2005, 6, 2190

CPP 9.9 Mon 16:45 Poster A

N-V center in diamond as spin-selective sensor — •Bernhard Grotz, Gopalakrishnan Balasubramanian, Inam Mirza, Fedor Jelezko, and Jörg Wrachtrup — 3. Physikalisches Institut, Universität Stuttgart, Germany

Due to its biocompatibility and chemical stability, diamond is a promising candidate for biological applications. In particular fluorescent properties of N-V colour centers in diamond have attracted interest because of unlimited photostability [1]. We show the concept and first experiments how such colour centers can be used as a sensor for biomolecules absorbed on diamond surfaces. Since N-V centers are paramagnetic, their fluorescence can be employed as spin-selective sensor.

[1] A. Gruber et al., Science 276, 2012 (1997)

CPP 9.10 Mon 16:45 Poster A

A detailed theoretical analysis of the optical spectra of the prototype molecules tetracene and rubrene — •Taras Petrenko, Olga Krylova, Moritz Sokolowski, and Frank Neese — Institute for Physical and Theoretical Chemistry, Bonn University, Wegelerstrasse 12, 53115 Bonn, Germany,

Tetracene and rubrene are two prototype fluorescent molecules which are presently intensively studied. Interestingly, both molecules exhibit the same fluorescent backbone. However, due to electric repulsion between the phenyl groups, the backbone of rubrene is twisted, whereas it is planar for tetracene. Optical spectroscopy reveals that the $S_0 \rightarrow S_1$ transition in rubrene is redshifted with respect to tetracene by $\sim$2000 cm^{-1} and that rubrene exhibits a considerably larger Stokes shift. In order to unravel the physical effect responsible for these differences we have performed normal coordinate analysis and frequency calculations using density functional theory in conjunction with linear response time-dependent density functional theory energy scan calculations. This yielded dimensionless normal coordinate displacements of the excited-state origin that were employed to calculate and fit the vibrational finestructure in absorption and fluorescence spectra. The analysis reveals that the $\sim$2000 cm^{-1} red shift of 0-0 vibronic band of rubrene relative to tetracene is mainly caused by the inductive effect of the phenyl substituents that leads to destabilization of the donor MO. (Funded by the DFG research unit 557 and the university of Bonn)

CPP 9.11 Mon 16:45 Poster A

A detailed theoretical analysis of the optical spectra of the prototype molecules tetracene and rubrene — •Taras Petrenko, Olga Krylova, Moritz Sokolowski, and Frank Neese — Institute for Physical and Theoretical Chemistry, Bonn University, Wegelerstrasse 12, 53115 Bonn, Germany,

Tetracene and rubrene are two prototype fluorescent molecules which are presently intensively studied. Interestingly, both molecules exhibit the same fluorescent backbone. However, due to electric repulsion between the phenyl groups, the backbone of rubrene is twisted, whereas it is planar for tetracene. Optical spectroscopy reveals that the $S_0 \rightarrow S_1$ transition in rubrene is redshifted with respect to tetracene by $\sim$2000 cm^{-1} and that rubrene exhibits a considerably larger Stokes shift. In order to unravel the physical effect responsible for these differences we have performed normal coordinate analysis and frequency calculations using density functional theory in conjunction with linear response time-dependent density functional theory energy scan calculations. This yielded dimensionless normal coordinate displacements of the excited-state origin that were employed to calculate and fit the vibrational finestructure in absorption and fluorescence spectra. The analysis reveals that the $\sim$2000 cm^{-1} red shift of 0-0 vibronic band of rubrene relative to tetracene is mainly caused by the inductive effect of the phenyl substituents that leads to destabilization of the donor MO. Funded by the DFG research unit 557 and the university of Bonn)

CPP 9.12 Mon 16:45 Poster A

Understanding Molecular Transport — •Angelica Zacarias and Eberhard K.U. Gross — Institut für Theoretische Physik, Freie Universität Berlin, Germany

In the past, computers have grown increasingly powerful as their basic elements became smaller. Present-day silicon technology allows integrated circuits on the micron scale. With the advent of the new generation of High-k transistors the gate length reach sizes between 85-45nm. However to further reduce the size, device designs have to be replaced by new concepts which make use of the quantum mechanical effects that dominate the atomic scale. The basic idea of molecular electronics is to use single-molecules as the basic elements of the electronic devices. The flexibility of such "molecular transistors" originates in the sensitivity of the IV-characteristics to the subtle details of the molecules. Theoretical simulations of such systems can play a key role in unveiling the mechanisms that control molecular transport. Calculations have so far shown that the shape of IV characteristics is determined primarily by the electronic states of the molecule, as they evolve as a function of an applied bias, whereas the overall magnitude of the current is controlled by the details of the molecule-electrode contacts. Using a combined density-functional theory (DFT) and Green's function approach we present the IV-characteristics of C$_{60}$ sandwiched between two gold metallic tips. Among other results we will present an encouraging comparision with experimental results of the conductance properties of C_{60} on Au(111).

CPP 9.13 Mon 16:45 Poster A

Nanopatterning of functional protein arrays — •Mark Schnietz[1], Helge Grossmann[2], Harun Solak[3], Robert Tampé[2], Andrey Turchanin[1], and Armin Gölzhäuser[1] — [1]Department of Physics, Physics of Supramolecular Systems, University of Bielefeld, D-33615 Bielefeld — [2]Institute of Biochemistry, Biocenter, Johann Wolfgang Goethe-University, D-60438 Frankfurt — [3]Laboratory for Micro and Nanostructuring, Paul Scherrer Institut, CH-5232 Villigen PSI

The ability to anchor oriented and functional protein arrays at the nanoscale affords useful materials for both fundamental research in biophysics/-chemistry and biotechnological and tissue engineering applications. In this contribution we present a novel approach to the fabrication of protein nanoarrays based on the combination of extreme UV interference lithography (EUV-IL) of self-assembled monolayers for the generation of chemical nanopatterns [1] (top-down) and biochemical tweezers, multivalent surface chelators [2] (tris-nitrilotriacetic acid, tris-NTA), for high affinity capturing of His-tagged proteins (bottom-up). The functionality of the generated protein arrays was demonstrated under physiological conditions via specific, homogeneous, oriented and reversible immobilization of His6-tagged 20S proteasome and fluorescence labeled His10-tagged maltose-binding proteins [3]. Various highly periodic dot and line patterns with areas up to ˜10 mm2 and features from 1000 nm to 50 nm were built in this way. [1] A. Turchanin et al., Small 2007. [2] A. Tinazli et al., Chem. Eur. J. 2005, 11, 5249. [3] A. Turchanin et al., Adv. Mater. 2007.

CPP 9.14 Mon 16:45 Poster A

Linear and nonlinear mechanics of bundles of semiflexible filaments — •Felix Schueller[1], Claus Heussinger[1,2], and Erwin Frey[1] — [1]Ludwig-Maximilians-Universitaet Muenchen, Muenchen, Germany — [2]Université de Lyon I, LPMCN, Villeurbanne, France

Bundles formed from semiflexible polymers play an important role in many physiological processes inside and outside of the cell.

We have previously defined a simple model ("wormlike bundle", WLB [1]) that describes the dynamical and statistical mechanical properties of semiflexible polymer bundles in terms of a mode-number dependent bending stiffness $\kappa(q)$.

While this treatment was restricted to in plane deformations of the bundle, we show here, how the WLB can be extended to a fully three-dimensional model that, in particular, includes twist deformations.

In this framework, we examine buckling instabilities under external force or torque. We solve the eigenvalue problem for determining the critical load as well as integrate numerically the nonlinear Euler-Lagrange equations to find the post-buckling bundle shapes.

[1] C. Heussinger, M. Bathe, and E. Frey, Phys. Rev. Lett. 99, 048101 (2007)

CPP 9.15 Mon 16:45 Poster A

High energy reflectivity studies of protein adsorption on functionalized surfaces — •Kaveh Shokuie[1], Michael Paulus[1], Florian Evers[1], Federica Venturini[2], Sebastian Schoeder[2], and Metin Tolan[1] — [1]Experimentelle Physik Ia/ DELTA, Technische Universität Dortmund, Maria-Goeppert-Meyer Str. 2, 44221 Dortmund — [2]European Synchrotron Radiation Facility, Grenoble, France

Adsorption of several proteins (Lysozyme, Hemoglobin, α-lactalbumin) on functionalized surfaces was investigated using high energy X-ray reflectivity. The main interest is the effect of different substrate surfaces on the protein adsorption behaviour (e.g. conformational changes of the protein). The applied technique, X-ray reflectivity, makes it possible to determine the sample's density profile perpendicular to its surface with Angstrom resolution. The high energy reflectivities were taken at the ID15 beamline of the ESRF using 72.5 keV radiation. The high photon energy allows the in situ investigation of the protein adsorption at the solid-liquid interface.

CPP 9.16 Mon 16:45 Poster A

Biofilm adsorption on tailored substrates: Ellipsometry, AFM, SPR and neutron scattering results — •Hendrik Hähl, Hubert Mantz, Yvonne Schmitt, and Karin Jacobs — Saarland University, Experimental Physics, D-66123 Saarbrücken, Germany

Whenever a protein solution is in contact with a material, the proteins will adsorb onto the surface. Everyday examples for this process are biofilms on teeth. This study aims to reveal the influence of surface properties on the adsorption process. Our results show that the adsorption kinetics of e.g. α-amylase is sensitive to the thickness of the oxide layer on top of the Si wafer. This is astonishing since the chemistry of the offered surfaces is identical, meaning that the short-range forces are not varied. Only the long-range forces are altered by a variation of the oxide layer thickness, and they play a central role for the adsorption kinetics. Theoretical models and simulations suggest that a variation of long-range forces can lead to conformational changes of the proteins during the adsorption. To test this hypothesis, experiments with atomic force microscopy (AFM), surface plasmon resonance (SPR) spectroscopy and ellipsometry as well as neutron reflectivity measurements have been performed.

CPP 9.17 Mon 16:45 Poster A

Nonlinear rheology of a glassy solution of semiflexible polymers — •Christian Hubert[1], Jens Glaser[1], and Klaus Kroy[1,2] — [1]ITP,Universität Leipzig, PF 100920,04009 Leipzig — [2]HMI,Glienicker Str. 100, 14109 Berlin

Recent experimental studies on purified solutions of the semiflexible biopolymer F-actin show a pronounced transition of shear softening to shear stiffening behavior as a function of different physiological parameters. The results suggest a surprising invariance of the rheology of the F-actin solution with respect to the choice of the control parameter. This property is successfully explained by the recently introduced glassy wormlike chain (GWLC) model, where the nonlinear response is traced back to a strong stretching of the relaxation spectrum of an ordinary wormlike chain. The model incorporates two stretching parameters corresponding to the height of free energy barriers due to stickiness and steric (free volume) interactions respectively, slowing down the relaxation of the polymer. A comprehensive overview of the dependence of the stretching parameters and the shear modulus on the physiological parameters is given.

[1] Semmrich, Storz, Glaser, Merkel, Bausch, Kroy,
PNAS, In Press (2007)
[2] arXiv: 0705.0490, arXiv: 0711.2427

CPP 9.18 Mon 16:45 Poster A

AFM Studies of Langmuir-Blodgett Films of Acidic Peptides — •Manuela Pluntke[1], Haofei Gong[2], Yi Yang[3], Norbert Sewald[3], Dirk Volkmer[2], and Othmar Marti[1] — [1]Institute of Experimental Physics, Ulm University, D-89069 Ulm — [2]Institute of Inorganic Chemistry II, Ulm University, D-89069 Ulm — [3]Faculty of Chemistry (AC 1), University of Bielefeld, PO Box 100 131, 33501 Bielefeld

Acidic proteins are found to play an important role in biomineralization. Extracted from different calcified tissues, they were shown to control polymorph selection, texture and morphology of $CaCO_3$ crystals. We recently fabricated Langmuir-Blodgett Monolayers of different artificial acidic peptides with β-hairpin conformation (H-Asp-(Phe-Asp)$_3$-D-Pro-Gly-Asp-(Phe-Asp)$_3$OH, H-Glu-(Phe-Glu)$_3$-D-Pro-Gly-Glu-(Phe-Glu)$_3$OH). Circular Dichroism Spectra show that these two peptides take a random coil and β-sheet structure in HFIP solution, respectively. At the air/water interface, significant differences of the peptide monolayer properties were found as revealed by surface pressure-area isotherms and BAM, although they have similar primary structure. Moreover, crystallization of $CaCO_3$ beneath these monolayers revealed different crystal morphologies. For a more detailed analysis of the peptide arrangement at interfaces we transfered the monolayers on mica and investigated them by means of high resolution AFM. Based on preliminary studies we assume that only the peptide H-Glu-(Phe-Glu)$_3$-D-Pro-Gly-Glu-(Phe-Glu)$_3$OH forms a highly ordered lattice of hairpin structures.

CPP 9.19 Mon 16:45 Poster A

Carbon dioxide hydrate formation at the carbon dioxide - water interface — •Felix Lehmkühler[1], Michael Paulus[1], Christian Sternemann[1], Daniela Lietz[1], Federica Venturini[2], and Metin Tolan[1] — [1]Technische Universität Dortmund, Experimentelle Physik I/DELTA, Maria-Goeppert-Mayer-Str. 2, 44221 Dortmund, Germany — [2]ESRF, BP 220, 38043 Grenoble Cedex 9, France

The formation of gas hydrate at the water - carbon dioxide interface was studied by x-ray reflectivity and x-ray diffraction experiments. CO_2 forms under high pressures and low temperatures cubic water cages with a lattice constant of 12 Å (structure I hydrate) and a CO_2 molecule in the center. At a temperature of 0°C a minimum pressure of 12.5 bar is required for CO_2 hydrate stability. In nature this formation takes usually place at the water - gas interface due to a higher gas concentration in comparison with the water bulk. However, the microscopic formation process is still not understood.

The water - CO_2 interface was investigated at a temperature of 0°C and gas pressures up to the condensation pressure of CO_2 of 35 bar. A pressure dependent adsoprtion of thin CO_2 layers is observable, but no hydrate formation. In contrast, after rising the gas pressure to condensate a macroscopic thick CO_2 layer hydrate crystallites could be observed at the liquid-liquid interface using x-ray diffraction.

To investigate this formation more precisely diffraction patterns were measured at different height positions of the sample. Hydrate clusters were observable at all positions except the gas phase. However, the highest formation rate is found at the water - liquid CO_2 interface.

CPP 9.20 Mon 16:45 Poster A

Lysozyme Adsorption at the Silica/Water Interface: an in situ High Energy X-ray Reflectivity Study — •Florian Evers, Kaveh Shokuie, Michael Paulus, Christian Sternemann, and Metin Tolan — TU Dortmund, Fakultät Physik/DELTA, Maria-Goeppert-Mayer-Str. 2, 44221 Dortmund, Germany

Lysozyme adsorption at the silica/water interface has been studied using high energy x-ray reflectivity which is a well-established method to study the structure of thin films. Data on protein layers adsorbed at solid/liquid interfaces are still rare. The dispersion profile of adsorbed lysozyme layers at hydrophilic silica interfaces, the effect of pH and protein concentration of the aqueous solution on the adsorption, and the time-dependence of the adsorption process were studied. Our observation of lysozyme monolayer adsorption is partially in contrast to former measurements with neutrons and to predictions.

CPP 9.21 Mon 16:45 Poster A

The Effect of electrolytes on interactions in thin aqueous wetting films — •Natascha Schelero, Katarzyna Hänni-Ciunel, and Regine von Klitzing — Stranski-Laboratorium, Institut der Chemie, TU Berlin, Strasse des 17. Juni 124, D-10623 Berlin

The (de)stability and functionality of thin wetting films plays an important role for processes in technical applications. The forces between the opposing interfaces depend on the composition of the film interfaces and of the film fluid. In the present paper the sum of interactions between the film surfaces is determined quantitatively by the disjoining pressure isotherm and it is measured by varying the outer pressure in a thin film pressure balance. Usually, this apparatus is used for disjoining pressure measurements at free-standing foam films (air/liquid/air). In recent studies we showed that it also can be used for the investigation of wetting films (air/liquid/solid) [1]. Water films in presence of 0.1 mM NaCl are stable against negatively charged interfaces like bare Silicon or Silicon coated with negatively charged polyelectrolytes, but unstable against positively charged surfaces. The films become thinner and less stable with increasing ionic strength indicating that the forces within the water film are controlled by electrostatic interactions [2]. The results give a clear evidence for negative charges at the free air/water interface [3]. Further on, the effect of specific ions on the stabilisation by electrostatic interfacial repulsion is investigated. [1] R. v. Klitzing, Adv. Coll. Interf. Sci., 2005,114/115:253 [2] Hänni-Ciunel K. et al., Soft Materials, 2007, 5 (2), 61-73 [3] Ciunel K. et al., Langmuir 2005 21 4790 - 4793

CPP 9.22 Mon 16:45 Poster A

Investigations on the Structure and Dynamics of DMPC-Monolayers used as Stabilizers in Colloidal Dispersions — •Sebastian Busch, Christoph Smuda, and Tobias Unruh — Forschungsneutronenquelle Heinz Maier-Leibnitz and Physik Department E13, Technische Universität München, Munich, Germany

Many modern drugs are not water-soluble. To facilitate their intravenous applicability, a drug carrier has to be employed. Dispersions of lipid nanoparticles stabilized by dimyristoylphosphatidylcholine (DMPC) are promising candidates. It has been shown [1] that not only the drug release rate but also the storage stability of these systems highly depends on the properties of the stabilizer. These properties were investigated i. a. by small angle X-ray scattering [2], revealing that the structure of the monolayer is clearly distinct from the well-known structure of bilayers. A series of experiments aiming to determine the dynamic characteristics of DMPC-monolayers was carried out at the cold neutron time–of–flight spectrometer TOFTOF at the Forschungsneutronenquelle Heinz Maier-Leibnitz in Garching bei München. First results are presented and discussed.

[1] K. Westesen, B. Siekmann, Int. J. Pharm., 151 (1997) 35; H. Bunjes, M. H. J. Koch, K. Westesen, J. Pharm. Sci. 92 (2003) 1509; H. Bunjes, F. Steiniger, W. Richter, Langmuir 23 (2007) 4005

[2] T. Unruh, J. Appl. Cryst. 40 (2007) 1008

CPP 9.23 Mon 16:45 Poster A

Microscopic theory of liquid-vapour interface of simple fluids — •Vitalie Botan and Martin Oettel — Institut für Physik, WA 331, Johannes-Gutenberg-Universität Mainz, Mainz, Germany

The liquid-vapor interface of Lennard-Jones fluids is examined by combining integral equation and density functional theory. In this approach a closure of reference hypernetted chain type to the inhomogeneous Ornstein-Zernike equation for the correlations functions is developed employing a bridge functional (instead of a bridge function) of a suitably chosen hard-sphere reference system. Using Tarazona's free energy functional for the reference system, the obtained self-consistent solutions for the density profiles and inhomogeneous two-body correlation functions are analyzed with respect to the mesoscopic capillary wave picture.

CPP 9.24 Mon 16:45 Poster A

Temperature dependent (2D) ordering in monolayers of amphiphile molecules — •Saskia Schmacke[1], Bernd Struth[2], Lutz Wiegart[3], Henri Gleyzolle[3], Michael Paulus[1], and Metin Tolan[1] — [1]Fakultät Physik /DELTA, Technische Universität Dortmund, D-44221 Dortmund, Deutschland — [2]DESY, D-22602 Hamburg, Deutschland — [3]ESRF, B.P. 220, 38043 Grenoble Cedex, France

Layers of amphiphile molecules on liquid substrates show a different phase behaviour depending on environmental parameters such as temperature, surface pressure and subphase. In this work the solid phase of the Phospholipid monolayer DPPC (dipalmitoylglycerophosphocholine) was analysed in order to investigate the influence of temperature on the crystaline structure of the layer. The latter was determined by the use of the Gracing Incidence X-Ray Diffraction technique (GID) at the beamline ID10b, ESRF. The obtained diffraction spectra are analysed in two steps: First the information about the 2D unit cell of the crystalline phase, e.g. lattice spacings, lattice type (2D Bravais lattice) and the deformation of the lattice was determined. In the second step the intensity dependence on the wave vector transfers perpendicular to the surface was analysed leading to information about the scatterer itself. Thus, chain length, diameter, tilt angle and orientation within the lattice of the molecules forming the monolayer are determined. A temperature induced phase transition from a centred rectangular to a hexagonal lattice with decreasing temperature was observed.

CPP 9.25 Mon 16:45 Poster A

Estimation of spinodals in pure fluids from interfacial properties obtained from equilibrium molecular dynamics and lattice Boltzmann simulations — Attila Imre[1], Gusztav Mayer[1], Gabor Házi[1], Roberto Rozas[2,3], and •Thomas Kraska[3] — [1]Simulator Development Department, KFKI Atomic Energy Research Institute — [2]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt, Linder Höhe, D-51147 Köln — [3]Institut für Physikalische Chemie, Universität zu Köln, Luxemburger Str. 116, D-50939 Köln

In this work, local pressure and density profiles of a liquid film in contact with its vapor at equilibrium are calculated. Two methods are employed; molecular dynamics and lattice Boltzmann simulations. The set of local values of tangential pressure and density along a liquid-vapor interface exhibits a van der Waals-like loop. The loci of the extreme values of local tangential pressure in the interfacial profile are related to the spinodal state. The maximum and minimum values of the tangential pressure are linearly related to the vapor and liquid spinodal pressures, respectively. The coefficient of the relationship appears to be universal and of geometrical origin. Comparison of the spinodal curves obtained from equations of state shows good agreement with the simulation results. Based on this investigation a method is proposed for the estimation of the liquid spinodal from experimental data. Estimations for water and helium are presented.

CPP 9.26 Mon 16:45 Poster A

Heterogeneous nucleation and growth of high wettable systems studied by molecular dynamics simulations — •Roberto Rozas[1,2] and Thomas Kraska[2] — [1]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt, Linder Höhe, D-51147 Köln — [2]Institut für Physikalische Chemie, Universität zu

Köln, Luxemburger Str. 116, D-50939 Köln

Heterogeneous nucleation and growth of supersaturated argon vapor at polyethylene surfaces is investigated by molecular dynamics simulations. The system serves as a model for high wettable systems. A non-equilibrium ensemble which allows the development of gradients in the system is employed; Nosé-Hoover thermostat is applied to the polymer substrate only while the vapor condenses. Simulations along an isotherm at different initial saturation of the vapor indicate a transition, close to the binodal, from adsorption to heterogeneous nucleation. At moderate saturation the layer-by-layer growth mechanism dominates while at higher supersaturation a tendency to growth islands-on-layers growth is observed. We find for this system that a two-dimensional version of the classical heterogeneous nucleation theory (HEN2D) is most suitable to describe the nucleation rate data versus saturation obtained from simulation.

CPP 10: POSTERS New Materials, Organic Semiconductors

Time: Monday 16:45–19:00 Location: Poster A

CPP 10.1 Mon 16:45 Poster A

Optical properties of Biaxial Nematogens — •David Polster[1], Christiane Köhn[2], Jens Seltmann[2], Matthias Lehmann[2], Harald Graaf[1], Jörg Schuster[1], and Christian von Borczyskowski[1] — [1]Center of Nanostructured Materials and Analytics, TU Chemnitz, 09107 Chemnitz, Germany — [2]Juniorprofessur Nichtklassische Synthesemethoden, TU Chemnitz, 09107 Chemnitz, Germany

Typical liquid crystalline molecules (nematogens) are characterized by a linear shape with one permanent dipol and are known to form a nematic phase. In biaxial nematogens (V-shaped molecules) instead two perpendicular dipoles can be found. For such mesogens the tendency to form the so illusive biaxial nematic phase is proposed for which up to 100fold faster switching times are expected.

We will present here a new class of unsymmetric substituted V-shape molecules. These mesogens consists of a bent core which defines the dihedral angle of the V-shaped molecule and two rigid arms with cyano substituted terminal aromatic units. They are characterized by two different dipole moments along the short and the long molecular axis. The thermotropic behavior of these new materials has been investigated and its nematic phase was characterized. The orientation of the nematogens in a typical liquid crystal cell will be shown and the influence of an applied electric field will be discussed. An alignement along the short axis of the molecule under electric field plays the major role for low voltages.

CPP 10.2 Mon 16:45 Poster A

Switchable Fluorescence Cell — •Frank Friedriszik, Harald Graaf, Jörg Schuster, and Christian von Borczyskowski — Center of Nanostructured Materials and Analytics, TU Chemnitz, 09107 Chemnitz, Germany

Calamitic liquid crystaline materials are well known and used in a wide spread of display applications. One of the most common material is the 4-pentyl-4-cyanobiphenyl (5CB) which is in the nematic phase at room temperature. Rubbed polyimid films can be used for an orientation of these calamitic liquid crystals in a liquid crystal cell where the molecules are aligned parallel to the substrate and with its axis along the rubbing direction. Due to the permanent dipole moment of the LC molecule an applied electric field perpendicular to the substrate surface will switch the orientation of the molecules parallel to the electric field.

Here we present recent results on the alignment of a rod like organic dye molecule doped into the liquid crystal and which orients within the liquid crystal parallel to the 5CB molecules. Thus, in the liquid crystal cell the organic molecules are oriented parallel to the substrate surface and its orientation will be switched together with the liquid crystal in an electric filed. As the transition dipol of the dye molecule is oriented along the axis of the molecule its luminescence is also switched by the electric fields. Thus we are able to demonstrate a prototype of a switchable fluorescence cell. Besides potential display applications, such a dye which aligns with the liquid crystal is also a perfect probe of local liquid crystal structure.

CPP 10.3 Mon 16:45 Poster A

Chemical modification and radiation induced degradation of the photoresist SU-8 — •Angela Keppler[1], Marcel Himmerlich[1], Christoph Kremin[1], Jens T. Schumacher[2], Andreas Grodrian[2], Juergen A. Schaefer[1], Josef Metze[2], Martin Hoffmann[1], and Stefan Krischok[1] — [1]Institut für Mikro- und Nanotechnologien, TU Ilmenau, P.O. Box 100565, 98684 Ilmenau, Germany — [2]Institut für Bioprozess- und Analysenmesstechnik e.V., Rosenhof, 37308 Heilbad Heiligenstadt, Germany

An increasing interest in using the epoxy-based photoresist SU-8 for producing bio-MEMS or microfluidic devices is noticeable. In biological applications, sterilisation processes using chemical treatments or UV radiation are common practice and the analysis of their interaction with SU-8 is of great interest. Employing X-ray photoelectron spectroscopy and contact angle measurements, we have investigated the changes in the surface chemical composition upon IR, UV and X-ray irradiation as well as the impact of contact with chemicals. The treatment of SU-8 with H_2SO_4 results in oxidation (formation of C=O bonds) while at NaOH treated surfaces, a reduction of ether bonds is found. Radiation induced changes and degradation of the polymer induced by X-ray, UV and IR irradiation were characterised. In contrast to X-ray and IR radiation where no modification was found, UV photons preferentially attack the ether bonds in SU-8, resulting in a strong degradation of the material. The chemical changes are correlated to differences in the contact angle of the material as well as its optical properties.

CPP 10.4 Mon 16:45 Poster A

A co-axial dielectric elastomer actuator — •Hristiyan Stoyanov, Guggi Kofod, and Reimund Gerhard — Applied Condensed-Matter Physics, University of Potsdam, Am Neuen Palais 10, D-14469 Potsdam,Germany

Dielectric elastomer actuators based on Maxwell-stress induced deformation, are considered for many potential applications where high actuation strain and high energy density are required. They usually rely on a planar actuator configuration, however, a string-like actuator would be less bulky, and more versatile for several applications. A co-axial dielectric elastomer actuator was developed and evaluated. The proposed geometry is fabricated through alternating dip-coating steps with thin insulating and conductive elastomer layers. Actuators with single and multiple active layers have been successfully demonstrated. The actuation strain and force generated by the actuators were determined at different levels of pre-strain. Voltage-dependent actuation strain measurements were obtained. The experimental results were compared to a straightforward electromechanical model for cylindrical elastomer actuators.

CPP 10.5 Mon 16:45 Poster A

Nano/micro-structure formation driven by local protonation of polymer thin films via dip-pen nanolithography — •Carsten Mädler[1,2], Sailaja Chada[2], Andres La Rosa[2], and Mingdi Yan[2] — [1]Center of Nanostructured Materials and Analytics, TU Chemnitz, 09107 Chemnitz, Germany — [2]Portland State University, PO Box 751, Portland OR 97207, US

While dip-pen nanolithography uses a sharp tip to anchor molecules on the substrate to form nanostructures, an alternative approach is presented here to exploit the responsiveness of the substrate. Acidic phosphate buffer molecules are delivered into ultraviolet-crosslinked films to swell the polymer material by a protonation-based mechanism. The experiment aims to provide the first demonstration of stimulating the mechanical response of polymer materials by confining protonation reaction locally and in a controlled manner. A series of experiments suggests that the structures are indeed due to swelling of the polymer. The process was studied at different dwell times and contact forces. A dependence of the structure height on the contact force was found, which is rather unusual for DPN processes.

CPP 10.6 Mon 16:45 Poster A

Charge transfer between covalently bound oligothiophenes and fullerene — •Wichard J D Beenken — Technische Universität

Ilmenau, FG Theoretische Physik I, Weimarer Str. 25, 98693 Ilmenau

Understanding the charge transfer between conjugated polymers, esp. poly-thiophenes, and fullerenes or their derivates is of high interest, since this is the key process for polymer-based organic solar cells. Nevertheless, there exist only very few theoretical studies about this system. The main problem is the undefined conformation between the two constituents. Using quantum-chemical methods, esp. TD-DFT, we calculated several oligo-thiophenes of various lengths, which were covalently bound to the fullerene C60. We identified several charge transfer states by plotting the respective charge-difference densities. Thereby it turns out that the kind of bridge between thiophene and C60 is crucial for the charge transfer energetics. We will show how one may try to eliminate this effect.

CPP 10.7 Mon 16:45 Poster A

Supermolecular structure and charge carriers mobilities of perylene diimides — •Valentina Marcon[1], James Kirkpatrick[1,2], Wojtek Pisula[1], and Denis Andrienko[1] — [1]Max-Planck-Institut für Polymerforschung, Mainz, Germany — [2]Department of Physics, Imperial College London, London, United Kingdom

Perylene diimides form columnar phases, where the molecules stack on top of each other and the columns arrange in a regular lattice. The self-organization into well-ordered columns results in the one-dimensional charge transport along the stack of the aromatic cores of the molecules. Most of the discotic molecules which organize in columns are p-type semiconductors, while the class of rylene diimide molecules, to which perylene belongs, forms n-type organic semiconductors.

Using atomistic molecular dynamics (MD) simulations we study the columnar phases of perylene diimides and establish correlations between the molecular structure, packing, and dynamical properties of these materials.

By using a scheme which combines electronic structure calculations, MD and kinetic Monte Carlo simulations, a correlation is then established between the molecular structure and charge mobility of perylenes columnar mesophases.

This work was partially supported by DFG. V. M. acknowledges the Alexander von Humboldt foundation. J. K. acknowledges the EPSRC.

CPP 10.8 Mon 16:45 Poster A

Atomistic force field and electronic properties of carbazole: melt and macrocyle — •Thorsten Vehoff[1], James Kirkpatrick[2], Kurt Kremer[1], and Denis Andrienko[1] — [1]Max-Planck-Institut für Polymerforschung, Ackermannweg 10, 55128 Mainz, Germany — [2]Department of Physics, Imperial College London, Prince Consort Road, London SW7 2B W, United Kingdom

Processable polymers with a conjugated backbone, e.g. carbazole, are interesting for use as hole conducting materials. Hole transport characteristics strongly depend on the local arrangement of molecules; for this reason, to obtain an efficient device, it is necessary to control the morphology of the material: very often, small changes of the structure (e.g. longer alkane side chains) or processing conditions (annealing regime, choice of solvents) result in a significant change of the morphology and, hence, charge carrier mobility.

In this contribution, we study the columnar mesophase of a carbazole macrocycle1. First an atomistic force field is developed for carbazole furnished with alkyne side chains as well as carbazole dimers and then tested on a melt of carbazole oligomers by evaluating properties such as the density and diffusion coefficient and comparing with experimental results. The mobility of charge carriers along the columns is calculated by first computing charge hopping rates between carbazole monomers and macrocycles according to Marcus theory and then solving the master equation for charge dynamics.

CPP 10.9 Mon 16:45 Poster A

Electronic Excitation Transfer in PPV-Mesoporous Silica Matrix — •Gil Claudio[1] and Eric Bittner[2] — [1]The University of Houston, 4800 Calhoun Road, Houston, Texas 77204, USA. Currently at the Max Planck Institute for Polymer Research, D-55021 Mainz, Germany — [2]The University of Houston, 4800 Calhoun Road, Houston, Texas 77204, USA.

Electronic excitation transfer as described by Förster theory has been shown to occur in various multi-chromophore systems such as conjugated polymers. The direction of energy transfer towards the low energy states is usually random due to the random distribution of chromophores in the system. Schwartz and co-workers synthesized a system with MEH-PPV conducting polymers inserted in the channels of mesoporous silica matrices. In this system, energy transfers from the high-energy randomly oriented chromophores of polymers outside the channels to the low-energy chromophores inside the well-ordered channels. We calculated several configurations of the polymer-silica matrices and the excitation transfer in these systems. These calculations confirm the energy transfer to the targeted sites as hypothesized in experiment. Lastly, we present criteria that allow efficient energy transfer to specific targeted areas.

CPP 10.10 Mon 16:45 Poster A

Optical and electronic properties of oligothiophene dendrimers — •Thomas Hartmann and Peter Reineker — Institute of Theoretical Physics, University of Ulm, 89069 Ulm, Germany

Dendrimers, regular star like polymers, are of interest from a fundamental point of view, but also because of various possible applications, such as in light harvesting systems, in solar cells, as carriers for drug delivery or for gene manipulation, or in catalysis, etc. In our investigation of the dendrimers we have focused on optical and energy transport properties of oligothiophene dendrimers with C2 symmetry. Our calculation of optical and energy transport properties is based on a Frenkel exciton model. This model takes into account the geometry of the dendrimers, local electronic excitation energies, transfer integrals, and the influence of vibrational degrees of freedom via a stochastic description. We have calculated optical absorption line shapes and the time dependence of the energy transport in dependence on the size of the dendrimer. Furthermore the influence of neighboring thiophenes in different branches of the denrimers is considered.

CPP 10.11 Mon 16:45 Poster A

Investigation of phosphorescent blue organic light emitting diodes — •Chien-Shu Chiu[1,3], Ralf Krause[2,3], Fryderyk Kozlowski[3], Arvid Hunze[3], and Wolfgang Kowalsky[1] — [1]Department of Electrical Engineering & Information Technology, Technical University of Braunschweig, Germany — [2]Department of Materials Science VI, University of Erlangen-Nuremberg, Germany — [3]Siemens AG, CT MM 1, Günther-Scharowsky-Str. 1, 91058 Erlangen, Germany

Recently, rapid development of phosphorescent materials has significantly improved the efficiency of organic light emitting diodes (OLEDs). By using efficient phosphorescent emitter materials white OLEDs with high power efficiency values could be demonstrated. But especially blue phosphorescent devices, due to stability issues, need to be further investigated und optimized. In this work, blue OLED devices based on the phosphorescent emitter FIrpic were investigated. Single-carrier hole-only as well as electron-only devices were fabricated and characterized to study the impact of charge carriers on device performance.

CPP 10.12 Mon 16:45 Poster A

Optimization of Emission Color and Efficiency of Organic Light Emitting Diodes for Lighting Applications — •Stefan Seidel[1,2], Ralf Krause[1,2], Fryderyk Kozlowski[2], Günter Schmid[2], Arvid Hunze[2], and Albrecht Winnacker[1] — [1]Department of Materials Science VI, University of Erlangen-Nuremberg, Germany — [2]Siemens AG, CT MM 1, Günther-Scharowsky-Str. 1, 91058 Erlangen, Germany

In recent years the performance of organic light emitting diodes (OLEDs) has reached a level where OLED lighting presents an interesting application target. Research activities therefore focus amongst other things on the development of high efficient and stable white light emitting devices. We demonstrate how the color coordinates can be adjusted to achieve a warm white emission spectrum, whereas the OLED stack contains phosphorescent red and green dyes combined with a fluorescent blue one. Detailed results are presented with respect to a variation of layer thicknesses and dopant concentrations of the emission layers. Furthermore the influence of various dye molecules and hence different energy level alignments between host and dopants on color and efficiency will be discussed.

CPP 11: DRG-DPG SYMPOSIUM Rheology III

Time: Tuesday 10:00–12:15 Location: C 264

CPP 11.1 Tue 10:00 C 264

Blood-Rheology on single drops before, during and after coagulation — •Wolfgang Pechhold, Theresia Gross, and Hubert Dammann — Institute for dynamic Materials Testing (IdM) at the University Ulm

Blood is a complex fluid in many respects. It contains about 45 p.c. of hematocrit (RBC, WBC and platelets) in low viscous plasma (1,8 mPa s), with dissolved proteins and clotting factors, including fibrinogen (2%). We report on its viscoelastic characterization ($\eta = \eta$'-iη") in the frequency range 1 Hz to 3 kHz using the dynamic squeeze flow of the Piezo Axial Vibrator (PAV) which needs only a droplet (10-50μl) of blood or plasma: in the anticoagulated state we varied the hematocrit from 0 to 92 p.c. and found an exponential increase of viscosity above 40 p.c. In full blood we measured η in the course of time before and during coagulation and found a strong gap dependence in the clotted state in both, intrinsic and extrinsic, clotting. Adding Heparin to the blood droplet, the clotting time becomes prolonged and exceeds 100 min for 1800 I.E. per 5 l. In platelet-free plasma no intrinsic coagulation takes place, and in high platelet-concentration (1,2 E6/mm3) we did not find any change in clotting time up to 3600 I.E. per 5 l Heparin added. For the used blood in all measurements of the coagulated state, i.e. after fibrin forming, the viscous part clearly dominated at all frequencies.

CPP 11.2 Tue 10:15 C 264

Combination of NMR relaxometry and mechanical testing during vulcanisation — Stefan Kahle[1,2], Manfred Hehn[2], Hans-Peter Raich[2], Walter Nussbaum[1], Peter Blümler[3], and •Manfred Wilhelm[2,4] — [1]www.scarabaeus-gmbh.de — [2]www.mpip-mainz.mpg.de — [3]www.econmr.org/bluemler — [4]www.polymer.uni-karlsruhe.de

A new design for an in-situ combination of NMR and rheological measurements is presented. The NMR is based on a BRUKER MINISPEC spectrometer. The magnet is self-made via a construction of 64 permanent magnets in a so called MANDHALA arrangement. The magnetic field strength reaches about 0.23 T, corresponding to a 1H resonance frequency of about 9.5 MHz. For the in-situ rheological measurements a Scarabaeus SISV50 instrument with modified sample cells is utilized. This unique combination and first measurements are presented.

CPP 11.3 Tue 10:30 C 264

Rheo-NMR Studies of Liquid Crystals in Shear Flow — Gönül Ar, Shahram Shafaei, and •Claudia Schmidt — Department Chemie, Universität Paderborn, Warburger Str. 100, 33098 Paderborn, Germany

Nuclear magnetic resonance spectroscopy has proven a useful tool for the investigation of shear-induced phenomena in liquid crystals [1,2]. Due to the anisotropy of the interactions of nuclear spins, information about shear-induced orientations can be obtained. In deuterium NMR, the quadrupolar interaction is used to probe the orientation of the liquid crystalline director. In situ observations of director orientations under shear can reveal the microscopic origin of macroscopic rheological phenomena. Recent examples for deuterium NMR investigations of shear phenomena in different types of liquid crystals, such as nematic, lamellar and hexagonal phases will be presented.

[1] P. T. Callaghan, Rep. Prog. Phys., 62, 599 (1999).

[2] C. Schmidt, in: Modern Magnetic Resonance, Vol. 3, Springer, New York, 2006.

CPP 11.4 Tue 10:45 C 264

Flow at the interface of immiscible fluids — Ute Böhme, Frank Bagusat, and •Ulrich Scheler — Leibniz Institute of Polymer Research Dresden, Hohe Str. 6, D-01069 Dresden

Flow in a modified Couette cell with a region of high shear has been investigated at the interface of oil and water. Flow NMR, which is a combination of PFG NMR for the measurement of displacements with NMR imaging has been applied to measure the flow with spatial resolution. NMR contrast has been generated from longitudinal relaxation which enable the measurement of both the spatial distribution and the flow field of each of the components separately. Upon shear in the Couette cell the interface between water and oil becomes bent. Flow measurements reveal, that this bending results from strong axial velocity in the region of high shear. While in homogeneous systems stable eddies in plane are found at the region of high shear, at the interface region between oil and water an eddy out of plane is found as well. The eddies depend on shear reate and viscosity. The out-of-plane eddy is attributed to the difference in viscosity between the two components.

break

CPP 11.5 Tue 11:15 C 264

Bridging the gap between microrheology and tribology — •Christian Clasen[1], Pirouz Kavehpour[2], and Gareth H. McKinley[3] — [1]Department of Chemical Engineering, Katholieke Universiteit Leuven (KUL), 3001 Leuven, Belgium — [2]Mechanical and Aerospace Engineering Department, University of California Los Angeles (UCLA), Los Angeles, CA90095, USA — [3]Department of Mechanical Engineering, Massachusetts Institute of Technology (MIT), Cambridge, MA 02139, USA

Tribology and elastohydrodynamic lubrication have traditionally been considered to be a subject apart from classical bulk rheology and the rapidly developing area of microrheological investigation. The principal reason for this separation is that although fluid properties in each field are key to the observed flow and friction phenomena, the experimental approach and the resulting terminology differ substantially and prohibit a direct translation of the results. In particular the lack of well-defined viscometric kinematics for tribological experiments and the difficulties in achieving sufficiently-precise fixture alignment in regular rheometry on the microscale have inhibited the merging of the results from these fields.

We show in this paper how recent developments in the area of sliding plate microrheometers with controlled gaps on the order of micro- to nanometers, and triborheometers with defined plate-and-plate geometry parameters and normal stress control can bridge this gap between classical tribology and rheology.

CPP 11.6 Tue 11:30 C 264

Polymer Solutions under Circular Couette Flow — •Andreas Zell and Christian Wagner — Technische Physik, Universität des Saarlandes, D-66123 Saarbrücken

We investigate the behaviour of dilute polymer solutions in a Taylor-Couette cell with independently rotatable cylinders. The focus of our interest lies on the examination of the elongation of the solved polymers and their response on the imposed flow. Our measurements show that we are able to detect these counteracting forces and that we can relate them to the polymer relaxation time of the respective solution. In addition we give a summary of a mathematical discussion of possible laminar flow states in a Taylor-Couette system, where the final argumentation is pointing to the usefulness of one of these flow states to our investigations.

CPP 11.7 Tue 11:45 C 264

Diffusion of Linear Macromolecules and Spherical Nanoparticles in Semidilute Polymer Solutions and Gels — •Sebastian Seiffert and Wilhelm Oppermann — Institute of Physical Chemistry, Clausthal University of Technology, Arnold-Sommerfeld-Strasse 4, D-38678 Clausthal-Zellerfeld, Germany

The dynamics of fluorescently labeled linear macromolecules and spherical particles that are enclosed in polymer matrixes were studied by fluorescence recovery after photobleaching. The experiments were designed such that the transition from a semidilute solution to a permanent network could be covered. This was achieved by employing a matrix polymer, polyacrylamide, carrying pendent dimethylmaleimide groups. Stepwise irradiation of such samples causes dimerization of the moieties via photochemical [2+2]-addition leading to progressive crosslinking. Thus, studies on the diffusion of linear and spherical tracers are enabled especially within the interesting transition region between a physically entangled system and a covalently crosslinked matrix. Comparability of the results is ensured since the same sample is analyzed merely at different degrees of crosslinking, respectively. The parameters varied were the concentration of matrix polymer and the molar mass of the enclosed linear chains as well as the size of the spheres. The aim of this study is to point out differences between the dynamics of linear tracers in contrast to spherical particles and to work out the behavior of the system when a semidilute polymer solution is chemically crosslinked. A central problem in this context is the adaptability of the reptation model in fairly dilute systems.

CPP 11.8 Tue 12:00 C 264

Near-surface dynamics explored by grazing incidence neutron techniques — •Marco Walz[1], Max Wolff[2], Nicole Voss[1], Hartmut Zabel[2], and Andreas Magerl[1] — [1]Chair for Crystallography and Structural Physics, University of Erlangen-Nürnberg, Staudtstr. 3, 91058 Erlangen — [2]Chair for Condensed Matter Physics, Ruhr-University Bochum, Universitätsstr. 150, 44780 Bochum

An understanding of boundary slip requires a knowledge of the structural and dynamical properties of interface regions on short length scales, and experimental methods with pronounced interfacial response are needed. To highlight the properties of the boundary layer we carried out for the first time a neutron spin-echo experiment under condition of grazing incidence (GINSE). With an aqueous solution of a tri-block copolymer with micellar orderings we could verify that the investigation of the dynamics of the sample is well feasible with GINSE, and we present first data taken near the critical angle of total reflection. It appears that the diffusive motion at the hydrophilic (attractive) interface is reduced as compared to a hydrophobic (repulsive) interface.

The authors gratefully acknowledge the financial support by the DFG grants MA801/12-1 and ZA161/18-1 within the priority program (SPP) 1164 and the BMBF grant ADAM 04ZAE8BO.

CPP 12: Confined Fluids

Time: Tuesday 11:00–12:30 Location: C 230

CPP 12.1 Tue 11:00 C 230

Direct measurement of the critical Casimir force in a binary liquid using TIRM — •Christopher Hertlein, Laurent Helden, and Clemens Bechinger — 2. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany

A colloidal particle suspended in a binary liquid at the critical composition close to a substrate experiences a critical Casimir force upon approaching the critical temperature of decomposition T_c. We have measured interaction potentials for a single polystyrene particle suspended in a mixture of water and $2,6$ -lutidine approaching T_c using Total Internal Reflection Microscopy (TIRM). TIRM is a technique for precise measurements of colloid - wall interaction potentials based on single particle evanescent wave light scattering. The measured interaction potentials display a clear contribution of the critical Casimir force which becomes stronger upon approaching T_c and is either attractive or repulsive depending on the preference for water or lutidine of substrate and/or particle. Theoretical calculations are in excellent agreement with experimental results. Switching the interaction from attraction to repulsion *in situ* is currently under investigation and could prove useful to control and fine-tune particle substrate potentials.

CPP 12.2 Tue 11:15 C 230

Fluctuation-induced interaction between ellipsoidal colloids at fluid interafce — •Ehsan Noruzifar and Martin Oettel — Institut fuer Physik, WA 331, Johannes-Gutenberg-Universitaet Mainz,D-55099 Mainz, Germany

One part of the effective interaction between colloids trapped at the fluid interface originates from capillary wave fluctuations. The very presence of colloids at the interface of two fluids restricts the allowed spectrum of long-ranged capillary wave fluctuations, thereby the resulting force is of Casimir-Polder type and adds a long-ranged part to the effective inter-colloidal interaction [1]. This interaction is calculable by integrating over all admissible interface configurations weighted by a capillary wave Hamiltonian. In the present work, the Casimir interaction between ellipsoidal colloids placed at a fluid interface is calculated as an interaction energy between multipole fields on the interface boundaries generated by thermal fluctuations [2]. The results obtained are an explicit example for an anisotropic Casimir force which is caused by the colloid shape.

[1] H. Lehle and M. Oettel, Phys. Rev. E 75, 011602 (2007) ; H. Lehle, M. Oettel, and S. Dietrich, Europhys. Lett. 75, 174 (2006). [2] T. Emig, N. Graham, R. L. Jaffe and M. Kardar, Phys. Rev. Lett. 99, 170403 (2007).

CPP 12.3 Tue 11:30 C 230

Broadening of solid-liquid phase transitions due to influence of surrounding interfaces — •Ralf Köhler and Hans Riegler — MPI KGF, Abt. Grenzflächen, 14424 Potsdam, Germany

In objects with reduced dimensionality (films, particles), surfaces and interfaces become important for their physical behaviour like phase transitions. Despite its importance for fundamental and applied science (nucleation, sintering, etc.) relatively little is known about the influence of the surrounding interfaces on the phase behaviour due to the lack of quantitative experimental data. With Contrast Enhanced Interference Microscopy (1) we investigate long-chain alkanes which form two-dimensional aggregates (domains) of nanometer thickness on planar silicon oxide surfaces. Thus, we quantify the influence of the surrounding interface on the liquid-solid phase transition of the domains. The domains melt gradually below the bulk phase transition temperature, forming a coexisting liquid film, which wets the adjacent substrate surface. The film thickness varies with temperature i.e., the liquid and solid phases exchange reversibly alkanes, whereby converting melting enthalpy into interfacial energy. The melting behaviour is quantitatively described in a thermodynamic approach. The behaviour is universal for the phase behaviour of any adsorbed material, which wets surrounding interfaces.

1) R.Köhler, P.Lazar, and H.Riegler, Appl.Phys.Lett. 89, 241906 (2006) 2) H.Riegler and R.Köhler, Nature Physics, 754 (2007)

CPP 12.4 Tue 11:45 C 230

Statics and dynamics of confined cluster forming systems — •Sven van Teeffelen and Christos N. Likos — Institut für Theoretische Physik II, Heinrich–Heine–Universität Düsseldorf, Universitätsstrasse 1, D-40225 Düsseldorf, Germany

Ultrasoft repulsive particles are known to crystallize into BCC and FCC cluster crystals [1,2]. Here, we study with the help of accurate density functional theory how a system of ultrasoft repulsive particles, such as dendrimers, behaves under planar confinement.

In particular, we present the phase diagram and we show how the emerging equilibrium fluid and crystal structures differ from those in the bulk. Extending our considerations to non-equilibrium phenomena, we employ a Dynamical Density Functional Theory (DDFT) to examine the growth or loss of local crystallinity in confinement, induced by compression or expansion of the confinining walls.

[1] B. Mladek, et. al., Phys. Rev. Lett. 96, 045701 (2006)

[2] M. A. Glaser, et. al., Europhys. Lett. 78, 46004 (2007)

CPP 12.5 Tue 12:00 C 230

Crystallization in layered films of confined charged colloids — •Stefan Grandner[1] and Sabine H. L. Klapp[1,2] — [1]Stranski-Laboratorium, Technische Universität Berlin, Straße des 17. Juni 115, D-10623 Berlin, Germany — [2]Institut für theoretische Physik, Technische Universität Berlin, Hardenbergstraße 36, D-10623 Berlin, Germany

We consider a system of spherical charged colloids between two parallel walls. A characteristic property of such colloids is the screening of the Coulomb potential of the macroions due to the counterions and additional salt, which we take into account via DLVO theory. An earlier comparison of Monte-Carlo results with colloidal probe AFM experiments has demonstrated the applicability of the DLVO potential for confined systems [1]. Typical for confined fluids is a layering parallel to the walls, which was observed for charged colloids as well [1,2]. In our current investigations we employ grand canonical Monte-Carlo simulations to study the in-plane structure in dense states. In particular, by computing bond angle order parameters we search for evidence of crystallization in the layers. Previous work for bilayers discovered several crystal-like structures such as square, hexagonal or rhombic ordering [3]. Furthermore we discuss the dependence of the onset of crystallization on pore size and bulk density.

[1] S. H. L. Klapp, D. Qu, and R. v. Klitzing, J. Phys. Chem. B **111**, 1296-1303 (2007).

[2] M. Kittner, and S. H. L. Klapp, J. Chem. Phys. **126**, 154902 (2007).
[3] R. Messina, and H. Löwen, Phys. Rev. Lett. **91**, 146101 (2003).

CPP 12.6 Tue 12:15 C 230

Structuring of colloidal suspensions confined in thin liquid films — •Yan Zeng[1], Sabine Klapp[1,2], and Regine v.Klitzing[1] — [1]Stranski-Laboratorium für Physikalische & Theoretische Chemie, Institut für Chemie, TU Berlin — [2]Institut für Theoretische Physik, TU Berlin

In order to study the structuring of colloidal suspensions Ludox silica solutions are confined between a microsphere and a flat interface in a colloidal probe AFM [1]. Oscillatory forces are measured due to layer by layer expulsion of the particles [2]. The period scales with the concentration with an exponent -1/3, this period has the same value as the particle distance in the corresponding bulk solution calculated from the position of the structure peak of SAXS measurements. The addition of salt decreases the period of oscillation, the amplitude and the scaling exponent of the particle distance in dependence of the salt concentration. In addition, simulations show that the scaling behavior changes from exponent -1/3 at low ionic strength to a concentration independent length at high ionic strength [3].

[1] M.Piech, J.Y.Walz, J.Colloid Interface Sci. 2002,8,2985

[2] J.Israelachvili, Intermolecular and surface Forces; Academic Press: San Diego, CA, 1992; Chapter 13

[3] S.Klapp, D.Qu, R.v.Klitzing, J.Phys.Chem.B 2007,111,1296.

CPP 13: Colloidal and Nanoparticles

Time: Tuesday 15:00–18:45 Location: C 264

CPP 13.1 Tue 15:00 C 264

Micromechanics of gas filled Microballoons — •Paulo Fernandes[1,2], George Tzvetkov[3,4], Rainer Fink[3], and Andreas Fery[1] — [1]Physikalische Chemie II, Universität Bayreuth, Bayreuth, Germany — [2]Max-Planck-Institut für Kolloid- und Grenzflächenforschung, Potsdam, Germany — [3]Physikalische Chemie II,Universität Erlangen-Nürnberg, Erlangen, Germany — [4]Swiss Light Source, Paul Scherrer Institut, 5232 Villigen, PSI, Switzerland

Gas filled MicroBalloons (MBs) are today highly valued research subjects mainly due to their potential use in medical applications where they impose themselves as targeted drug delivery systems and contrast agents for ultrasonic imaging. Intense research has been devoted to the development of MB systems. Their mechanical and adhesion properties are of interest since these determine the micro containers behavior and stability in applications. We introduce novel AFM-based methods for quantifying both mechanics and adhesion properties.

We use a combination of the colloidal probe AFM technique and an inverted optical microscope. The deformation behavior of individual MBs is characterized with AFM Force Spectroscopy measurements. We analyze the dependence of the profiles with MB radius at different temperatures (room and body temperature). Scanning Transmission X-ray Microscopy (STXM) experiments proved to be very appropriate to study the MBs. Quantitative analysis of the resulting transmission profiles allowed us to characterize the MBs properties.

CPP 13.2 Tue 15:15 C 264

Fabrication of novel metal oxide hollow spheres with tailored shell thickness — •Mukesh Agrawal[1], Andrij Pich[2], Nikolaos E. Zafeiropoulos[1], and Manfred Stamm[1] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., Hohe Strasse 6, 01069 Dresden, Germany — [2]Technische Universität Dresden, Institut für Makromolekulare Chemie und Textilchemie, Mommsenstr. 4, 01062 Dresden, Germany

Sub-micrometer sized polystyrene-metal oxide core-shell composite particles and hollow metal oxide spheres with tunable shell thickness and void size have been fabricated exploiting the sol-gel process. A controlled precipitation of ZnO/TiO2/Ta2O5 nanoparticles has been carried out on the template surface by hydrolyzing the metal oxide precursors and subsequently polymer core was removed either via chemical treatment with toluene or calcination at elevated temperature to achieve the hollow spheres. Thickness of the ZnO/TiO2/Ta2O5 shell, precipitated on polystyrene core during coating process has been tuned by varying the concentration of metal oxide precursors in reaction media. The obtained core-shell composite particles and hollow microspheres have been characterized by scanning electron microscopy, transmission electron microscopy, infra-red spectroscopy, X-ray diffraction and thermo gravimetric analysis. Due to the unique optical and dielectric properties, these nanostructured materials are envisaged to be used in applications such as novel building blocks for the fabrication of advanced materials, surface coatings, catalysts and drug delivery systems.

CPP 13.3 Tue 15:30 C 264

Temperature, pH, and ionic strength induced changes of the swelling behavior of PNIPAM-Poly(Allylacetic-Acid) copolymer microgels. — •Thomas Hellweg[1] and Matthias Karg[2] — [1]Universität Bayreuth, Physikalische Chemie I, Universitaetsstr. 30, 95447 Bayreuth, Germany — [2]TU Berlin, Institut f. Chemie, Stranski-Lab. f. Theoretische und Physikalische Chemie, Strasse des 17.Juni 124, 10623 Berlin, Germany

The volume transition of colloidal microgels made of N-isopropylacrylamide (NIPAM) can be affected by copolymerization. Therefore, a series of poly(N-isopropylacrylamide-co-allylacetic acid) copolymers with different contents of allylacetic acid (AAA) was synthesized by means of emulsion polymerization. The thermo-responsive behavior of these particles was studied using dynamic light scattering (DLS). Further characterization was done employing transmission electron microscopy (TEM) and zeta potential measurements. The measured zeta potentials provide information about the relative surface charge. Since these copolymers are much more sensitive to external stimuli such as pH and ionic strength than their pure PNIPAM counterparts the volume phase transition was investigated at two different pH values and various salt concentrations. At pH 10 for some of the copolymer microgels a significant shift of the volume phase transition temperature towards higher temperatures is found. For higher AAA contents a change in pH from 8 to 10 can induce a change in radius of 100 nm making the particles interesting as pH controlled actuators.

CPP 13.4 Tue 15:45 C 264

Switchable photoluminiscent CdTe nanocrystals by temperature responsive microgels — Mukesh Agrawal[1], Smrati Gupta[1], Vera Cimrova[2], Nikolai Gaponik[3], Alexander Eychmüller[3], Spyros Tzavalas[1], Rosana Rojas-Reyna[1], •Jorge Rubio-Retama[1], Manfred Stamm[1], and Nikolaos E. Zafeiropoulos[1] — [1]Leibniz-Institut für Polymerforschung Dresden, Hohe Strasse 6, Dresden 01069, Germany — [2]Institute of Macromolecular Chemistry Praha, Czech Republic — [3]3Physcal-Chemistry Department, Teknische Universität Dresden, Dresden 01069 Germany

Microgels are perhaps of the most promising responsive systems due to their high specific surface, which yields materials with very short response time. In the present study we report a facile and reproducible method for preparing fluorescence thermo-sensitive hybrid material based on monodispersed and thermosensitive P(NIPAM) microgels covered with nanocrystals of CdTe of 3.2 nm of diameter. The CdTe nanocrystals were covalently immobilized on the surface of the microgels. Through temperature variation it was possible to modify the chemical environment around the CdTe nanocrystals. This change provoked a variation in the nanocrystal photoluminescence properties in such way that when the temperature was under the LCST of the polymer the photoluminescence of the nanocrystals was strongly quenched, while when the temperature was above the LCST of the microgels (36 C) the photoluminescence properties of the nanocrystals were strongly enhanced.

CPP 13.5 Tue 16:00 C 264

Smart Hybrids made of poly-NIPAM and Gold Nanoparticles: — •Matthias Karg[1], Isabel Pastoriza-Santos[2], Jorge Pérez-Juste[2], Luis M. Liz-Marzán[2], and Thomas Hellweg[3] — [1]Berlin, Stranski-Laboratorium, Strasse des 17. Juni 124, 10623 Berlin, Germany — [2]Universidade de Vigo, Grupo de Quimica Fisica, 36310 Vigo, Spain — [3]Universität Bayreuth, Physikalische Chemie I, Universitätsstrasse 30, 95440 Bayreuth

Recently, composite materials made of organic polymers and inorganic matter are of high interest. Typically, the aim for the preparation of such kind of hybrids is the combination of the properties of both components, which can be e.g. thermoresponsive behavior for the polymer and optical or magnetic properties for the inorganic component. Here, we present hybrid particles, which were made of thermoresponsive poly-N-isopropylacrylamide (poly-NIPAM) microgels and gold nanoparticles. Chracterization of the particles has been done using Dynamic Light Scattering (DLS), Atomic Force Microscopy (AFM), Transmission Electron Microscopy (TEM) and Small Angle Neutron Scattering (SANS). The thermoresponsive optical properties were investigated using UV-VIS spectroscopy and were found to be fully reversible. [1] M. Karg, I. Pastoriza-Santos, L.M. Liz-Marzán, T. Hellweg, ChemPhysChem., 2006, 7, 2298-2301 [2] M. Karg, I. Pastoriza-Santos, J. Pérez-Juste, T. Hellweg, L. M. Liz-Marzán, Small, 2007, 3, 1222-1229

CPP 13.6 Tue 16:15 C 264

TiO2 nanoparticles by PEOMA-PDMS-PEOMA block copolymer — •Mine Memesa[1], Jan Perlich[2], Sebastian Lenz[1], Sebastian Nett[1], Sebastian Emmerling[1], Peter Müller-Buschbaum[2], and Jochen S. Gutmann[3] — [1]Max-Planck Institute for Polymer Research, Ackermannweg 10, D-55128, Mainz, Germany — [2]TU München, Physik-Dept. LS E13 James-Franck-Str. 1, 85747 Garching, Germany — [3]Institute of Physical Chemistry, University Mainz, D-55099, Mainz, Germany

The effect of titanium oxide (TiO2) nanoparticles on the efficiencies of conjugated polymer photovoltaics has been widely studied. Preparation of TiO2 nanoparticles by using an amphiphilic block copolymer as a templating agent via a sol-gel process resulted in different morphologies. In this study, TiO2 nanoparticles are prepared by a poly(dimethylsiloxane) (PDMS) containing block copolymer, poly(ethyleneoxide)methacrylate(PEOMA)-block-PDMS-block-PEOMA via sol-gel chemistry. By varying the components of the sol gel, the morphology of the particles formed is investigated by Scanning Electron Microscopy (SEM), Atomic Force Microscopy (AFM) and Grazing Incidence Small Angle X-ray Scattering (GISAXS). The ability of PDMS to turn into silicon-oxi carbide (Si-O-C) after being heated to elevated temperatures is believed to act as an alternative to the conventional blocking layer between conducting transparent electrode (FTO) and the photoactive layer in hybrid organic solar cells. The results of the ongoing study on the morphology of the particles and resultant physical properties will be presented.

CPP 13.7 Tue 16:30 C 264

Depletion-Driven Aggregation Kinetics and Protein Resistance of Surface Decorated Au Nanoparticles — •Fajun Zhang[1], Donald G. Dressen[1,2], Maximilian W. A. Skoda[1,3], Robert M. J. Jacobs[3], Stefan Zorn[1], Richard A. Martin[4], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen, Germany — [2]Department of Physics and Astronomy, University of Denver, USA — [3]CRL, University of Oxford, UK — [4]Department of Physics, University of Bath, UK

Self-assembled monolayers with oligo(ethylene glycol) (OEG) termination are of great importance in biomedical applications due to their protein resistance. We have successfully prepared OEG-thiol decorated gold colloids and studied various interactions, stability and aggregation kinetics of colloid in the mixture of protein and colloid by SAXS and UV-vis spectroscopy [1]. Results proved the protein resistance of the OEG SAM at curved interfaces. Above a critical protein concentration, c*, the colloids lose their stability and form aggregates due to the depletion-attraction [1]. Depletion-driven aggregation kinetics was studied under various protein concentrations and ionic strength. A kinetic crossover from RLCA to DLCA is observed at low salt addition, which is caused by the effective repulsive interaction barrier between colloids within the oscillatory depletion potential. Above 0.5 M NaCl, the surface charge of proteins is screened significantly, and the energy barrier disappeares, thus the growth kinetics becomes DLCA only [1]. [1] F. Zhang, et al., J. Phys. Chem. B. 2007, 111, 251. J. Phys. Chem. A. 2007, DOI: 10.1021/jp074293v. Euro. Biophys. J. Submitted.

break

CPP 13.8 Tue 17:00 C 264

Frustration-induced magic number clusters of colloidal magnetic particles — •Larysa Baraban[1], Denys Makarov[1], Manfred Albrecht[2], Nicolas Rivier[3], Paul Leiderer[1], and Artur Erbe[1] — [1]University of Konstanz, Department of Physics, Konstanz, Germany — [2]Chemnitz University of Technology, Surface and Interface Physics, Chemnitz, Germany — [3]Institut de Physique et Chimie des Materiaux de Strasbourg, Strasbourg, France

We report the formation of stable two-dimensional clusters consisting of long-range interacting colloidal particles with pre-defined direction of macroscopic magnetic moments. The colloids can find the global minimum of the structure driven by magnetic frustration. This solution coincides with the ground state configuration of a two-dimensional triangular antiferromagnet, which is consistent with an XY-spin model. By satisfying the criteria of stability, a series of 'magic number' clusters is formed. Since the ground state follows the rules for compensation of magnetic moments and chirality, it is likely that conclusions can be drawn for spin systems as well, although the exact nature of the interactions is different. Thus, the system can be regarded as a mesoscopic model system for spin arrangements in antiferromagnets.

CPP 13.9 Tue 17:15 C 264

Metal-precursor loaded polymer-particles: a basis for ordered arrays of nanoparticles — •Achim Manzke[1], Fabian Enderle[1], Stefan Wiedemann[1], Christian Pfahler[1], Alfred Plettl[1], Paul Ziemann[1], Eyk Schreiber[2], Ulrich Ziener[2], and Katharina Landfester[2] — [1]Institut für Festkörperphysik, Universität Ulm, D-89069 Ulm — [2]Institut für Organische Chemie III, Universität Ulm, D-89069 Ulm

The fabrication of metal precursor loaded colloidal polystyrene (PS) particles in aqueous solution is carried out by a miniemulsion technique. We will report on colloids loaded with Pt-, Fe- as well as with Fe- and Pt-complexes. Dropped on hydrophilic Si substrates, hexagonally ordered monolayers of colloids are generated. By applying optimized plasma and temper processes, metallic nanoparticles can be obtained which still exhibit the original ordered arrangement. The metal content in the colloid defines the size of the final particle, which could be varied between 6 and 14 nm, so far. The interparticle distances is determined by the diameter of the starting PS-particles and could be varied between 80 and 230 nm. This new technique has the potential to extend the limits of the micellar technique [1] regarding the particle distance and order.

[1] G. Kästle et al. , Adv. Funct. Mat. 13, 853 (2003)

[2] A. Manzke et al. Adv. Mater. 19, 1337 (2007)

CPP 13.10 Tue 17:30 C 264

X-ray investigations for determining the aspect ratio in CdSe nanorods — Ullrich Pietsch and •Özgül Kurtulus — Festkörperphysik , Universität Siegen, Siegen, Germany

Semiconductor based 1D nanostructures are of high technological interest due to potential application in 1D conductivity measurements and optical devices. Catalyst assisted solution-liquid-solid synthesis is a new method where nanocrystal catalysts are used to grow CdSe nanorods (NR) from solution. The aim of this study is to investigate CdSe samples prepared with this new method by means of x-ray diffraction. The measurements have been performed at DELTA synchrotron using a beam of wavelength 1.127 Å and an image plate system. It is found that the CdSe NRs have a crystal structure of wurtzite with an aspect ratio changing between 2 and 10. This is in contradiction with the results obtained from TEM measurements, according to which the lengths of the NRs are in the order of 1μ and the widths are around 20nm. Presently the results are interpreted by the appearance of stacking faults which separate uniformly stacked AB, AB layers from each other. It is planned to measure an individual NR using a nanofocused x-ray beam. Once an individual NR could be observed, the next step is to measure the powder spectrum using a CCD as a function of the position of the beam spot along the nanorod. Depending on this information, the parameters affecting the structure of the NRs would be clear by making experiments with samples prepared in different conditions.

CPP 13.11 Tue 17:45 C 264

A new method to detect and characterize single metallic nanoparticles using confocal microscopy — •Tina Züchner[1], Antonio Virgilio Failla[1], Achim Hartschuh[2], and Alfred Johann Meixner[1] — [1]Institut für Physikalische und Theoretische Chemie, Universität Tübingen, Germany — [2]present address: Department für Chemie und Biochemie, LMU München, Germany

A new confocal microscopy method for imaging single metallic nanoparticles is presented. It provides information about the particle's shape, size and orientation. For excitation azimuthally and radially polarized doughnut modes [1] were used. The particles were immobilized on glass or embedded in media of different refractive indices. Both the scattered light from the particles and the light reflected at the glass slide were collected and contributed to the image. The resulting patterns were studied experimentally and theoretically. Particles of different shapes (spheres, rods and triangles) could be distinguished [4] and the refractive index mismatch at the sample interface could be detected. For metallic nanorods the 2-dim. orientation can be directly imaged [2] with high precision [3]. Preliminary data shows that the method also allows to determine the 3-dim. orientation of nanorods.

[1] R. Dorn, S. Quabis and G. Leuchs, Phys. Rev. Lett. 91, 233901 (2003). [2] A.V. Failla, H. Qian, H. Qian, A. Hartschuh and A.J. Meixner, Nano Lett. 6, 1374 (2006). [3] A.V. Failla, S. Jäger, T. Züchner, M. Steiner and A.J. Meixner, Opt. Expr. 15, 8532 (2007). [4] T. Züchner, A.V. Failla, A. Hartschuh and A.J. Meixner, J. Microsc., in print (2007).

CPP 13.12 Tue 18:00 C 264

Femtosecond Spectroscopy Study of the Exciton Relaxation Dynamics in Silicon Quantum Dots — •Carola Kryschi[1], Volker Kuntermann[1], Carla Cimpean[1], and Dietrich Haarer[2] — [1]Institut für Physikalische Chemie I, FAU, Egerlandstr. 3, D-91058 Erlangen — [2]BIMF, Universität Bayreuth, D-95440 Bayreuth

This contribution is targeted to the development of surface-modified silicon quantum dots (Siqdots) with tailored luminescence properties. The surface modification of Siqdots with sizes between 1 and 5 nm has been successfully achieved via two different synthesis routes, first, by controlled oxidation followed from silanization and second, by thermal hydrosilylation with chromophores. The luminescence properties of ethanolic Siqdots dispersions were characterized using stationary and time-resolved luminescence spectroscopy techniques, whereas the ultrashort exciton relaxation dynamics were examined using femtosecond transient absorption spectroscopy. Silanized Siqdots were observed to exhibit two species of photoluminescence (PL): the blue emission at 380 nm is assigned to localized surface states, whereas radiative recombination of quantum confined excitons gives rise to a broad PL band around 800 nm. Whereas the latter is ascribed to Siqdots with sizes larger than 3 nm, for Siqdots smaller than 1.5 nm exciton relaxation dynamics is understood to occur predominantly by trapping due to lower-lying surface states which may radiatively decay. Siqdots terminated with suited chromophores were observed to exhibit only one PL band in the visible that is ascribed to exciton states involving resonant couplings to the conjugated electron system of the chromophores.

CPP 13.13 Tue 18:15 C 264

Spectroscopic fingerprints of single dye - quantum dot nanoassemblies — •Danny Kowerko, Jörg Schuster, and Christian von Borczyskowsi — Center of nanostructured materials and analytics, TU-Chemnitz, 09107 Chemnitz

Self assembled nanoassemblies of semiconductor quantum dots (QDs) and organic molecules are of interest for numerous applications in science and technology. However, physics and chemistry of coupling mechanisms and possible interactions (i.e. energy transfer) are complex and thus not yet fully understood. Spectroscopic analysis of nanoassemblies in solution is difficult, since many complex dynamical process are involved [1]. We have chosen an alternative approach to study nanoassemblies by freezing all of the solution dynamics while depositing the nanoparticles in a low concentration on a silicon oxide surface. The solution which we deposit the nanoassemblies from always contains the unbound building blocks too. We may compare spectroscopic properties of the free and bound species on one and the same sample under identical conditions. By recording series of emission spectra of individual quantum dots, dyes and nanoassemblies we obtain very detailed spectroscopic information which allows us to compare the spectroscopic observable quantities for the free and the bound species. We are thus able to extract spectroscopic fingerprints of the nanoassemblies. In this talk we will present results for CdSe quantum dots and functionalized perylene bisimide dye molecules as building blocks for the aforementioned nanoassemblies.

[1] E. I. Zenkevich, C. von Borczyskowski, J. Lum., 122, 784, 2007

CPP 13.14 Tue 18:30 C 264

Optical mesurements on periodically ordered nanoscopic metal clusters on glass substrates — •Michael Weinl, Daniel Kraus, Jörg K. N. Lindner, and Bernd Stritzker — University of Augsburg, Institute of Physics, 86135 Augsburg

Nanosphere lithography (NSL) is a versatile, fast developing tool for fabricating large areas of nanoscopic, highly ordered metallic particles on a substrate surface. NSL uses self-assembled monolayers of colloidal particles as a deposition mask with the empty space between three adjoining nanospheres acting as mask opening. In comparison to e-beam lithography, NSL produces a great amount of defects but on the other hand it is a very fast and cost-effective technique. The fixed triangle geometry of pure nanosphere lithography can be augmented by angle-resolved evaporation or by plasma and ion beam modification of the masks. In this work, polystyrene nanospheres with a diameter of 200 to 1000 nm were used to fabricate colloidal mono- and doublelayers on glas and silicon substrates. Double layers can be used as masks with smaller mask openings and larger pitch, as compared to monolayers. Regular arrays of metallic nanodots were formed by physical vapour deposition of Au and Ag through these masks. The metal particle shape and size was determined by ESEM, AFM and TEM. An apparatus for the spatially resolved mesurement of optical absorption and transmission in the spectral range of 400 to 950 nm was developed to examine the optical properties of regular metal dot arrays. The lateral resolution also allows to observe the optical properties of structures created at mask defects.

CPP 14: Membranes

Time: Tuesday 15:00–16:30 Location: C 230

CPP 14.1 Tue 15:00 C 230

Free Volume and Permeability in Boltorn-modified Gas Separation Membranes — •Klaus Rätzke[1], Jan Kruse[1], Franz Faupel[1], Dana Sterescu[2], Dimitrios Stamatialis[2], Matthias Wessling[2], and Eduardo Mendes[3] — [1]3. Technische Fakultät Universität Kiel, Germany — [2]1. University of Twente, The Netherlands — [3]2. Delft University of Technology, The Netherlands

This paper describes the the permeation properties of poly (2, 6-dimethyl-1,4-phenylene oxide) (PPO) dense polymer films containing aliphatic hyperbranched polyesters, Boltorn (H40) which are dispersed at various concentrations. Focus is on the correlation between permeation and free volume, which was determined by positron annihilation lifetime spectroscopy, using a well established correlation between orthopositrionium lifetime and average free volume size. The gas permeability of PPO with 1.0 wt % of Boltorn is 2-3 times higher than the pure polymer, while at higher concentration (9.1 wt %) of Boltorn the permeability becomes almost 50 % of the pure polymer. The gas pair selectivity, however, stays constant. The increase in permeability at low concentration of Boltorn is due to the increase of the free volume, probably due to hydrogen bonds between Boltorn and the oxygen of PPO backbone. The decreased permeability of PPO containing higher concentration of Boltorn (9.1 wt %) is due to two reasons: decrease in free volume as determined by PALS as well as phase separation. D. Sterescu, D. Stamatialis, E. Mendes, J. Kruse, K. Rätzke, F. Faupel, M. Wessling Macromolecules, 40 (2007) 5400.

CPP 14.2 Tue 15:15 C 230

Novel carbon nanomembranes as support for ultrahigh resolution structural analysis of nanoparticles — •Christoph Nottbohm[1], André Beyer[1], Alla Sologubenko[2], Inga Ennen[1], Andreas Hütten[1], Harald Rösner[3], Wolfgang Eck[4], Joachim Mayer[2], and Armin Gölzhäuser[1] — [1]Fakultät für Physik, Universität Bielefeld — [2]RWTH Aachen — [3]Forschungszentrum Karlsruhe — [4]Universität Heidelberg

The resolution in transmission electron microscopy (TEM) has reached values as low as 0.08 nm. However, these values are not accessible for very small objects in the size range of a few nanometers or lower as they have to be placed on some support, which contributes to the overall electron scattering signal, thereby blurring the contrast. Here, we report on the use of nanomembranes made from cross-linked aromatic self-assembled monolayers as TEM sample supports. When transferred onto a copper grid, a single 1.6 nm thick nanomembrane can cover the entire grid and is free-standing within the micron-sized openings. Despite its thinness, the membrane is stable under the impact of the electron beam. Micrographs taken from nanoclusters onto these nanomembranes show highly increased contrast in comparison to images taken from amorphous carbon supports. In scanning transmission electron microscopy with nanomembrane support, a size analysis of sub-nanometer Au clusters was performed and single Au atoms were resolved.

CPP 14.3 Tue 15:30 C 230

Mechanical properties of freestanding nanomembranes from self-assembled monolayers — •Xianghui Zhang, Nils Mellech, Christoph Nottbohm, Andre Beyer, and Armin Gölzhäuser — Fakultät für Physik, Universität Bielefeld, Postfach 100131, 33501 Bielefeld, Germany

Ultrathin membranes are promising materials in science and nanotechnology. Here we report the characterization of nanomembranes with a thickness of approximately 1.5 nm, which have a remarkable high tensile strength and excellent elasticity. The nanomembranes are aromatic self-assembled monolayers (SAMs) that are laterally crosslinked by electron irradiation. The SAMs are prepared on silicon-nitride windows, supported by a silicon frame. Afterwards the silicon nitride is dissolved, providing freestanding nanomembranes that cover openings in silicon substrate with sizes from 10 μm to 50 μm. Bulge testing is used to determine Young´s modulus and residual stress of the freestanding nanomembranes. Rupture testing is performed to measure tensile strength. The nanomembranes display outstanding performance in tensile strength of up to 700 MPa, which is 4$\sim$7 times higher than the highest currently known value for nanomembranes. The electron dose dependences of tensile strength, the Young´s modulus and the residual stress of the nanomembranes have been systematically studied. This allows to tailor its mechanical properties for the fabrication of nanoelectromechanical (NEMS) devices.

CPP 14.4 Tue 15:45 C 230

Polyelectrolyte-surfactant interactions in foam films — •Nora Kristen[1], Vasile Simulescu[1,2], and Regine v. Klitzing[1] — [1]Stranski-Laboratorium, Institut für Chemie, Technische Universität Berlin, Str. d. 17.Juni 124, 10623 Berlin — [2]West University Timisoara, 300223 Timisoara, Rumania

Interactions between polyelectrolytes and surfactants in foams are of interest for many technical applications, e.g. in cleaning processes. Foam consists of many single free-standing films; to investigate these foam films a so called Thin Film Pressure Balance (TFPB) is used. With this apparatus disjoining pressure isotherms are measured (disjoining pressure vs. film thickness).

Depending on the charge combination of the surfactant and the polyelectrolyte, two different types of films can be formed: either a Common black Film (CBF, mainly stabilized by electrostatic forces) or a Newton Black Film (NBF, mainly stabilized by steric forces).

The addition of polyelectrolytes affects the interactions within the foam due to complexation between the surfactant and the polyelectrolyte at the surfaces. With a cationic surfactant like C(n)TAB a film with positive charged surfaces is formed. After addition of negative polyelectrolyte, the charge at the surface is reversed. In both cases, a CBF is formed due to the electrostatic repulsion of the two interfaces. But what happens at isoelectric point of the surface charge: Is a NBF formed or does the film break? The addition of very low polyelectrolyte concentrations leads to a low net surface charge. Therefore the stability of films with a low polyelectrolyte concentration is investigated.

CPP 14.5 Tue 16:00 C 230

Dynamics of Phospholipids in the Stabilizer Layer of Dispersed Lipid Nanoparticles Investigated by Quasielastic Neutron Spectroscopy — •Tobias Unruh, Sebastian Busch, and Christoph Smuda — Technische Universität München, Forschungsneutronenquelle Heinz Maier-Leibnitz (FRM II) and Physik Department E13, Garching, Germany

Dispersions of colloidal lipid particles such as triglyceride nanoparticles are used as delivery systems for intravenous administration of drugs. The stabilizing properties of the surfactant layer in the interface between the nanoparticles and the aqueous dispersion medium are determined i.a. by the dynamics of the stabilizer molecules, which holds in particular if the dispersed particles undergo rapid shape or size changes as e.g. during their production in a homogenizer or their crystallization after preparation [1].

Investigations on the dynamics of phospholipid molecules in dispersions of alkanes and triglycerides performed by quasielastic neutron spectroscopy (QENS) will be presented. The measurements were carried out at the high resolution time–of–flight spectrometer TOFTOF of the FRM II in Garching. Due to the high neutron flux of the instrument the investigation of samples with only 20 mg of phospholipid in the beam was possible. The dynamics of the phospholipids is compared to their dynamics in the bilayers of small unilamellar vesicles (SUVs) and the effect of the addition of a co–surfactant on the phospholipid dynamics will be discussed.

[1] K. Westesen, B. Siekmann, Int. J. Pharm., 151 (1997) 35

CPP 14.6 Tue 16:15 C 230

Nanoporous Templates from Supramolecular Assembly of Block Copolymers — •Bhanu Nandan, Marcus Böhme, Radim Krenek, and Manfred Stamm — Leibniz Institute of Polymer Research Dresden, Hohe Strasse 6, 01069 Dresden

Highly ordered arrays of nanostructures derived from block copolymer self-assembly have attracted lot of attention for nanotechnological applications, such as in nanostructured networks and membranes, nanoparticles templates and nanoreactors, photonic crystals, and high density information storage media. In the present work, we investigated nanotemplates based on supramolecular assembly (SMA) of polystyrene-*block*-poly(4-vinylpyridine) (PS-*b*-P4VP) and a low molar mass additive 2-(4'-hydroxyphenylazo)benzoic acid (HABA). The strong repulsion between PS and P4VP in this system allowed fabrication of templates with characteristic length-scale which was not accessible in the past with other block copolymers. Moreover, the morphology of these nanotemplates could be tailored by (1) choosing block copolymer of appropriate block length ratio, (2) varying concentration of HABA, or (3) by blending the SMA with respective homopolymers. Long range order was improved by solvent annealing under controlled conditions and using substrates of low roughness. It is further shown that the SMA fabricated in this work can be used to template various functional inorganic nanostructures by electrodeposition, physical vapour deposition or by soaking in nanoparticle solutions.

CPP 15: Single Molecules

Time: Tuesday 17:00–19:00 Location: C 230

CPP 15.1 Tue 17:00 C 230

Single molecule probes in soft materials — •Jörg Schuster and Christian von Borczyskowski — TU Chemnitz, Institut für Physik, 09107 Chemnitz

Within the past years, single molecule spectroscopy has become a routine tool which is extensively used to study soft, mostly biological, materials. The success of single molecule spectroscopy is due to the fact, that single molecule probes are sensitive to the structure and dynamics of their local nanoscale environment. Fluctuations of single molecule observables such as dipole orientation, spectral positions, excited state lifetime which would be averaged out in ensemble experiments are exploited in order to detect static and dynamic heterogeneities in combination with a nano scale resolution.

The present talk will be focussed on the application of single molecule probes in the field of nonbiological, soft materials, including simple and complex liquids as well as polymers. A number of very different single molecule based techniques is used, including single molecule tracking in a wide field microscope as well as spectroscopy in a confocal instrument. The application of special dye probes will be demonstrated by some recent experiments from our group. In addition, we report on a very recent finding, namely to use the so called power law intermittency (blinking), as a probe of local dielectric relaxations and charge trapping in nonconducting polymer materials.

CPP 15.2 Tue 17:15 C 230

Molecular Wires in Single Molecule Junctions: Charge Transport and Vibrational Spectra — •Stefan Ballmann[1], Daniel Secker[1], Heiko B. Weber[1], Wolfgang Hieringer[2], and Andreas Görling[2] — [1]Lehrstuhl für Angewandte Physik, Universität Erlangen-Nürnberg, Staudtstrasse 7, 91058 Erlangen — [2]Lehrstuhl für Theoretische Chemie, Universität Erlangen-Nürnberg, Egerlandstrasse 3, 91058 Erlangen

Quantum transport through single molecules is accompanied by internal molecular vibrations, detectable in principle as vibronic sidepeaks in the conductance spectra. We use the mechanically controllable break-junction (MCBJ) technique for the investigation of single-molecule contacts. The molecules under investigation are oligoynes, with a string-like atomic chain unit consisting of eight carbon atoms with alternating single and triple bonding, spanned between two platinum atoms and protected by bulky ligands. In our experiments, suppressed conductance at low bias, characteristic step-like features at higher voltages and strong sample-to-sample fluctuations are observed in the I-V-characteristics. In order to obtain a better understanding of the experimental results, density functional theory (DFT) calculations were performed. The experimental data show strong indications for the observation of vibrational features as peaks in dI/dV at a temperature of 75 Kelvin. In comparison to the theoretically observed values for the vibrational frequencies of the carbon chain, the peaks are in excellent agreement with the four energetically lowest-lying longitudinal modes.

CPP 15.3 Tue 17:30 C 230

Numeric force ramp spectroscopy for polymer stretching: the role of thermal fluctuations — •Felix Hanke[1,2], Douglas B Staple[2], and Hans Jürgen Kreuzer[2] — [1]Fritz-Haber Institut der MPG, Faradayweg 4-6, 14195 Berlin — [2]Dept of Physics, Dalhousie University, Halifax, NS, B3H 3J5, Canada

Force ramp spectroscopy is aimed at stretching single polymer molecules in an Atomic Force Microscope (AFM) such that the external force applied to the molecule increases linearly. This approach differs from the more commonly used constant velocity experiments in the observed thermal noise of the molecule-cantilever system. Recent experiments on Dextran [1], doubted the applicability of the often-used Gibbs (or fixed force) ensemble based on a thermal fluctuations argument. Here we use a Transfer Matrix formalism to describe the Dextran-cantilever system [2], which is coupled to a master equation description of the pulling process [3]. This theory enables a numerical imitation of the force ramp experiment from which the molecular force response and thermal noise of the force ramp setup are calculated. We find that the thermodynamics governing the force ramp experiment always depends significantly on the AFM cantilever. Specifically, the thermal noise of the system always remains restricted by the cantilever. This leads us to suggest that the interpretation of every single-molecule AFM experiment must account explicitly for the effect both, molecule and cantilever. [1] Walther et al, Biophys J 90 3806 (2006); [2] Hanke, Kreuzer, Eur Phys J B, 22 163 (2007); [3] Hanke, Kreuzer, Phys Rev E, 72 031805 (2005)

CPP 15.4 Tue 17:45 C 230

Time-resolved photoluminescence studies on individual single carbon nanotubes — •Tobias Gokus[1], Hayk Harutyunyan[1], Frank Hennrich[2], Manfred Kappes[2], and Achim Hartschuh[1] — [1]Department Chemie und Biochemie, Ludwig-Maximilians-Universität München and CeNS, D-81377 München — [2]Forschungszentrum Karlsruhe, Institut für Nanotechnologie, D-76021 Karlsruhe

The photoluminescence lifetime of individual semiconducting single-walled carbon nanotubes (SWCNTs) dispersed on glass substrates has been measured using time correlated single photon counting (TCSPC) at room temperature. We observe mono-exponential decay dynamics of the exciton recombination over more than four orders of magnitude in agreement with previous measurements at low temperature [1]. All photoluminescence transients show fast decay times in the range of few picoseconds (˜10 ps) with large variations from nanotube to nanotube of the same chirality (n,m). To clarify the origin of these lifetime variations we studied the effects of finite tube-length, excitation energy and nanotube environment for different nanotube chiralities.

[1] A. Hagen et al., Phys. Rev. Lett. 95, 197401 (2005).

CPP 15.5 Tue 18:00 C 230

Unravelling single polymers on surfaces by scanning force microscopy manipulation — •Wei Zhuang[1], Edis Kasemi[2], Fikri E. Alemdaroglu[3], A. Dieter Schlüter[2], Andreas Herrmann[3], and Jürgen P. Rabe[1] — [1]Department of Physics, Humboldt University Berlin, Newtonstr. 15, 12489 Berlin, Germany — [2]Institute of Polymers, Swiss Federal Institute of Technology, ETH-Hönggerberg, HCI J 541, 8093 Zürich, Switzerland — [3]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

Scanning Force Microscopy (SFM) has become a powerful tool to reveal the superstructure of single polymer molecules as well as to manipulate individualized polymers on solid substratesinto supermolecular functional entities, which would not form spontaneously. The manipulation can be brought about by either exerting a heterogeneous point force with an SFM tip in contact to a single polymer, or by a so called blowing manipulation with a tapping tip, which can exert a homogeneous force to the single polymer with circular topology. Here, we report an SFM tip manipulation of single dendronized polymers (denpols), which allows to determine the self-organized superstructure of denpols and can finally unravel the duplex superstructure of single charged denpols absorbed on solid substrate upon vacuum drying. In addition, we report an SFM blowing manipulation of single DNA-PEG-DNA triblock copolymer, so that the ds-DNA and the organic polymer chain have been unravelled against random coil, which afforded for the first time to visualize all three blocks of a single linear triblock copolymer chain with recognizable contours by SFM.

CPP 15.6 Tue 18:15 C 230

Probing polymer dynamics by interfacial heat transfer at single gold nanoparticles — •Romy Radünz and Frank Cichos — Molecular Nanophotonics Group, University of Leipzig, Linnéstr. 5, 04103 Leipzig

A new time-resolved photothermal microscopy technique has been developed, which allows to follow the release of heat from a single nanoparticle to the local surrounding. Photothermal microscopy is based on the conversion of light absorbed by a single nanoparticle into heat, which is released into the polymer matrix and induces a local refractive index change on a length scale on the order of 100 nm. Finally, this refractive index change can be detected optically with a confocal microscope by heterodyne optical techniques. Within this all-optical setup gold nanoparticles with a diameter down to 10 nm can be detected. By following the temporal evolution of the photothermal signal we are able to probe heat transfer across nanoscale interfaces between single metal nanoparticle and polymer matrix, that depends on the interfacial heat transfer resistance and the heat conductivity of the polymer. Furthermore, it is possible to probe thermal properties of the polymer at various states of matter of the polymer. Temperatures even above melting temperatures of polymers are achievable due to the high absorption cross section and heat conversion efficiency of gold nanoparticles. The lengthscale on which these properties are probed can be controlled by applying an intensity modulated laser beam, since the heat diffusion length decreases with increasing modulation frequency.

CPP 15.7 Tue 18:30 C 230

Mesopore functionalization as highly specific tool for the control of single molecule dynamics in silica materials — •Timo Lebold[1], Julia Blechinger[1], Christophe Jung[1], Johanna Kirstein[1], Klaus Müllen[2], Lea Mühlstein[1], Thomas Bein[1], and Christoph Bräuchle[1] — [1]Center for Nanoscience (CeNS), Ludwig-Maximilians-Universität München, Department of Chemistry and Biochemistry, Butenandtstraße 11, 81377 München — [2]Max Planck Institute for Polymer Research, Ackermannweg 10, 55021 Mainz, Germany

Nanoporous channel systems form a class of very promising host systems in many fields of modern science. Various guests can be embedded into their nanometer-sized pores. Yet, directly influencing the diffusion dynamics of the incorporated guest molecules is not an easy task, even though a broad range of applications (e.g. drug-delivery, catalysis) could profit from this ability. Covalently attached organic functionalizations within the porous network of the silica material could be an efficient tool for realizing this aim. Hence, this study examines the influence of different functionalizations onto the diffusion dynamics of single TDI dye molecules as guests within the mesoporous network of a hexagonal thin silica film. The films were synthesized with the non-ionic Block-copolymer Brij 56 as template. Within the pores the template micelles coexist with an organic carpet of functional groups. The specific choice of this functional groups then allows for a precise tuning of the host-guest interactions and thus the guest dynamics. Furthermore this work will offer detailed mechanistic insights into the diffusion processes within a mesopore.

CPP 15.8 Tue 18:45 C 230

Visualizing single molecule diffusion in nanoporous materials — •Christophe Jung, Johanna Kirstein, Andreas Zürner, Babara Platschek, Thomas Bein, and Christoph Bräuchle — Department of Chemistry and Center for Nanoscience (CeNS), Ludwig-Maximilians-Universität, Butenandtstrasse 11, 81377 München

Nanostructured host-guest materials are important for various applications (e.g. catalysis, molecular sieving, drug-delivery systems). Therefore a thorough understanding of the dynamics and the interactions of the guest molecules inside the host matrix is needed. Whereas measurements of ensemble diffusion provide information about the overall behaviour of the guests in a porous host, tracking individual molecules provides insights into heterogeneities, mechanistic details of molecular diffusion and the host structure. Thin mesoporous silica films containing a hexagonal and lamellar phase mixture were investigated. The dye molecules act as beacons while they diffuse through the different structural phases of the host: the structure of the trajectories, the diffusivities and the orientation of single molecules are distinctive characteristics, for molecules travelling in each mesophase or on the film surface. Moreover, we combine single molecule microscopy techniques with transmission electron microscopy in order to directly correlate individual molecular trajectories with the underlying structure of the porous host. It can be investigated in great detail how the luminescent molecule diffuses within the mesoporous channel system, how it changes speed, direction or traffic lanes in the porous network.

CPP 16: SYMPOSIUM Driven Soft Matter I

Time: Tuesday 9:30–12:30 Location: C 130

Invited Talk CPP 16.1 Tue 9:30 C 130

Imaging the flow of concentrated colloidal suspensions — •Wilson Poon, Lucio Isa, and Rut Besseling — The University of Edinburgh, Scotland, UK

Recent advances in confocal microscopy allow us to image the flow of concentrated colloidal suspensions at single-particle resolution in real time. I will describe results from recent experiments on suspensions of hard spheres at packing fractions of 60% or higher. At zero applied stress, these suspensions behave like amorphous solids ('colloidal glasses'). We have used fast confocal imaging to study the yielding of such suspensions under simple shear, as well as their flow in rectangular capillaries. In both cases, direct imaging has revealed a rich variety of phenomena not predicted by traditional rheological theory treating dense suspensions as yield stress fluids. In the case of pipe flow, we find that a theory previously proposed for granular materials can give a good account of certain aspects of our observations.

Invited Talk CPP 16.2 Tue 10:00 C 130

Stochastic thermodynamics of driven soft matter — •Udo Seifert — II. Institut fuer Theoretische Physik,Universitaet Stuttgart

Stochastic thermodynamics provides a conceptual framework for describing small systems embedded in a heat bath and mechanically or by external flow driven to non-equilibrium. Both the first law and entropy production can be consistently defined along single trajectories. An infinity of integral fluctuation theorems hold, among which the Jarzynski relation and the one on total entropy production are prominent ones [1]. After briefly reviewing and illustrating these foundations using a driven colloidal particle as paradigm, I will present within this scheme our recent work concerning (i) optimal finite-time processes and (ii) extended fluctuation-dissipation theorems (FDTs) and generalized Einstein relations. The optimal protocol of an external control parameter minimizes the mean work required to drive the system from one given equilibrium state to another in a finite time. Explicit solutions both for a moving laser trap and a time-dependent strength of such a trap show finite jumps of the optimal protocol to be typical both at the beginning and the end of the process [2]. The Einstein relation connecting diffusion constant and mobility is violated beyond the linear response regime. Based on our recent extension of the FDT [3], we have derived and measured an additive correction term which involves an integral over measurable correlation functions [4].

[1] U. Seifert, PRL 95: 040602, 2005. [2] T. Schmiedl and U. Seifert, PRL 98: 108301, 2007. [3] T. Speck and U. Seifert, EPL 74: 391, 2006. [4] V. Blickle, T. Speck, U.S., C. Bechinger, PRL 98: 210601, 2007.

Invited Talk CPP 16.3 Tue 10:30 C 130

Spatial cooperativity in soft glassy flows — •Lydéric Bocquet — Lyon University and Technical University Munich

Amorphous glassy materials of diverse nature – concentrated emulsions, granular materials, molecular glasses – display complex flow properties, intermediate between solid and liquid, which are at the root of their use in many applications. A classical feature is the very non-linear nature of the flow rule relating stresses and strain rates. In this talk, I will present recent experimental results for the flow of thin layers of concentrated emulsions which, beyond the classical non-linearities of the rheological behaviour, demonstrate the existence of finite size effects in the flow behavior and the absence of an intrinsic local flow rule. In contrast, a rather simple non-local flow rule is shown to account for all the velocity profiles. This non-locality of the dynamics is quantified by a length, characteristic of the cooperativity of the flow at these scales, that is unobservable in the liquid phase (lower concentrations) and that increases with concentration in the jammed phase. These results will be discussed in the context of a generic elasto-plastic description for the flow dynamics, describing the non-local collective dynamics of the localized plastic events occuring during the flow. Beyond its practical importance for applications involving thin layers, e.g. coatings, our assessment of non-locality and cooperativity echoes observations on other glassy, jammed and granular systems, suggesting a possible fundamental universality.

break

CPP 16.4 Tue 11:15 C 130

Experimental investigation of shear banding in wormlike micelles — •Sébastien Manneville[1], Lydiane Bécu[2], Jean-Baptiste Salmon[3], and Annie Colin[3] — [1]Laboratoire de Physique - Ecole Normale Supérieure de Lyon, 46 allée d'Italie, 69364 Lyon cedex 07, France — [2]CNRS - Université du Maine, Avenue Olivier Messiaen, 72085 Le Mans, France — [3]Rhodia Lab of the Future - CNRS, 178 avenue du Docteur Schweitzer, 33608 Pessac, France

Under simple shear some complex fluids may separate into bands of widely different viscosities. This phenomenon is known as "shear banding" and involves inhomogeneous flows where macroscopic bands bearing different shear rates coexist in the sample. In the last decade, "wormlike micelle" solutions have emerged as a model system to study shear banding. Depending on the concentration, these self-assembled surfactant systems constituted of long, cylindrical, semi-flexible aggregates undergo a shear-induced transition from a viscoelastic state of entangled micelles to a state of highly aligned micelles.

In this talk, we will describe two velocimetry techniques, based on dynamic light scattering and ultrasonic velocimetry respectively, that may be used in combination with conventional rheometry to investigate shear banding with high spatial and temporal resolutions. Experimental results will be presented, where shear-banded flows of wormlike micelles are shown to involve complex spatiotemporal behaviors and apparent wall slip. Such observations, confirmed by recent measurements from other groups, raise lots of open questions that we shall address in the last part of the talk.

CPP 16.5 Tue 11:30 C 130

Rheology and particle tracking on soft colloidal suspensions with tunable glassines — Eko Hari Purnomo, •Dirk van den Ende, Michel Duits, Siva Vanapalli, and Frieder Mugele — Physics of complex fluids, University of Twente, the Netherlands

We studied both the macro- and micro- rheology of soft thermosensitive microgel suspensions that can be tuned continuously and reversibly between the glassy state at low and the liquid state at high temperature. In the glassy state, the rheological properties (G', G'', and J) of the suspensions depend strongly on their age [1]. They can be described quantitatively by the soft glassy rheology (SGR) model. The underlying mechanism for the aging is the increase of the structural relaxation time τ_s as the system ages. To test for micro-rheological propertiesc we determined the mean square displacement (MSD) of probe particles, embedded in the system. The MSD values were obtained from particle tracking using a Confocal Scanning Laser Microscope. This technique provides not only the MSD values but also the displacement distributions and the time evolution of single particle displacements, which are indicative for heterogeneity of the suspension. In this paper we will discuss the non Gaussian properties of our suspension at different levels of glassines as well as the relation between these properties and the macro-rheology.

[1] E.H. Purnomo, D. van den Ende, J. Mellema, and F. Mugele, Phys. Rev. E. 76, 021404 (2007).

CPP 16.6 Tue 11:45 C 130

Diffusion and Taylor dispersion in a simple glass under shear — •Fathollah Varnik — Max-Planck Institut für Eisenforschung, Düsseldorf, Germany

We investigate, via MD simulations of a simple glass, large scale dynamics under homogeneous shear by evaluating the time dependence of the mean square displacements for temperatures ranging from the supercooled state to far below the mode coupling critical temperature of the model. Particularly long simulations are performed allowing an accurate determination of the diffusion constant. For low temperatures and at not too high shear rates, the mean square displacements exhibit the well known two step relaxation behavior with a long time diffusive motion along the spatial directions perpendicular to the flow. In the flow direction, on the other hand, a third regime follows the diffusive motion, where Taylor dispersion with the typical t^3 time dependence clearly dominates the long time behavior of the particle displacements. Once this contribution is subtracted, normal diffusive behavior is recovered in the limit of long times. Comparing diffusive motion along the flow, the shear gradient and the vorticity (neutral) directions reveals small but systematic anisotropy in particle dynamics.

CPP 16.7 Tue 12:00 C 130

A binary Yukawa mixture under shear: A computer simulation study of the transient dynamics — •Jochen Zausch[1] and Jürgen Horbach[2] — [1]Inst. f. Physik, Universität Mainz, Staudinger Weg 7, 55099 Mainz — [2]Inst. f. Materialphysik im Weltraum, DLR, Linder Höhe, 51147 Köln

Very recently, experiments and computer simulations have demonstrated that shear strongly affects transport properties of an undercooled liquid. If the shear rate $\dot{\gamma}$ exceeds the typical relaxation time τ of the system, an acceleration of the dynamics is observed which is reflected, e.g., in a decrease of the shear viscosity (shear thinning). The underlying mechanism of this change is still not well understood on a microscopic level.

We use extensive molecular dynamics simulations to elucidate the transient dynamics of a sheared binary Yukawa mixture from equilibrium to steady state, after a constant shear field is switched on. By inspection of the density-density correlation function we find that the steady state is reached after a time of the order of $\dot{\gamma}^{-1}$. The same is true for the stress that is built up upon increasing strain. The linear velocity profile on the other hand develops in a much shorter time. Similar simulations are performed for the case when a sheared system falls back to equilibrium after shear is switched off. Interestingly, the stress decays as fast as it was built up although the system is still far from equilibrium.

CPP 16.8 Tue 12:15 C 130

Slip and shear-banding in hard-sphere colloidal glasses — •Rut Besseling[1], Pierre Ballesta[1], Lucio Isa[1], George Petekidis[2], and Wilson Poon[1] — [1]School of Physics, University of Edinburgh, Scotland, UK — [2]Inst. Elec. Structure and Laser-FORTH, Heraklion, Crete, Greece

We study slip and flow of colloidal hard-sphere glasses by cone-plate rheometry and simultaneous confocal microscopy, both for microscopically smooth shearing surfaces and for surfaces with particle scale roughness. For smooth walls, the global rheology shows a crossover from Bingham-like slip behaviour at small applied shear rates to a Herschel-Bulkley response at large rate. The velocity profiles show that the *slip to shear* transition is position dependent and we present a phenomenological model that quantifies both local and global rheology. We show that Bingham-type slip is directly connected with the onset of yield stress and that it is generic for hard-sphere glasses at smooth, non-sticky walls.

For rough boundaries, we find global Herschel-Bulkley flow curves, but the associated velocity profiles show marked non-linearity's, developing into strong localization (coexistence of solid and sheared regions) just above the yield stress. This localization has its onset at the glass transition -i.e. flow is uniform for the colloidal fluid- and becomes more pronounced at larger densities. We discuss the possible role of microscopic stress fluctuations as origin for the shear localization.

CPP 17: SYMPOSIUM Driven Soft Matter II

Time: Tuesday 14:00–16:00 Location: C 130

Invited Talk CPP 17.1 Tue 14:00 C 130

Soft Matter under Flow — •Gerhard Gompper — Institut für Festkörperforschung, Forschungszentrum Jülich, D-52425 Jülich, Germany

The dynamics of soft matter systems – such as colloidal suspensions, polymer solutions, and suspensions of fluid vesicles or cells – is often dominated by the hydrodynamic behavior of the solvent. For example, the flow properties of blood in micro-vessels is determined by the rheological properties of the red blood cells, and polymers unfold, tumble and collapse in shear flow. Furthermore, microfluidic devices allow the manipulation of small amounts of suspensions of particles or cells.

Multi-particle collision dynamics (MPC), a particle-based off-lattice mesoscopic simulation techniques has been shown be able to bridge the large length- and time-scale gap between the atomic and the mesoscopic domain in soft matter systems, and to describe hydrodynamic interactions at low Reynolds numbers very well [1]. In particular, it has then be applied recently to study the dynamical behavior of fluid vesicles and model red blood cells both in shear and capillary flows [2].

[1] M. Ripoll, K. Mussawisade, R.G. Winkler and G. Gompper, Europhys. Lett. **68**, 106 (2004); I.O. Götze, H. Noguchi, and G. Gompper, Phys. Rev. E **76**, 046705 (2007).

[2] H. Noguchi and G. Gompper, Phys. Rev. Lett. **93**, 258102 (2004); Proc. Natl. Acad. Sci. USA **102**, 14159 (2005); Phys. Rev. Lett. **98**, 128103 (2007).

Invited Talk CPP 17.2 Tue 14:30 C 130

Viscoelasticity of gels — •Annette Zippelius and Peter Müller — Institut für Theoretische Physik, Georg-August-Universität, D-37077 Göttingen

We study shear relaxation of randomly crosslinked macromolecular networks. The sol phase is characterized by a stretched exponential decay of shear relaxation, which can be traced to the random connectivity of molecular clusters such that weakly connected regions dominate the relaxation of shear. The transition from the sol to the gel is - like the glass transition - characterized by a diverging static shear viscosity, if the transition point is approached from the fluid side, respectively by a vanishing shear modulus, if the approach is from the amorphous solid side. The critical behaviour can be calculated exactly within the Rouse model, including the coefficients of normal stresses. A variational principle can be used to derive an exact lower bound for the static shear viscosity in the presence of excluded volume interactions. The divergence of the lower bound is stronger than in the Rouse model, proving the relevance of excluded volume interactions for the dynamic critical behaviour.

CPP 17.3 Tue 15:00 C 130

Giant DNA Diffusion — •Ralf Eichhorn, Jan Regtmeier, Alexandra Ros, Dario Anselmetti, and Peter Reimann — Universität Bielefeld, Fakultät für Physik, D-33615 Bielefeld

It has been predicted theoretically that particle diffusion in non-equilibrium systems can be enhanced by orders of magnitude, for instance, when the particle is moving in a periodic potential and the non-equilibrium conditions are established by an external static (tilting) force [1,2]. Recently, this effect has been demonstrated experimentally for colloidal particles [3]. We investigate this phenomenon experimentally and theoretically for λ (48.5 kbp) and T2 (164 kbp)

DNA in a structured microfluidic device. The periodic potential landscape is created by electrodeless dielectrophoresis, and the tilting force is realized by electrophoresis. The observed giant diffusion is sensitive to the length of the DNA-fragment, and thus has potential application in DNA purification.

[1] P. Reimann, C. Van den Broeck, H. Linke, P. Hänggi, J.M. Rubi, and A. Perez-Madrid, Phys. Rev. Lett. **87**, 010602 (2001).

[2] P. Reimann, C. Van den Broeck, H. Linke, P. Hänggi, J.M. Rubi, and A. Perez-Madrid, Phys. Rev. E **65**, 031104 (2002).

[3] S. H. Lee, D. G. Grier, Phys. Rev. Lett. **96**, 190601 (2006).

CPP 17.4 Tue 15:15 C 130

Are we built of glass? — •Klaus Kroy[1,3], Pablo Fernandez[2], Jens Glaser[1], Christian Hubert[1], Sebastian Sturm[1], and Lars Wolff[1] — [1]Universität Leipzig, Leipzig, Germany — [2]Technische Universität München, Garching, Germany — [3]Hahn-Meitner Institut, Berlin, Germany

Recently B. Fabry and J. Fredberg [1] discovered that biological cells fall into the broad class of materials exhibiting 'soft glassy rheology' [2]. The glassy wormlike chain (GWLC) is a minimal extension of the standard WLC model of a stiff biopolymer, which establishes a link between this observation and the microscopic interactions of the polymeric constituents of the cytoskeleton [3]. Some of its major predictions for the nonlinear and non-equilibrium mechanical response of biopolymer networks to large driving forces will be outlined and compared to experimental data. On this basis, fundamental aspects of mechano-transduction, nonlinear cell elasticity and plasticity become accessible to theory.

[1] Fabry B, Maksym G. N, Butler J. P, Glogauer M, Navajas D, Fredberg J. J., Phys. Rev. Lett. 87 (2001) 148102

[2] Sollich P, Lequeux F, Hebraud P, Cates M. E., Phys. Rev. Lett. 78 (1997) 2020.

[3] arXiv:0705.049, arXiv:0711.2427

CPP 17.5 Tue 15:30 C 130

Entangled Dynamics of a Stiff Polymer — •Thomas Franosch, Felix Höfling, Tobias Munk, and Erwin Frey — Arnold Sommerfeld Center for Theoretical Physics and Center for NanoScience (CeNS), Department of Physics, Ludwig-Maximilians-Universität München, Theresienstrasse 37, D-80333 München, Germany

Entangled networks of stiff biopolymers exhibit complex response, emerging from the topological constraints that neighboring filaments impose upon each other. The relevant dynamic processes cover many decades in time, posing a tremendous challenge both to experiments and simulations. Pioneered by Edwards and de Gennes, the many-filament interaction was condensed in the picture of reptation in a confining tube. To achieve progress beyond simple scaling arguments, we propose a class of reference models for entanglement dynamics that allows us to provide a quantitative foundation of the tube concept for stiff polymers. For the fundamental limiting case of an infinitely thin needle exploring a planar parcours of point obstacles, we have performed large-scale simulations. Our results unambiguously prove the conjectured scaling from the fast transverse equilibration to the slowest process of orientational relaxation. In the highly entangled regime, the slow dynamics becomes attainable by employing a novel simulation algorithm based on interval analysis. We determine the rotational diffusion coefficient of the tracer, its angular confinement and the tube diameter. In addition, the tube concept is extended to a theoretical description of the complete orientational dynamics including a two-step relaxation, which is corroborated by our simulation results.

CPP 17.6 Tue 15:45 C 130

Flow NMR of polymers in external fields — Ute Böhme, Frank Bagusat, and •Ulrich Scheler — Leibniz Institute of Polymer Research Dresden, Hohe Str. 6, D-01069 Dresden

Pulsed-field gradient NMR is applied to study the motion of polymers in an external electric field and under mechanical shear. The application of an electric field drives motion of charged species. In conjunction with the diffusion coefficient from th electrophoreitc mobility the effective charge per molecule is derived [1-3]. The electric field applicable in the aqueous system is too weak to deform the polymer or even abstract counterions.

In a shear flow established in a Couette cell partial orientation of polymer chains is measured via residual dipolar couplings. The entire flow field in a non-symmetric flow cell is monitored by a combination of PFG NMR and NMR imaging exhibiting regions of high shear and locally low shear, where polymers relax [4].

[1] U. Böhme, U. Scheler, Colloids and Surfaces A, 222, (2003), 35 [2] U. Böhme, C. Vogel, J. Meier-Haack, Us. Scheler, J. Phys. Chem. B 111, (2007), 8344 [3] U. Böhme, U. Scheler, Journal of Colloid and interface science 309, (2007), 231 [4] A. Gottwald, U. Scheler, Polymer Preprints, 44, (2003), 273

CPP 18: SYMPOSIUM Driven Soft Matter III

Time: Tuesday 16:30–18:30 Location: C 130

Invited Talk CPP 18.1 Tue 16:30 C 130

Bifurcations in complex fluids — •Ingo Rehberg and DFG-Forschergruppe 608 — Universität Bayreuth

The dynamic behavior of complex fluids in the neighborhood of bifurcation points is considered as particularly interesting, because here small changes of the external field lead to a maximal response. Moreover, the reaction of the fluid if often accompanied by symmetry breaking processes, which can be experimentally detected with great precision. In particular, we will present measurements of the reorientation of liquid crystalline gels under electric fields [1], and of the dynamic response of magnetic fluids to the change of external magnetic fields [2,3].

[1] Freedricksz transition in a thermoreversible nematic liquid gel; Matthias Müller, Wolfgang Schöpf, Ingo Rehberg, Günter Lattermann, Andreas Timme (submitted).

[2] Reorientation of a hexagonal pattern under broken symmetry: The hexagon flip; Christopher Groh, Reinhard Richter, Ingo Rehberg, and F. H. Busse, Phys. Rev. E 76, 055301(R) (2007).

[3] Response of a ferrofluid to travelling stripe forcing; Achim Beetz, Christian Gollwitzer, Reinhard Richter, Ingo Rehberg (submitted).

CPP 18.2 Tue 17:00 C 130

Dynamics in inhomogeneous liquids and glasses via the test particle limit — •Matthias Schmidt[1,2], Paul Hopkins[1], and Andrew J. Archer[3] — [1]H. H. Wills Physics Laboratory, University of Bristol, Tyndall Avenue, Bristol BS8 1TL, United Kingdom — [2]Institut für Theoretische Physik II, Heinrich-Heine-Universität Düsseldorf, Universitätsstraße 1, D-40225 Düsseldorf, Germany — [3]Department of Mathematical Sciences, Loughborough University, Loughborough, Leicestershire, LE11 3TU, United Kingdom

We show that one may view the self and the distinct part of the van Hove dynamic correlation function of a simple fluid as the one-body density distributions of a binary mixture that evolve in time according to dynamical density functional theory. For a test case of soft core Brownian particles the theory yields results for the van Hove function that agree quantitatively with those of our Brownian dynamics computer simulations. At sufficiently high densities the free energy landscape underlying the dynamics exhibits a barrier as a function of the mean particle displacement, shedding new light on the nature of glass formation. For hard spheres confined between parallel planar walls the barrier height oscillates in-phase with the local density, implying that the mobility is maximal between layers, which should be experimentally observable in confined colloidal dispersions.

CPP 18.3 Tue 17:15 C 130

Dynamic density functional theory of fluids of platelike colloidal particles — •Markus Bier and Rene van Roij — Institute for Theoretical Physics, Utrecht University, The Netherlands

Fluids of platelike colloidal particles, e.g., suspensions of clay, exhibit a large range of phenomena such as flocculation, glass transitions, gelation, aging, and even liquid crystal phase transitions because of the interplay between translational and orientational degrees of freedom.

In recent years dynamic density functional theories (DDFT) for simple fluids, i.e., for particles with only translational degrees of freedom, have been derived based on Langevin dynamics, which can be considered as a reasonable description of dilute colloidal dispersions. DDFT is a convenient formalism to describe nonequilibrium configurations of inhomogeneous fluids given one knows a sufficiently precise density functional to descibe the equilibrium behaviour.

We proposed a DDFT for fluids of platelike colloidal particles based on a density functional for platelike colloidal particles within the Zwanzig approximation in order to investigate the relaxation within an external field [M. Bier and R. van Roij, Phys. Rev. E 76, 021405 (2007)] as well as the formation of nonequilibrium steady states under the influence of reservoirs which are not in equilibrium with each other [M. Bier and R. van Roij, submitted (see preprint arxiv:0710.5439v1)]. In this contribution we will briefly motivate the formalism and afterwards report in detail on the numerical findings.

CPP 18.4 Tue 17:30 C 130

Hydrodynamical jet oscillations and band structures in the flow of nano-rods — •Sebastian Heidenreich, Siegfried Hess, and Sabine H. L. Klapp — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergst. 36, D-10623

The flow properties of nano-rods are strongly affected by the dynamical behavior of molecular alignment. A theoretical description can be made by an relaxation equation [1] of the order parameter tensor. For plane Couette flow geometry the model implies a rather complex orientational behavior [2] even in the case where the alignment is spatially homogeneous and the flow profile is linear. In the last years the dynamics of the inhomogeneous alignment and the effect on the velocity profile was investigated intensively [3]. In our contribution we model fluid-wall interactions by boundary conditions for the alignment tensor (strong anchoring). Our numerical analysis for the plane Couette flow yields oscillating local spurts of the velocity profile, referred to as hydrodynamical jets which are caused by the competition of elasticity and flow coupling. Moreover, we observe time-dependent shear bands in startup flows.

[1] S. Hess, Z. Naturforsch. **30a**, 728, 1224 (1975)
[2] G. Rienäcker, M. Kröger, and S. Hess, Phys. Rev. E **66**, 040702(R) (2002);
[3] B. Chakrabarti, M. Das, C. Dasgupta, S. Ramaswamy, and A. K. Sood, Phys. Rev. Lett. **92**, 055501 (2004); S. Heidenreich, P. Ilg and S. Hess, Phys. Rev. E 75, 066302 (2007)

CPP 18.5 Tue 17:45 C 130

Dynamical density functional theory for anisotropic colloidal particles — •Martin Rex, Henricus Herman Wensink, and Hartmut Löwen — Institut für Theoretische Physik II: Weiche Materie, Universität Düsseldorf, Germany

We generalize the formalism of dynamical density functional theory for translational Brownian dynamics towards that of anisotropic colloidal particles which perform both translational and rotational Brownian motion. Using a mean-field approximation for the density functional and a Gaussian-segment model for the rod interaction, the dynamical density functional theory is then applied to a concentrated rod suspension in a confined slab-geometry made by two parallel soft walls. The walls are either expanded or compressed and the relaxation behavior is investigated for an equilibrated starting configuration. We find distinctly different orientational ordering during expansion and compression. During expansion we observe preferential parallel ordering of the rods relative to the wall while during compression there is homeotropic ordering perpendicular to the wall. We find a nonexponential relaxation behavior in time. Furthermore an external field which aligns the rods perpendicular to the walls is turned on or switched off and similar differences in the relaxational dynamics are found. Comparing the theoretical predictions to Brownian dynamics computer simulation data, we find good agreement.

CPP 18.6 Tue 18:00 C 130

Novel estimators for the effective charge of polyelectrolytes during electrophoresis — •Kai Grass[1] and Holm Christian[1,2] — [1]Frankfurt Institut for Advanced Studies, Ruth-Moufang-Strasse 1, D-60438 Frankfurt am Main, Germany — [2]Max-Planck-Institut für Polymerforschung, Ackermannweg 10, D-55128 Mainz, Germany

In this contribution, we present two novel estimates for the effective charge (Q_{eff}) of strongly charged polyelectrolyte chains during free solution electrophoresis by means of coarse-grained molecular dynamics simulations.

First, we show that it is possible to calculate Q_{eff} from the electrophoretic mobility obtained from Langevin simulations. Second, we are able to directly obtain Q_{eff} from the number of comoving counter ions. Both estimators yield similar results and show that the effective charge of polyelectrolyte chains grows linear in the number of monomers as previously predicted.

The effective charge is used to evaluate the scaling behavior of the hydrodynamic friction of the polyelectrolyte-counterion-complex. We show the violation of the Nernst-Einstein equation during free solution electrophoresis by obtaining a linear dependence on chain length for the hydrodynamic friction which differs from the scaling of the hydrodynamic size.

CPP 18.7 Tue 18:15 C 130

Dynamical properties of magnetic nanoparticles in ferrofluids investigated by Brownian dynamics — Guillaume Meriguet[1], •Marie Jardat[1], Emmanuelle Dubois[1], Vincent Dupuis[1], Bela Farago[2], Regine Perzynski[1], and Pierre Turq[1] — [1]Universite Pierre et Marie Curie-Paris6, Paris, France — [2]Institut Laue Langevin, Grenoble, France

The dynamical properties of real ferrofluids, charge-stabilized aqueous dispersions of magnetic particles bearing a permanent dipole, are investigated with and without an external magnetic field by Brownian dynamics simulations. On the one hand, since the magnetic particles have an anisotropic optical index, their rotational properties have been studied experimentally: an external magnetic field induces a macroscopic birefringence the relaxation of which is followed after the magnetic field is suppressed. A non-equilibrium simulation procedure is proposed that mimics the experimental operating mode: after equilibrium simulations under magnetic field, the birefringence decay is recorded once the field is suppressed. On the other hand, the translational dynamics of the nanoparticles is investigated. The diffusion coefficient of the particles has been experimentally determined at several wave-vectors using neutron spin echo spectroscopy, with and without an external magnetic field. The same quantities are computed from Brownian dynamics simulations. The comparison between experimental and theoretical results allow us to evaluate the influence of several factors on the dynamics, such as the volume fraction, the dipolar interactions or hydrodynamic interactions.

CPP 19: SYMPOSIUM Driven Soft Matter IV

Time: Wednesday 14:00–16:00 Location: C 130

CPP 19.1 Wed 14:00 C 130

Simulating rare events in nonequilibrium systems: nucleation in a driven Ising system — •Rosalind Allen — SUPA School of Physics, Edinburgh University, Edinburgh, UK

I will describe the application of the recently developed Forward Flux Sampling method [1-4] for simulating rare events to a nonequilibrium transition - nucleation in a sheared two dimensional Ising system. I will describe an analysis of the transition state ensemble to understand the reaction mechanism and rationalise the observed nonmonotonic dependence of the nucleation rate on the shear rate.

[1] Sampling rare switching events in biochemical networks. R. J. Allen, P. B. Warren and P. R. ten Wolde, Phys. Rev. Lett. 94, 018104 (2005)

[2] Simulating rare events in equilibrium or nonequilibrium stochastic systems. R. J. Allen, D. Frenkel and P. R. ten Wolde, J. Chem. Phys. 124, 024102 (2006)

[3] Forward flux sampling-type schemes for simulating rare events: Efficiency analysis. R. J. Allen, D. Frenkel and P. R. ten Wolde, J. Chem. Phys. 124, 194111 (2006)

[4] Computing stationary distributions in equilibrium and nonequilibrium systems with forward flux sampling. C. Valeriani, R. J. Allen, M. Morelli, D. Frenkel and P. R. ten Wolde, J. Chem. Phys. 127, 114109 (2007)

CPP 19.2 Wed 14:15 C 130

Driven polymer blends: criticality and structure formation in inhomogeneous temperature fields — •Werner Köhler, Al-

bert Voit, and Alexei Krekhov — Physikalisches Institut, Universität Bayreuth

Even moderately inhomogeneous temperature fields, as generated by localized laser heating, couple to the order parameter (the composition) and can drive polymer blends far out of equilibrium. Close to the critical point this Soret effect can be four to five orders of magnitude stronger than in conventional liquid mixtures. Global equilibrium phase diagrams loose their meaning, and even UCST-mixtures can be quenched into phase separation by local heating. Close to the critical point we observe critical scaling, and almost arbitrary composition patterns can be written into a PDMS/PEMS blend using a galvano laser scanner. Below the spinodal the prescribed patterns compete with the intrinsic length scale of the correlation length, and surface tension effects become increasingly important. The theoretical modelling of the structure formation is based on a modified Cahn-Hilliard-equation, and 2D-models are able to reproduce the essential spatio-temporal features. While the susceptibility (Soret coefficient) diverges at the critical point of the liquid-liquid phase transition, it is completely insensitive to a glass transition due to a cancellation of local friction being effective on the molecular length scale of a few monomers.

[1] A. Voit, A. Krekhov, W. Enge, L. Kramer, W. Köhler, PRL 94 (2005) 214501; [2] A. Voit, A. Krekhov, W. Köhler, Macromolecules 40 (2007) 9; [3] A. Voit, A. Krekhov, W. Köhler, PRE 70 (2007) 011808

CPP 19.3 Wed 14:30 C 130

Super-heterodyne light scattering as versatile tool to characterize multiphase flow — •Thomas Palberg[1], Tetjana Köller[1], and Gerhard Nägele[2] — [1]Institut f. Physik, Johannes Gutenberg Universität, Mainz — [2]Institut für Festkörperforschung, Forschungszentrum Jülich GmbH., Jülich

Condensed matter put to extreme mechanical impact may react by crack formation, creep flow or even (partial) melting behaviour. Soft matter model systems may help in elucidating such phenomena due to both their softness, implying significant mechanical response even for small loads and their enlarged length and time scales, facilitating convenient optical access. Colloidal crystals in particular may display shear induced straining, local or global shear melting or shear induced crystallization, if subjected to shearing fields. Structural evolution may be monitored in detail using either video microscopy or time resolved static light scattering. We here show that incoherent scattering contributions (dominant at low scattering angles or selectively detected in VH geometry) can be exploited to provide the complementary information on the complex flow behaviour, without interference with the structural distribution. Super heterodyning in addition renders the data of interest free of homodyne contributions and low frequency noise. The combination of coherent and incoherent scattering experiments therefore may help in clarifying the coupling between structure and motion under shear. We exemplify our method studying an aqueous charged sphere suspension driven under the influence of different fields.

CPP 19.4 Wed 14:45 C 130

Fluid interfaces under shear: Studying the Ising model under drive. — Tom Smith[1], Oleg Vasilyev[2], Douglas B. Abraham[3], •Anna Maciolek[2], and Matthias Schmidt[1] — [1]H. H. Wills Physics Laboratory, University of Bristol, Tyndall Avenue, Bristol BS8 1TL, UK — [2]Max-Planck-Institut fuer Metallforschung, Heisenbergstr. 3, D-70569 Stuttgart, Germany — [3]Theoretical Physics, Department of Physics, University of Oxford

We use a phase-separated driven two-dimensional Ising lattice gas in order to model liquid-liquid interfaces exposed to shear flow parallel to the interface. The model is confined between two parallel walls and two different types of external field with direction parallel to the walls are used to drive the system out-of-equilibrium : i) the field acts locally at the walls, or ii) the field varies linearly with distance across the slit. From computer simulations using Kawasaki (conserved order parameter) dynamics we obtain structural information such as the lateral and transversal correlation lengths at the interface. In equilibrium the confinement of the interface due to the presence of walls reduces its width and the characteristic transverse (correlation) length, while increasing the interfacial free energy. We find that shear induces similar effects. Furthermore we test whether the roughness of the driven interface decreases as compared to the equilibrium case. The global effects of shear on the system are in particular surprising for case i) where only particles at the boundaries of the system are driven. The relationship of our findings to recent experimental results in sheared phase-separated colloidal dispersions is discussed.

CPP 19.5 Wed 15:00 C 130

2d-Motion of magnetic particles in external fields — •Artur Erbe, Peter Henseler, Michael Koeppl, Marcin Zientara, Peter Nielaba, and Paul Leiderer — Universitaet Konstanz, FB Physik, Konstanz, Germany

Magnetic colloidal particles are ideal model systems to study the behavior of particles, which interact via dipole-dipole interactions, under various conditions. Here we present studies of a two-dimensional system of micron-sized particles moving under the influence of an external field. The external force acting on the particles is either given by gravity or a gradient in the magnetic field. We study the motion of the particles by video microscopy and compare the results to molecular dynamics simulations. Layering and layer-reduction effects are observed, when the particles are driven through narrow channels. This behavior is explained by the interplay of the interparticle interactions and the influence of the confining walls. In unbounded systems we observe laning of the particles. We discuss possible origins for this behavior.

CPP 19.6 Wed 15:15 C 130

Bridging scales in a phase separating binary fluid: From Cahn-Hilliard to Doi-Ohta model — •Asja Jelić, Patrick Ilg, and Hans Christian Öttinger — ETH Zurich, Department of Materials, Polymer Physics, CH-8093, Switzerland

Mixtures of immiscible fluids are systems that can be studied at various length and time scales. The General Equation for the Non-Equilibrium Reversible-Irreversible Coupling (GENERIC) framework is used to connect two different levels of description of a phase separating binary fluid. We start from the Cahn-Hilliard model of spinodal decomposition in a binary fluid mixture under flow from which we derive the coarse-grained description. The familiar Doi-Ohta model is recovered in the long wavelength limit. The key ingredient required for this procedure is a mapping of the variables of one level to another, so that a statistical formulation of GENERIC framework in a generalized mixed ensemble enables one to develop a thermodynamically consistent formulation and simulation algorithms for non-equilibrium systems and sets the framework for their multi-level description. The present state of the study relates the two levels by giving the expected reversible time evolution and shedding new light on the irreversible processes and the interpretation of the parameters in the Doi-Ohta model.

CPP 19.7 Wed 15:30 C 130

Thermodynamically consistent coarse-graining in unentangled polymer melts: mapping microscopic dynamics to conformation tensor theory — •Patrick Ilg, Martin Kröger, and Hans Christian Öttinger — ETH Zürich, Polymer Physics, 8093 Zürich, Switzerland

The dynamics of polymer melts both, in equilibrium and under flow is extremely interesting from a theoretical and application point of view. We here propose a systematic and thermodynamically consistent coarse-graining method that uses a combination of Monte-Carlo and molecular dynamics simulations in order to break the time-scale problem present in polymer systems. The method relies on the splitting of reversible and irreversible contributions to the dynamics and explicitly accounts for the entropy generated in the coarse-graining step. This work uses a general framework of nonequilibrium thermodynamics [1] and builds upon similar studies on the derivation of hydrodynamics for rarefied gases [2].

Starting with a classical bead-spring model of unentangled polymer melts, we coarse-grain to the frequently used conformation tensor level. We verified the method for the case of planar shear flow, where we obtain the correct viscosity and normal stress differences in the low shear rate regime.

[1] H. C. Öttinger. Beyond-Equilibrium Thermodynamics. Wiley, 2005. [2] M. Kröger and H. C. Öttinger. Beyond-equilibrium molecular dynamics of a rarefied gas subjected to shear flow. J. Non-Newtonian Fluid Mech., 120:175–187, 2004.

CPP 19.8 Wed 15:45 C 130

Correlations in granular media with volume driving — •Wolf Till Kranz[1], Timo Aspelmeier[1], and Annette Zippelius[1,2] — [1]Max-Planck-Institut für Dynamik und Selbstorganisation, Göttingen — [2]Universität Göttingen

Due to the dissipative nature of the interaction of granular particles an input of energy is needed in order to reach a stationary state. The simplest example of energy injection, volume driving by randomly forcing each particle, leads to an unphysical divergence of the structure factors at long wavelengths. We show that this divergence is removed when the driving is modified to obey momentum conservation. The length scale l on which momentum is conserved determines the length scale on which correlations build up: on lengths scales shorter than l the remnants of the divergence are still visible while it is suppressed on longer scales. We discuss the long wavelength behaviour of the static structure factor and the longitudinal current correlation function.

CPP 20: POSTERS Driven Soft Matter

Time: Wednesday 16:00–18:30 Location: Poster A

CPP 20.1 Wed 16:00 Poster A

Alignment of microphase separated block-copolymers by ionic polarization — •Peter Kohn, Klaus Schröter, and Thomas Thurn-Albrecht — Department of Physics, Martin Luther University Halle-Wittenberg, 06120 Halle, Germany

Microphase separated block-copolymers display well defined local periodic structures. In the absence of an external field the domains are oriented isotropically on a macroscopic scale. It is well known that by applying a static external electric field, which couples to the dielectric contrast of the domains, the system's thermodynamic equilibrium is changed to the state where the domain interfaces are oriented along the electric field direction.

In contrast to this approach we show that alignment can also be achieved with AC-electric fields which induce an additional polarization caused by mobile ions in a system with selective ion solubility in one block. In such a dissipative conducting system the resulting structure is governed by stability considerations rather than thermodynamic equilibrium, but an orientation of the interfaces parallel to the field is the stable domain-orientation with no torque acting on the domains. We use impedance spectroscopy to characterize the induced ionic polarization in a styrene-methylmethacrylate block-copolymer doped with lithium triflate. By small-angle x-ray scattering the effect of electric fields of different frequency and strength on the domain orientation is studied. Orientation based on mobile ion polarization is more efficient than the dielectric mechanism of orientation.

CPP 20.2 Wed 16:00 Poster A

Bistable and chaotic solutions in polar nano-rod systems under shear — •Stefan Grandner[1], Sebastian Heidenreich[2], Siegfried Hess[2], and Sabine H. L. Klapp[1,2] — [1]Stranski-Laboratorium, TU Berlin, Straße des 17. Juni 115, D-10623 Berlin, Germany — [2]Institut für theoretische Physik, TU Berlin, Hardenbergstraße 36, D-10623 Berlin, Germany

The orientational dynamics of rod-like particles with permanent dipole moment shows a time dependent response in a plane Couette flow. This behavior can be described by nonlinear mesoscopic relaxation equations for the alignment tensor [1] and the polarization [2] combined with a generalized Landau free energy. This yields an eight-dimensional coupled system of differential equations. For simplicity we assume a spatially homogeneous system. Numerical results are presented for longitudinal dipoles where the equilibrium state is a polarized nematic. The large variety of periodic, transient chaotic and chaotic states is summarized in solution diagrams [3]. Compared to the non-polar case we observe a preference of dynamic states out of the shear plane and a higher sensitivity to initial conditions, resulting in larger bistability regions. The time dependence of the electric polarization generates magnetic fields of measurable strength.

[1] S. Hess, Z. Naturforsch. **30a**, 728, 1224 (1975).
[2] S. Grandner, S. Heidenreich, P. Ilg, S. H. L. Klapp, and S. Hess, Phys. Rev. E **75**, 040701(R) (2007).
[3] S. Grandner, S. Heidenreich, S. Hess, and S. H. L. Klapp - Polar nano-rods under shear: From equilibrium to chaos (submitted).

CPP 20.3 Wed 16:00 Poster A

Growth instabilities of thin colloidal crystals prepared by convective self assembly. — José Marqués-Hueso and •Hans Joachim Schöpe — Johannes Gutenberg-Universität Mainz, Institut für Physik, Staudinger Weg 7, 55099 Mainz, Deutschland

Colloidal particles have proved to be a suitable precursor to the formation of nanoscaled materials. More explicitly, crystalline arrays of colloidal particles (synthetic opals) show interesting optical properties with potential application as new types of optical gratings or optical filters. They further serve as a starting material of 3D photonic band gap materials. Their performance heavily relies on the material quality. One of the less studied defects in the case of colloidal crystals produced by vertical deposition is the modulation of the film thickness. Often a near regular periodic horizontal modulation in the thickness of the crystalline film can be observed. In our manuscript we present the first systematic measurements of the thickness modulation as a function of the volume fraction and the salt concentration of the suspension, of the tilting angle of the substrate, of the substrate material and of the pulling speed. We observe a variation of the growth velocity suggesting an inconstant behavior of the meniscus with a stick-slip motion like observed in simple droplet drying experiments. We suggest that a stick-slip motion of the meniscus during the evaporation process can explain the stripes morphology in the case of colloidal crystals.

CPP 20.4 Wed 16:00 Poster A

Bouncing Droplets and Partial Coalescence with Polymer Solutions — •Stephan Gier[1], Stéphane Dorbolo[2], and Christian Wagner[1] — [1]Technische Physik, Universität des Saarlandes, D-66123 Saarbrücken — [2]GRASP, Université de Liège, B-4000 Liège

We investigate bouncing droplets consisting of different polymer solutions on a vibrated Newtonian liquid surface. It is known that Newtonian liquid droplets on a vibrated bath of a high viscosity oil undergo a bouncing motion. In our experiments we see that adding different polymers or surfactants changes the bouncing behaviour of the droplets. This holds for both the shape of the droplets and the acceleration threshold of the vibrated bath. If one puts a liquid droplet on an interface between two fluids, where the lower one is the same as the droplet fluid, then partial or total coalescence can occur depending on four dimensionless parameters (Bond number, Ohnesorge numbers of both fluids, relative density difference between the two fluids). This is well known for Newtonian liquids. For our non-Newtonian solutions the coalescence is only nearly partial in all the experiments because the elasticity of the polymer solutions suppresses the forming of a so-called daughter droplet.

CPP 20.5 Wed 16:00 Poster A

Colloids in non-equilibrium steady states - Direct measurement of a reponse function — •Maximilian Semmling, Valentin Blickle, and Clemens Bechinger — 2. Physikalisches Institut, Universität Stuttgart

The Brownian motion in equilibrium has been studied for long time. In recent times remarkable progress in the understanding of non-equilibrium systems was made. The Jarzynski Relation and other fluctuations theorems of non-equilibrium systems have been tested for different experimental setups.

As the simplest case we study non-equilibrium steady states of colloidal particles. In our setup we use a rotating laser trap to apply a tilted periodic potential to the particle. We obtain different non-equilibrium steady states by changing the driving force of the laser. We measure the time dependent velocity response of the system driven from one steady state to another.

CPP 20.6 Wed 16:00 Poster A

Salt concentration and particle density dependence of electrophoretic mobilities of spherical colloids in aqueous suspension — •Tetyana Köller[1], Holger Reiber[1], Thomas Palberg[1], and Felix Carrique[2] — [1]Institut für Physik, Johannes Gutenberg Universitaet, 55099 Mainz, Germany — [2]Departamento de Fisica Aplicada 1, Universidad de Málage, Campus de Teatinos, 29071 Málaga, Spain

Using Laser Doppler Velocimetry in the super-heterodyne mode, we conducted a systematic study of the electrophoretic mobility of dispersions of small silica spheres (a=18nm) suspended in water at different salinity and particle concentration. The concentration of NaCl was varied from 40μM up to 16mM, while the particle concentrations were varied between 4,2x10ˆ18 mˆ-3 and 2,1x10ˆ20 mˆ-3. We find a decrease of mobility with increasing salt concentrations and an increase with increased particle number densities. The latter observation is not backed by the standard cell model of electrophoresis with Shilov-Zharkikh boundary conditions. Rather, if the experimental data are interpreted within that model an unexpected change of the zeta potential at constant added salt concentration results. Interestingly, all experimental data collapse on a single master curve, if plotted versus the ratio C* of particle counter ions to added salt ions. We obtain a logarithmic increase of mobility for C*<1 and a plateau for C*>1. This may indicate a change of the Stern layer structure not yet included in the theoretical model.

CPP 20.7 Wed 16:00 Poster A

Polymer drift in a solvent by force acting on one polymer end — •Semjon Stepanow[1] and Norio Kikuchi[2] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany — [2]Centre for Condensed Matter Theory, Department of Physics, Indian Institute of Science, Bangalore 560 012 India

We investigate the effect of hydrodynamic interactions on the non-equilibrium drift dynamics of an ideal flexible polymer pulled by a constant force applied at one polymer end using the perturbation theory and the renormalization group method. For moderate force, if the polymer elongation is small, the hydrodynamic interactions are not screened and the velocity and the longitudinal elongation of the polymer are computed using the renormalization group method. Both the velocity and elongation are nonlinear functions of the driving force in this regime. For large elongation we found two regimes. For large force but finite chain length L the hydrodynamic interactions are screened. For large chain lengths and a finite force the hydrodynamic interactions are only partially screened, which in three dimensions results in unusual logarithmic corrections to the velocity and the longitudinal elongation.

CPP 20.8 Wed 16:00 Poster A

Instabilities in straight and curved microchannels — •Virginie Vergnat and Christian Wagner — Technische Physik, Universität des Saarlandes, D-66123 Saarbrücken

We present experimental measurements on flow instabilities of pressure driven polymer solutions in curved microchannels. We investigate how these instabilities develop at the end of the curvature, when the microchannel becomes a straight, flat channel. The pressure driven flow of elastic liquids in curved channels is linear unstable whilst in straight channels it is stable. But the form of, and the threshold to, a nonlinar instability is controversially discussed. We use Micro-PIV to determine the type of instability, e.g if there might be convective or global instability regimes.

CPP 20.9 Wed 16:00 Poster A

Fluctuation-dissipation theorem for soft matter systems in shear flow — •Thomas Speck and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, Germany

In equilibrium, the fluctuation-dissipation theorem (FDT) connects the response of an observable with the time-derivative of the correlation function between this observable and its conjugate with respect to the external perturbation. If we drive the system into a nonequilibrium steady state then entropy will be produced on average and the FDT breaks down. We have shown how to quantify the breakdown of the FDT for a single particle through an additive violation function [1]. We will extend this result to soft matter systems composed of many particles like polymers and colloidal suspensions. As an illustration, we calculate analytically the violation function in the case of a Rouse polymer in simple shear flow.

[1] T. Speck and U. Seifert, Europhys. Lett. **74**, 391 (2006).

CPP 20.10 Wed 16:00 Poster A

AC field-induced shape change of nematic liquid crystalline droplets — •Günter K. Auernhammer, Jinyu Zhao, Beate Ullrich, and Doris Vollmer — MPI Polymerforschung, Mainz, Germany

We investigate the influence of AC fields on nematic liquid crystalline droplets coexisting with and immersed in a continuous isotropic phase of the same mesogenic liquid. Its dielectric constant and (small but non-vanishing) electric conductivity depend on both the phase and the orientation. These dependences can give rise to convective motion in the nematic phase (electro-hydrodynamic convection, EHC) or near the droplet surface (leaky dielectric model, LDM). Due to the extremely low surface tension of nematic-isotropic interface, viscous stresses easily can induce substantial deformations visible under the microscope.

We follow the influence of frequency and electric field strength on the deformation of the droplets for liquid crystals with positive and negative dielectric anisotropy (5CB and MBBA). In both cases we find a disk-like (oblate) deformation which shows a maximum when plotted as a function of frequency at constant applied field. Isotropic droplets in a nematic surrounding behave in a similar manner but show an elongation (prolate deformation). Depending on the initial size of the droplets, the interaction between neighboring droplets is either attractive or repulsive. Added tracer particles in the isotropic phase reveal a convective motion around the nematic droplets driving the deformation of the droplet. We interpret our findings in the frame work of the LDM and find good agreement.

CPP 20.11 Wed 16:00 Poster A

Quantitative test of Mode Coupling theory for quasi-hard spheres — Fabian Weysser[1], Antonio Puertas[2], Thomas Voigtmann[3], and •Matthias Fuchs[1] — [1]Universität Konstanz, Fachbereich Physik, Germany — [2]Universidad de Almería, Departamento de Física Aplicada, Spain — [3]University of Edinburgh, School of Physics, Great Britain

Mode Coupling Theory (MCT), describes a dynamical phase transition to a glassy state for colloidal suspensions and molecular liquids. As only input to the theory the static structurefactor of the system is being used. The polydisperse hard sphere system is one of the simplest model system: While polydispersity prevents crystallization the system still exhibits a glass transition. Numerical solutions of the MCT equations were calculated for a Molecular Dynamics (MD) system of polydisperse quasi hard spheres. The structurefactor input originated from this MD system. The MCT solutions and the MD output were compared with special attention to the behavior of one and multi-component MCT calculations. The interesting dynamic quantities in these systems are the fluctuating density correlations describing the structural relaxation.

Fits to the dynamic output of the MD system were performed with the MCT results with the packing fraction as only fit parameter.

The final decay of the density correlations can be described better by multi-component systems than by one-component systems.

CPP 20.12 Wed 16:00 Poster A

Constitutive equation for dense colloidal dispersions — Brader Joe M.[1], Voigtmann Thomas[2], Cates Michael E.[2], and •Fuchs Matthias[1] — [1]Fachbereich Physik, Universität Konstanz, Germany — [2]SUPA, School of Physics, The University of Edinburgh, UK

We present a first principles approach to the rheology of dense colloidal suspensions subject to homogeneous but otherwise arbitrary flow. Starting from the fundamental Smoluchowski equation for interacting Brownian particles neglecting hydrodynamic interactions we derive exact results for calculating time dependent averages, which lead e.g. to a generalized Green-Kubo relation for the stress tensor. Using Mori-Zwanzig type projection operator steps we develop a formally exact equation of motion for the transient density correlator which captures structural relaxation under flow. Approximations to these quantities are then developed which lead to a general constitutive equation for dense dispersions under arbitrary homogeneous flow. As the approximations used are tailored to treat high density systems our final equations allow the time dependent rheology of glassy colloidal suspensions to be investigated. We demonstate the effectiveness of our approach by presenting numerical results for shear [1] and general flows, including step-strain/compression, steady-shearing and creep.

[1] J. Brader et al., Phys. Rev. Lett. 89, 058301 (2007); M. Fuchs and M.E. Cates, Phys. Rev. Lett. 89, 248304 (2002)

CPP 20.13 Wed 16:00 Poster A

Hard spheres under shear — •Erik Lange[1], Cristiano de Michele[2], Francesco Sciortino[2], and Matthias Fuchs[1] — [1]University of Konstanz — [2]Universita di Roma La Sapienza

Hard spheres are an important model system in equilibrium as well as in non-equilibrium statistical mechanics.

Adding Brownian motion, hard sphere systems serve as model for colloidal dispersions. Yet, the simulation of hard spheres with Brownian dynamics is difficult because of the singular nature of the interaction potential.

We develop an event-driven approach to simulate Brownian motion of (truly) hard spheres at high densities and present results for strongly sheared systems.

In particular we want to focus on the stress tensor:

$$\sigma_{xy} = \frac{1}{V} \left\langle \sum_i m_i (v_i)_x (v_i)_y + \sum_{i<j} (F_{ij})_x (r_{ij})_y \right\rangle .$$

This can be used to calculate not only the stress-stress correlation functions but also the viscosities, and non-linear flow curves.

These quantities can be measured directly in a sheared colloidal suspensions.

We present results from simulations of a system with a simple linear shear profile not including hydrodynamic interactions.

CPP 20.14 Wed 16:00 Poster A

The crossover of transport properties of polymer solutions from the high polymer limit to finite chain length — •Dominik Stadelmaier, Jürgen Rauch, Marianne Hartung, and Werner Köhler — Physikalisches Institut, Universität Bayreuth

In our contribution we discuss the influence of polymer chain length and solvent viscosity on the Soret effect in polymer solutions. The Soret effect (thermal diffusion) describes the mass flow in a binary system with a temperature gradient. In most polymer solutions the polymer is moving to the cold side (thermal diffusion coefficient D_T is positive) and D_T does not depend on the polymer chain length in the high polymer limit as already recognized by de Gennes in 1981 and observed in previous experiments. This suggests to interpret D_T as being a property of the monomer. Measurements of long chained polystyrene (PS) in different solvents in our group have identified the viscosity as the dominating solvent parameter. In order to investigate the crossover from the polymer regime to shorter chains we measured samples of polystyrene solutions with molar masses ranging from $4 \cdot 10^3 kg/mol$ down to the effective monomer ethylbenzene. Remarkably D_T decreases with decreasing polymer chain length but remains positive for all solvents down to the dimer. For the effective monomer there is a sign reversal in three of the solvents. Our results suggest an interpretation for D_T in terms of effective correlated segments acting as thermodiffusing entities that are much larger than a single monomer unit and approximately of the size of the Kuhn segment.

CPP 20.15 Wed 16:00 Poster A

Effects of spatio-temporal forcing on phase separation — •Vanessa Weith, Alexei Krekhov, and Walter Zimmermann — Theoretische Physik I, Universität Bayreuth, 95440 Bayreuth, Germany

Motivated by recent experiments on polymer blends with a large Soret effect [1,2] we have studied phase separation in the presence of an inhomogeneous temperature field. Within a generalized Cahn-Hilliard model [3] we have investigated the effects of an additive spatio-temporal forcing $\sim a\cos(qx - vt)$ on phase separation, which corresponds to a spatio-temporal temperature modulation in optical grating experiments [1,2].

For a stationary forcing with $v = 0$ one finds that beyond a critical forcing amplitude $a_0(q)$ spinodal decompostion is locked by the spatially periodic forcing. We show how this critical locking amplitude is changed by increasing the pulling velocity v. Furthermore we identify the changes of the bifurcation to the spatially periodic patterns as a function of v and we present results about the spatio-temporal behavior of the solution of the generalized Cahn-Hilliard model in one and two spatial dimensions.

[1] S. Wiegand and W. Köhler, in Thermal Nonequilibrium Phenomena in Fluid Mixtures, edited by W. Köhler and S. Wiegand (Springer, Heidelberg, 2002)

[2] W. Enge and W. Köhler, Phys. Chem. Chem. Phys. 6, 2373 (2004)

[3] A. P. Krekhov and L. Kramer, Phys. Rev. E 70, 061801 (2004)

CPP 20.16 Wed 16:00 Poster A

Isotope and isomer effect in thermal diffusion of binary liquid mixtures — •Steffen Hartmann, Gerhard Wittko, and Werner Köhler — Physikalisches Institut, Universität Bayreuth

A temperature gradient induces a diffusive mass flow in a multicomponent system, which is counterbalanced in the stationary state by the Fickian mass diffusion. The occuring concentration gradient can be described by the Soret coefficient, defined as the ratio of the thermal and the Fickian diffusion. There still exists no rigorous theory for thermal diffusion in liquids and a few transient holographic grating experiments have been performed in which well definied parameters are systematically varied. The isotopic substitution leaves most molecular parameters unchanged and mainly affects the molecular mass and moment of inertia. Deuteration of one component leads to a change of the Soret coefficient, which is independent of concentration and temperature. For many binary mixtures there exists a certain concentration where the temperature dependence of the Soret coefficient vanishes. In contrast to the isotope effect, the change of the Soret coefficient due to isomeric substitution depends on the concentration.

CPP 20.17 Wed 16:00 Poster A

Dynamic density functional theory: correlated Brownian motion in colloidal systems — •Joachim Dzubiella — Physics Department, Technical University Munich, Germany

Classical density functional theory (DFT) has been proven to be a powerful mathematical tool to describe the equilibrium structure and phase behavior of correlated many-body systems (e.g., dense colloidal or biological fluids) in bulk or under the action of external potentials. Using the equilibrium functional a dynamic DFT can be constructed which accurately reproduces and predicts the strongly inhomogeneous steady-state or even time-dependent structure of systems in non-equilibrium. Here we present selected examples of colloidal systems out of equilibrium, such as driven polymer solutions, diffusion-controlled reactions, and sedimenting colloids in confinement.

CPP 20.18 Wed 16:00 Poster A

Ultrafast Dynamics in Nanolayered Polyelectrolyte/ Metallic Structures Studied by Femtosecond Pump-Probe Spectroscopy — •Mareike Kiel[1,2], Wolfram Leitenberger[1], and Matias Bargheer[1,2] — [1]Max-Planck-Institut für Kolloid- und Grenzflächenforschung, Potsdam — [2]Universität Potsdam

The dynamic response of hybrid nanolayer systems composed of polyelectrolytes and metals upon optical excitation is studied by ultrafast pump-probe experiments. Relative intensity changes of transient absorption and reflection spectra are measured with light in the visible and near-infrared region, providing information on the photoinduced dynamics within the structure. We investigate multilayer stacks of (MEPE/PSS) that is, a metallofunctionalized polyelectrolyte-amphiphile multilayer complex fabricated by the layer-by-layer technique, as well as gold colloid particle strata separated by several PAH/PSS layers. We compare the results to investigations of equivalent crystalline solid state multilayer structures with dimensions on the nanometer length scale. We compare the generation and propagation of specific hypersound waves in the frequency range of 1 THz, which is given by the speed of sound in the respective material (∼2 nm/ps) and its artificial spatial layering period (∼2nm). The timescale of the expansion mode of the entire structure is measured to lie in the ∼20ps range.

CPP 20.19 Wed 16:00 Poster A

On multiplicative forcing effects in the Cahn-Hilliard model — •Christian Feller, Alexei Krekhov, and Walter Zimmermann — Theoretische Physik I, Universität Bayreuth, 95440 Bayreuth, Germany

Phase separation in the presence of a spatially periodic temperature modulation has been investigated theoretically. The linear stability analysis of the homogeneous basic state of the Cahn-Hilliard model with periodic modulation $G\cos(Qx)$ of the control parameter has been performed.

The threshold for the onset of the bifurcation has been determined as function of the modulation amplitude G and the modulation wave number Q. For harmonic and subharmonic solutions with respect to the modulation of the control parameter one obtains different thresholds for the bifurcation from the basic state. The threshold for the harmonic solutions is always lower. Beyond the threshold there exists a discrete set of periodic solutions characterized by the wave number Q/m (with integer m) which become stable only beyond a certain second threshold.

It has been found that in the two dimensional case additional longitudinal perturbations do not influence the bifurcation diagram obtained for one dimension. Numerical simulations of phase separation dynamics in a quenched system in two dimensions are compared with the results of linear stability analysis.

CPP 20.20 Wed 16:00 Poster A

Large deviation functions for the entropy production in

driven systems — •Jakob Mehl, Thomas Speck, and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, Pfaffenwaldring 57/III, D-70550 Stuttgart

In stochastic thermodynamics, notions like work, heat, and entropy production can be defined along a single trajectory. For systems coupled to a heat bath and driven into a nonequilibrium steady state, we study the probability function for the entropy produced in the surrounding medium. In the long time limit, this probability function is determined through the large deviation function. Instead of obtaining the large deviation function from the probability function directly, we apply an operator technique. As an example for linear stochastic systems, we study a dumbell consisting of two particles connected through a spring in simple shear flow. As an example for non-linear systems, we focus on a single colloidal particle moving in a spatial periodic potential confined to one dimension by a toroidal trap.

CPP 20.21 Wed 16:00 Poster A

Crystallizing hard spheres — •Sara Iacopini[1], Hans Joachim Schöpe[1], Eckhard Bartsch[2], and Thomas Palberg[1] — [1]Johannes Gutenberg Universität, Institut für Physik, Staudingerweg 7, D-55128 Mainz, Germany — [2]Albert Ludwigs Universität, Institut für Physikalische Chemie, Albertstraße 21, D-79104 Freiburg, Germany

Colloidal systems display phase transition that are totally analogous to those observed in atomic systems. In particular, a system of colloidal particles where only excluded volume interactions are relevant (a hard-spheres system) tends to form an ordered crystal phase upon increasing the particles volume fraction. Beyond the freezing line, the undercooling of the system acts as a driving force towards the formation of the solid phase. However, it is still a matter of theoretical and experimental investigations which path will the system actually follow in its journey towards the thermodynamically stable state, and which factors may influence it. We studied by means of light scattering the crystallization kinetics of polystyrene microgel colloids in an organic solvent, a system that has proved to display hard-sphere-like behaviour. Our experiments allowed for monitoring the phase transition from the metastable fluid, to the onset of nucleation and growth of the crystallites, up to the later stage of ripening of the polycrystalline material. We investigate how, with increasing particles volume fraction, the growing competition between the thermodynamic driving force and the approaching dynamical arrest modifies the crystallization scenario.

CPP 20.22 Wed 16:00 Poster A

Growth and Pattern Formation in the Kardar Parisi Zhang equation — •Hans Fogedby — Department of Physics and Astronomy, Aarhus University, Aarhus, Denmark

A nonperturbative weak noise scheme is applied to the Kardar-Parisi-Zhang equation for a growing interface in all dimensions. It is shown that the growth morphology can be interpreted in terms of a dynamically evolving texture of localized growth modes with superimposed diffusive modes. Applying Derrick's theorem it is conjectured that the upper critical dimension is four.

CPP 20.23 Wed 16:00 Poster A

memory in paste and its application to control crack pattern — •akio nakahara and yousuke matsuo — Nihon University, Funabashi, JAPAN

We experimentally find that paste (densely packed colloidal suspension) has memories of external mechanical fields such as vibration and flow. There is a transition in memory from memory of vibration to memory of flow as we decrease a volume fraction of colloidal particles in paste. These memories in paste are maintaned as anisotropic microstructures, and can be visualized as crack patterns which emerge when the paste is dried. When paste has a memory of vibration, the direction of crack propagation becomes perpendicular to the direction of the vibration. On the other hand, when paste has a memory of flow, the direction of crack propagation becomes parallel to the direction of the flow [1].

By using these memory effects, we can imprint direction of crack propagation into paste to control and produce various crack patterns, such as cellular, lamellar, radial, ring, spiral, and so on.

[1] A. Nakahara and Y. Matsuo, Phys. Rev. E 74, 045102(R) (2006).

CPP 20.24 Wed 16:00 Poster A

Active components at interfaces — •Thomas Fischer[1] and Pietro Tierno[2] — [1]Experimentalphysik V, Bayreuth, Germany — [2]Physics, Barcelona, Spain

We study the motion of paramagnetic colloidal particles placed above magnetic bubble domains of a uniaxial garnet film and driven through the lattice by external magnetic field modulation. An external tunable precessing field propels the particles either in localized orbits around the bubbles or in superdiffusive or ballistic motion through the bubble array. This motion results from the interplay between the driving rotating signal, the viscous drag force and the periodic magnetic energy landscape. We explain the transition in terms of the incommensurability between the transit frequency of the particle through a unit cell and the modulation frequency. Ballistic motion dynamically breaks the symmetry of the array and the phase locked particles follow one of the six crystal directions.

CPP 20.25 Wed 16:00 Poster A

CRYSTAL SUPERSTRUCTURES OF COLLOIDAL CRYSTALS IN CONFINEMENT — Ana Barreira Fontecha, •Hans Joachim Schöpe, and Thomas Palberg — Johannes Gutenberg-Universität Mainz, Institut für Physik, Staudinger Weg 7, 55099 Mainz, Deutschland

Colloidal model systems have been used over three decades investigating the structural and dynamic properties of liquids, crystals and glasses as well as crystallization and the glass transition. Crystal superstructures have been observed in binary systems of repulsive spheres as well as oppositly charged sphere systems showing structures well known from atomic solids. We study the structural transition of colloidal crystals confined to low angle wedge geometry. Restricting the available space leads to an adaptation of the crystalline bulk structures to the symmetry of the confinement and a rich variety of strutures is found as a function of colloid packing fraction and confinement dimension. In addition to the known sequence of crystalline structures, crystal superstructures with dodecagonal symmetry are observed in one component colloidal model system under confinemen having no atomic counterpart.

PRL, submitted

CPP 20.26 Wed 16:00 Poster A

Confined colloidal crystals. — Ana Barreira Fontecha, •Hans Joachim Schöpe, and Thomas Palberg — Johannes Gutenberg-Universität Mainz, Institut für Physik, Staudinger Weg 7, 55099 Mainz, Deutschland

The packing of spheres in confined geometry is of fundamental and practical interest for logistics, mathematics, condensed matter physics. For colloids in the bulk bcc packing is observed at long ranged repulsions, while fcc and hcp for short ranged interactions. Restricting the available space leads to adaptations of these structures to the symmetry of the confinement and a rich variety is found as a function of colloid packing fraction and confinement dimension. Their practical importance lies within their use as photonic and phononic materials, while at the same time there is a fundamental interest to understand this diversity in terms of thermodynamics, kinetics and the influence of external forces. We study the confinement of colloidal latex spheres subjected to lateral compression in a thin wedge, which allows us to investigate the structural changes taking place in the transition from 2 to 3 dimensions. In this presentation we extend former experimental work presenting new crystalline structures. In particular, we report on a vertically oriented hexagonally close packed (hcp) structure, a prism structure with triangular basis, a prism structure with square basis and a structure alternating between triangular and square symmetry. Following the maximum packing criterion we show that all these structures have their own range of maximum stability as function of the plate distance. PRE 76, 050402R (2007)

CPP 20.27 Wed 16:00 Poster A

Energy elastic effects in flowing polymeric liquids, and the concept of nonequilibrium temperature — •Markus Hütter, Clarisse Luap, and Hans Christian Öttinger — ETH Zürich, Department of Materials, Polymer Physics, CH-8093 Zürich, Switzerland

Entropy elasticity of rubbers serves as a starting point for most of the current models to describe the flow of polymeric liquids with an internal conformation tensor, while consideration of energetic effects is scarce. Such exclusive subscription to entropy elasticity can be considered a little surprising, in particular in view of microscopic modeling where potential forces between (united) atoms play a dominant role. In this regard, it is interesting to discuss the possible ramifications of energy elasticity on the flow behavior of polymeric liquids. After discussing previous approaches in literature for capturing energy elastic effects, we develop a thermodynami- cally consistent model in terms of the momentum density, the local entropy density, the mass density, and the conformation tensor as dynamic variables. The choice of the local entropy as a variable in contrast to temperature or total entropy is of primary importance, as will be explained in due detail. Specifically, we avoid working with a temperature concept that is ill-defined in flow. In order to render the conclusions of the model more specific, a microscopically motivated toy model with energetic effects is introduced, for which both the coarse-grained energy and entropy are calculated in a generalized canonical ensemble.

CPP 20.28 Wed 16:00 Poster A

Viscoelastic Instabilities — •Christian Wagner — Technische Physik, Universität des Saarlandes, 66123 Saarbrücken

Viscoelastic liquids are characterized by a complex viscosity with a dissipative and an elastic contribution. Similar to simple Newtonian liquids, above a critical threshold, one can observe a transition from laminar to complex flow situations. But other than in Newtonian liquids, the threshold might occur at Reynolds numbers Re << 1. The critical condition of the instability is mainly determined by the so called Weisenberg Number, the ratio of the flow rate to the characteristic relaxation time of the liquid. This leads to completely new instability mechanisms, like e.g. the subcritical formation of double whirl patterns in Taylor Couette flow, the occurrence of turbulent like flow in planar Couette flow at vanishing Reynolds numbers or the transition to elastic turbulence in Poiseuille flow that can lead to melt fracture, a severe problem in fiber spinning processes. We present a general introduction into the problem of elastic instabilities and present experimental and theoretical results on elastic instabilities in Poiseuille flow.

CPP 20.29 Wed 16:00 Poster A

Non-affine deformations of inherent structure as signature of cooperativity in supercooled liquids — •Emanuela Del Gado, Patrick Ilg, Martin Kroeger, and Hans Christian Oettinger — Polymer Physics, ETH Zürich

Experimental and theoretical investigations close to the glass transition indicate the presence of cooperatively rearranging regions of growing size, but it is still debated whether and how cooperativity can be related to structural changes. We search for a signature of the onset of cooperative dynamics in the structural features of supercooled liquids from a novel perspective [1]. We unveil the existence of non-affinely rearranging regions in the inherent structures (IS) by numerical simulations of model glass formers subject to static affine deformations combined with local energy minimizations [2]. In the liquid state IS, we find a broad distribution of rather large, non-affine displacements which are correlated only over small distances. At low temperatures, the onset of the cooperative dynamics corresponds to much smaller non-affine displacements correlated over larger distances. This indicates the presence of non-affinely rearranging domains of relevant size in the IS, which can be seen as the IS counterpart of the cooperatively rearranging regions in the dynamics. This idea suggests a new insight into possible structural signatures of slow cooperative dynamics of supercooled liquids and supports the connections with elastic heterogeneities found in amorphous solids.

[1] H. C. Oettinger, Phys. Rev. E 74, 011113 (2006). [2] E. Del Gado, P. Ilg, M. Kroeger and H.C. Oettinger, cond-mat/0711.1581.

CPP 20.30 Wed 16:00 Poster A

Optimal control of many-electron systems with time-dependent density-functional theory — •Alberto Castro and E. K. U. Gross — Institut für Theoretische Physik, Fachbereich Physik, Freie Universität Berlin, 14195 Berlin (Germany)

We propose the use of time-dependent density-functional theory (TDDFT) within the framework of quantum optimal control theory (QOCT). This amounts to controlling the time-dependent Kohn-Sham (KS) system of non-interacting particles, and driving it towards a desired objective. The obtained driving field will identically control the density of the real, interacting system – and those observables that can be written as simple density functionals. In practice, working with the KS system of equations implies the following peculiarities with respect to the usual QOCT formalism: (i) Since the system is non-interacting, the wave functions are restricted to be single Slater determinants. The basic variational variables are therefore the KS orbitals; (ii) The dependence of the KS Hamiltonian with the density forces us to consider a generalized QOCT formalism, able to tackle with non-linear propagation equations; (iii) The formulation of the target, which is an obvious task in standard QOCT, raises interesting theoretical questions when working with the KS system.

CPP 20.31 Wed 16:00 Poster A

Transitions of Smectic Systems under Shear Investigated by Nuclear Magnetic Resonance — Bruno Medronho[1,2], Shahram Shafaei[3], Gönül Ar[3], Michael Blaschke[3], Ulf Olsson[2], and •Claudia Schmidt[3] — [1]Department of Chemistry, University of Coimbra, 3004-535 Coimbra, Portugal — [2]Physical Chemistry 1, Center of Chemistry and Chemical Engineering, Lund University, Box 124, 221 00 Lund, Sweden — [3]Department of Chemistry, University of Paderborn, Warburger Str. 100, 33098 Paderborn, Germany

Smectic phases driven by shear show interesting structural transitions. Most interesting is the formation of monodisperse, close-packed, multilamellar vesicles (MLVs), also called onions, that is found in many lyotropic lamellar phases [1]. Other systems show transitions between different orientations of planar layers, when parameters such as shear rate or temperature are changed. These dynamic transitions, which can be continuous or discontinuous, have been investigated by deuterium NMR spectroscopy [2]. Results for the shear-induced formation and destruction of MLVs in an aqueous solution of the nonionic surfactant $C_{10}E_3$ will be presented [3].

[1] O. Diat, D. Roux, and F. Nallet, J. Physique IV, 3, 193 (1993).

[2] S. Müller, Claus Börschig, Wolfram Gronski, Claudia Schmidt, and D. Roux, Langmuir, 15, 7558 (1999).

[3] B. Medronho, S. Shafaei, R. Szopko, M. G. Miguel, U. Olsson, C. Schmidt, in preparation.

CPP 20.32 Wed 16:00 Poster A

Velocity Autocorrelation Function in Driven Granular Gases — •Andrea Fiege[1], Wolf Till Kranz[1], Timo Aspelmeier[1], and Annette Zippelius[1,2] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Institute of Theoretical Physics, University of Göttingen, Germany

We study a system of granular gas particles in 2 and 3 dimensions, i. e. spherical particles which suffer energy loss due to inelastic collisions. An energy source (volume bulk driving) provides a stationary state, allowing us to compute time-delayed correlation functions. Here we concentrate on the velocity autocorrelation function, which is studied with the help of the Mori-Zwanzig projector operator formalism and molecular dynamic simulations. Diffusion coefficients are calculated within the Green-Kubo framework and their enlargement compared to the corresponding Enskog values is shown to exhibit a nonmonotonic dependence on the density. We also discuss the possibility of long time tails in the velocity autocorrelation.

CPP 20.33 Wed 16:00 Poster A

Mesoscale hydrodynamics approach to viscoelastic fluids — •Ingo Goetze, Yu-Guo Tao, Hiroshi Noguchi, and Gerhard Gompper — Forschungszentrum Juelich, Juelich, Germany

Multi-particle collision (MPC) dynamics is a well-established, highly efficient particle-based hydrodynamics simulation technique for Newtonian fluids. The standard version of MPC does not conserve angular momentum. However, there are situations, where this leads to non-physical results. Therefore, we have developed a new method with angular momentum conservation.[1] We show that this method has to be employed, for example, to correctly describe circular Couette flow of multiphase fluids.[2]

Moreover, many complex fluids show viscoelastic behaviour. Therefore, an efficient MPC method for viscoelastic fluids is highly desirable. We present such an algorithm, that shows Maxwell fluid behaviour.

[1] H. Noguchi, N. Kikuchi, and G. Gompper, Europhys. Lett. **78**, 10005 (2007).

[2] I. O. Götze, H. Noguchi, and G. Gompper, Phys. Rev. E **76**, 046705 (2007).

[3] Y-G. Tao, I. O. Götze, and G. Gompper, submitted

CPP 20.34 Wed 16:00 Poster A

Event-Driven Simulation of Cluster Aggregation under Periodic and Steady Shear — •Daniel Rings and Klaus Kroy — Institut für theoretische Physik, Universität Leipzig, Vor dem Hospitaltore 1, 04103 Leipzig

Aggregation of colloids has an impact on various technological as well as biological systems. Consider for example the accumulation of dust in bearings, or the clotting within blood vessels.

In the framework of our toy model we study universal features as well as distinct differences of a two-dimensional colloidal suspension under steady shear stress and periodic driving. Especially, the gelling behavior and thus macroscopic observables differ in that there appears a transition from (quasi-)stationarity to irreversible gelation. We present improvements to our collision-driven dynamics simulation, by which the investigations have been conducted. Its main features comprise a spatial coarse-graining scheme as well as approximative reduction of local event queues, which results in good algorithmic efficiency at high precision.

CPP 20.35 Wed 16:00 Poster A

The concept of temperature in driven granular suspensions — •Matthias Schröter, Alexander Buck, Leen Alawieh, and Harry L. Swinney — CNLD, UT Austin, Texas

Dense granular suspensions driven by a flow field show signatures of glass formation like dynamical heterogeneities, rate-dependence, or increase of timescales. The possibility to describe such non-equilibrium phenomena with an effective temperature is still debated. Our measurements using a torsion pendulum and tracking of tracer particles test the applicability of fluctuation-dissipation theorem based temperature concepts.

CPP 20.36 Wed 16:00 Poster A

Colloids in AC fields: Edge localized instabilities in dielectrophoretic bottles — Jinyu Zhao, •Günter K. Auernhammer, and Doris Vollmer — MPI Polymerforschung, Mainz, Germany

Dielectric colloids dispersed in a dielectric liquid experience a body force in gradients of AC fields. This force is due to the contrast in the dielectric properties between the colloids and the surrounding liquid. It allows to tune the concentration of colloids in the dielectrophoretic bottle by changing the applied field.

We investigate the process of filling the dielectrophoretic bottle, i.e., directly after turning the field on. Our system consists of sterically stabilized PMMA colloids in a density-matching mixture of decaline and cyclohexyl bromide. At high frequencies of the applied field (100 kHz to 1MHz), we find that the spatially homogeneous migration of the colloids can be unstable against localized colloidal flows. Our experiments indicate a critical value of the driving force for the instability. The onset is at a field of $\approx 0.5V/\mu m$ in the dielectrophoretic bottle. We analyze this instability in analogy to the Rayleigh-Taylor instability. In contrast to the standard Rayleigh-Taylor instability, the driving body force is not due to gravity but due to the applied field gradient.

CPP 20.37 Wed 16:00 Poster A

Towards magnetic response of composite materials: Nanoparticle incorporation into polymer matrix — •Marta Kolasinska[1], Rumen Krastev[1], Thomas Gutberlet[2], and Helmuth Möhwald[1] — [1]Max Planck Institut für Kolloid- und Grenzflächenforschung, 14424 Potsdam/Golm, Deutschland — [2]Paul Scherrer Institut, 5232 Villigen PSI, Switzerland

Nanometer thick polymer materials with embedded nanoinhomogeneities possess a number of specific properties which depend strongly on the inter particle distances in the matrix. Fabrication of well-defined nanostructures is a prerequisites to obtain materials of desired functions.

We incorporated magnetite nanoparticles onto/into polyelectrolyte multilayers (PEMs) and found that a 2D ordering of particles into *monolayers* depends on treatment of underlying PEM changing it from metastable to equilibrium. The metastable glassy PEM were permeable for the nanoparticles while in the melted PEM the particle penetration was blocked. They were concentrated at the film *surface* forming 2D ordered layer. The magnetic moment of the sample was checked by neutron reflectometry. We found pronounced magnetic response in the reflectivity curves. This proves that structures with appropriate concentration of magnetic particles were achieved which makes such materials suitable to prepare new magnetic responsible materials.

CPP 21: POSTERS Colloids, Nanoparticles and Aggregates

Time: Wednesday 16:00–18:30 Location: Poster A

CPP 21.1 Wed 16:00 Poster A

Tuning the Surface Field at Liquid/Liquid Interfaces: New Wetting Behaviours and Surface Phase Transitions — •Christian Bahr[1], Erfan Kadivar[2], Yasutaka Iwashita[1], Holger Stark[3], and Stephan Herminghaus[1] — [1]MPI for Dynamics and Self-Organization, 37073 Göttingen — [2]Department of Physics, University of Isfahan, 81746 Isfahan, Iran — [3]Institute of Theoretical Physics, Technical University Berlin, 10623 Berlin

We present experimental and theoretical results concerning the ordering and wetting behaviour at interfaces between thermotropic liquid crystals and aqueous phases. The addition of a surfactant to either of the two bulk media provides the interface with an ordering potential which strongly influences the behaviour in the vicinity of the liquid-crystal – isotropic phase transition.

At nematic – isotropic transitions, the observed behavior changes from surface-induced order at higher surfactant concentrations to surface-induced disorder at lower surfactant concentrations. The experimental behavior can be well described within the framework of Landau-de Gennes theory. Current measurements concentrate on the realization of prewetting transitions.

At smectic – isotropic transitions, the variation of the surfactant concentration enables the observation of new surface layering transitions and surface triple points which were predicted by theoretical models but have experimentally not been demonstrated so far.

[1] E. Kadivar, Ch. Bahr, and H. Stark, Phys. Rev. E **75**, 061711 (2007); Ch. Bahr, Phys. Rev. Lett. **99**, 057801 (2007).

CPP 21.2 Wed 16:00 Poster A

Time resolved fluorescence studies of self-assembling porphyrins — •jędrzej szmytkowski[1,3], chilla malla reddy[2], mihaela carmen balaban[3], teodor silviu balaban[2,3], and heinz kalt[1,3] — [1]Karlsruhe Institute of Technology (KIT), Universität Karlsruhe (TH), Institute of Applied Physics, Karlsruhe, Germany — [2]Karlsruhe Institute of Technology (KIT), Forschungszentrum Karlsruhe, Institute of Nanotechnology, Karlsruhe, Germany — [3]Center for Functional Nanostructures (CFN), Karlsruhe, Germany

There is a great interest in biomimetic antenna systems, which can be used in hybrid solar cells. The self-assembly causes an increase in the harvesting of sunlight in such structures. In order to find novel artificial self-assembling compounds, we have studied the time resolved luminescence of several new diacetyl zinc porphyrins as well as push-pull porphyrins having an electron withdrawing group and an electron donating group directly grafted onto the porphyrin macrocycle and the data have been analyzed using decay associated spectra (DAS). The results show the formation of molecular aggregates in the investigated systems.

CPP 21.3 Wed 16:00 Poster A

Self–assembly driven pattern formation of dendron–like macromolecules on a structured surface — •Marta Balbás-Gambra, Erwin Frey, and Thomas Franosch — Arnold Sommerfeld Center for Theoretical Physics and Center for NanoScience, Ludwig-Maximilians Universität, München

Dendron–like macromolecules have been observed to self–assemble into a broad variety of patterns on top of graphite surfaces. We have developed a theoretical model to understand the nature of this assembly and explored the phase behavior as a function of temperature and density. The interaction between the macromolecules is described by an interaction–site model, which largely simplifies the complexity and reduces the model to a few points representing both the aromatic rings and carbonated chains of the molecule. The attraction between chains of different molecules is accounted for by a short ranged potential (Lennard–Jones), whereas the strong repulsion of the aromatic rings is encoded in a hard–sphere interaction. Suitable order parameters are introduced to describe the ensuing ordered phases and corresponding patterns. The phase behavior is explored employing extensive Monte–Carlo simulations.

CPP 21.4 Wed 16:00 Poster A

Influence of self assembled monolayers on local structuring

of silicon — •Harald Graaf, Thomas Baumgärtel, and Christian von Borczyskowski — Center of Nanostructured Materials and Analytics, TU Chemnitz, 09107 Chemnitz, Germany

The local anodic oxidation of hydrogen-terminated silicon by an atomic force microscope under ambient conditions is an established method for the preparation of silicon oxide nanostructures. The kinetics of this process have been studied in detail by several groups and the influence of humidity, applied electric field, shape of the cantilever and exposure time respectively tip veocity has been developed.

We will discuss here the influence of two organic alkenes with different headgroups (CH_3 and $COOCH_3$) covalently bond to silicon surfaces. Both monolayers showed similar trends in the influence of the oxidation e.g. higher threshold voltage compared to hydrogen terminated silicon. A decreasing hydrophobic character of the monolayer is accompanied by a broadening and flattening of the formed oxide structure. More hydrophilic surfaces led also to a lower increase in threshold voltage with increasing tip velocity.

CPP 21.5 Wed 16:00 Poster A

Polyelectrolyte coating of tubular J-aggregates investigated by cryo-TEM — •Omar Al-Khatib[1], Dörthe M. Eisele[2], Jürgen P. Rabe[2], Christoph Böttcher[3], and Stefan Kirstein[2] — [1]MPI-Golm, Inst. für Kolloid- und Grenzflächenforschung, Wissenschaftspark Golm, 14424 Potsdam — [2]HU-Berlin, Inst. für Physik, Newtonstr. 15, 12489 Berlin — [3]FU-Berlin, Forschungszentrum für Elektronenmikroskopie, Fabeckstr. 36a, 14195 Berlin

Amphiphilic carbocyanine dyes are able to form tubular J-aggregates in aqueous solutions by a self-assembly process [1]. The wall of the tubular aggregates is formed by a dye bilayer that encloses the hydrophobic alkyl chains and exposes negative surface charges to the water. The charged surface is utilized to adsorb oppositely charged polyelectrolytes in order to cover the aggregates by the polymer and gain mechanical stabilization and further functionalization. The addition of various polycations such as poly(diallyldimethylammonium chloride) (PDAC) and poly(allylamine hydrochloride) (PAH) was investigated by optical spectroscopy and cryogenic transmission electron microscopy (cryo-TEM). It is found that the relative concentration of the polyelectrolyte is a critical parameter for precipitation of the structures. This and other solvent conditions and their influence on the spectra and structure are discussed.

[1]S.Kirstein, S. Dähne, International Journal of Photoenergy, Volume 2006, Article ID 20363, 1-21

CPP 21.6 Wed 16:00 Poster A

Dissipative Structure Formation in Surfactant Films — •Peter C. Seitz and Motomu Tanaka — Physikalisch Chemisches Institut, INF 253, 69120 Heidelberg, Universität Heidelberg

We study the formation of dissipative microstructures in composite ultrathin surfactant films. Dissipation occurs at the three phase contact line during Langmuir-Blodgett transfer onto a solid substrate of lipid/lipopolymer films. Structures are stripe like and continuous over several cm, limited only by substrate size. Stripe to stripe distance is precisely controlled by transfer speed from several μm to below optical resolution.

The onset of the meniscus is observed using imaging ellipsometry. This allows the determination of the microscopic contact angle as well as the discrimination between domains in lateral direction. Data is analyzed using Off-Null ellipsometry and repeating null ellipsometry conditions giving access to Å scale resolution over a μm range. The close relation between the contact angle and the draining process during transfer allows a hydrodynamic modelling and thus a deeper insight to the nucleation leading to stripe patterns.

CPP 21.7 Wed 16:00 Poster A

Self-assembly and multi-compartment micellar hydrogel formation of amphiphilic di- and triblock copolymers containing fluorophilic blocks — •Ruzha Ivanova[1], Tune Bonné[1], Kell Mortensen[2], Klaus Pranzas[3], Thomas Komenda[4], Karin Lüdtke[4], Rainer Jordan[4], and Christine Papadakis[1] — [1]Physikdepartment E13, TU München, 85747 Garching — [2]Risø National Laboratory, Roskilde, Denmark — [3]GKSS, Geesthacht — [4]Department Chemie, TU München, 85747 Garching

The self-assembly of novel amphiphilic poly(2-oxazoline) di- and triblock copolymers containing hydrophilic and fluorophilic and/or lipophilic blocks in aqueous solutions was studied. Small-angle neutron scattering together with contrast matching was used to study the size and the shape of the micelles as well as the effect of the copolymer concentration and the length of the hydrophilic block on the structure. In addition, transmission electron microscopy was used to visualize the micelles. The diblock copolymers aggregate into core-shell micelles. The micelles formed by the lipophilic-hydrophilc copolymers are spherical, whereas those formed by the hydrophilic-fluorophilic copolymers are slightly elongated. The triblock copolymers aggregate into micelles, and at higher concentrations, hydrogels are formed. We could show that the scattering curves of the hydrogels can be described by a coexistence of spherical lipophilic and elongated fluorophilic micellar cores linked by the hydrophilic blocks. Thus the studied poly(2-oxazoline) copolymers have large practical potential as multi-compartment vehicle systems in e.g. medicine or cosmetics.

CPP 21.8 Wed 16:00 Poster A

Molecular Self-Organisation of Fréchet-Dendrons Probed by STM — C. Rohr[1], K. Gruber[1], M. Malarek[2], L. J. Scherer[2], C. E Housecroft[2], E. C. Constable[2], and •B. A. Hermann[1] — [1]Dept. of Physics / CeNS, LMU Munich and WMI, Walther-Meissner-Str. 8, 85748 Garching, Germany — [2]Dept. of Chemistry, Uni. of Basel, Spitalstrasse 51, 4056 Basel, Switzerland

Self-organised molecular layers provide a promising route to constructing new (switchable) nanodevices and optimising nanosensors. The design of suitable molecules involves the control of structure and stabilisation on the surface as well as the control of chemical functionality. The synthesis of molecules bearing functionality and at the same time exhibiting excellent self-organization properties is tedious and time consuming. Hence, the search for a potentially universal "adapter", that can control the self-organisation and stabilisation on a particular type of surface, is a worthwhile challenge. High-resolution nanoscale imaging using scanning tunnelling microscopy (STM) provides the means to significantly advance such studies. How powerfully Fréchet-dendrons can affect various central components (catalytic, switchable, redox-active) on a graphite surface is addressed by analysing self-organised monolayers of nine different molecules, each containing at least one first or second-generation Fréchet-type dendron. The arrangement of the molecules in the monolayer on the surface can further be influenced by small structural changes of the Fréchet-type dendron.

CPP 21.9 Wed 16:00 Poster A

To be or not to be - included? Heterogeneous Molecular Structures Probed by STM — K. Gruber[1], C. Rohr[1], M. Malarek[2], L. J. Scherer[2], C. E. Houscroft[2], E. C. Constable[2], and •B. A. Hermann[1] — [1]Dept. of Physics / CeNS, LMU Munich and WMI, Walther-Meissner-Str. 8, 85748 Garching, Germany — [2]Dept. of Chemistry, Uni. of Basel, Spitalstrasse 51, 4056 Basel, Switzerland

Complex molecular structures, e.g as are apparent in supramolecular chemistry, typically assemble through interactions mediated by weak intermolecular forces. Weak refers here to an interaction lower in strength than a covalent bond. Especially heterogeneous assemblies are of growing interest for biological and chemical processes as well as for technical applications and provide important contribution to the design of nanodevices such as small molecular machines. All heterogeneous assemblies presented in this poster are based on weak interactions of smaller inclusion molecules with Fréchet-dendrons. While adamantene could be successfully incorporated into existing patterns (host-guest structures), heterogeneous assemblies with the inclusion compound coronene resulted in the formation of a new (polymorph) molecular arrangement. The new polymorph pattern could further be influenced by employing two other molecules of slightly modified chemical structure, benzoperylene and benzopyrene, missing two and four carbon atoms, respectively. This work impressively demonstrates the versatility of the Fréchet-dendrons, allowing a high degree of control of heterogeneous structures and presents a first step towards controlled multilayer, multicomponent self-organization of complex systems.

CPP 21.10 Wed 16:00 Poster A

The influence of nano fillers on the dynamics of a PEP-Silsesquioxane composite - a NSE study — •Klaus Nusser[1], Gerald Johannes Schneider[2], Wim Pyckhout-Hintzen[2], Andreas Wischnewski[2], Lutz Willner[2], and Dieter Richter[2] — [1]Institut für Physik, Universität Regensburg, 93040 Regensburg — [2]Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich

Elastomer-filler composite materials are technically very important and widely used, because the addition of active fillers to the polymers significantly enhances the properties of the resulting blend material and helps to optimize its employment in distinct applications. Up to now mainly a reinforcing effect of the filler was observed. New results by Mackay et al., however, report a decrease in viscosity by the addition of nano-particles of a characteristic size. The impact of this effect is investigated by means of a mixture of polyethylene-propylene (PEP) with silsesquioxane. The silsesquioxan nano particles have a characteristic diameter, which can very well be compared to the tube diameter of the PEP melt within the reptation model. The changes of the dynamics after the addition of this nano-filler are investigated and supposed to give more insight into the mechanisms of interaction in polymer-filler nano composites. First results from neutron spin echo measurements at the ILL are presented.

CPP 21.11 Wed 16:00 Poster A

The role of interfaces in photoluminescence intermittency — •Cornelius Krasselt, Jörg Schuster, Harald Graaf, and Christian von Borczyskowski — TU Chemnitz, Institut für Physik, 09107 Chemnitz

Fluorescence intermittency characterized by a broad distribution of on- and off-periods, the so called power law blinking, has recently attracted great scientific interest since it appears to be a common feature of individual emitters [1]. Meanwhile it is generally accepted, that intermittency is due to the emission and trapping of charges. However, the physical nature of this charge trapping process is still unresolved and thus matter of debate. Even the most advanced available theoretical model, the diffusion controlled electron transfer model by Tang and Marcus (see references in[1]) will account for a few but not all experimental observations [1].

One of the most obvious findings is the omnipresence of interfaces in all of the observations of power law blinking reported so far, since usually various silicon oxide substrates are used as sample substrate or emitters are embedded in polymers in order to immobilize it. We show now very recent results of blinking in the presence of silicon dioxide surfaces which obviously modifies the blinking statistics. Since organic layers are knwon, to saturate interface related charge trapping centers on silicon oxides we conclude that those interface states play a key role for the blinking processes.

[1] F. Cichos, C. von Borczyskowski, M. Orrit: Curr. Op. Colloid Interface Science 12 (2007), 272

CPP 21.12 Wed 16:00 Poster A

Colloidal Adsorbate Structures on Quasicrystaline Light Fields — Jules Mikhael, •Laurent Helden, and Clemens Bechinger — 2. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart, Germany.

Quasicrystals are unusual materials since they exhibit no periodic structure but retain true long range order. Spontaneous formation of quasicrystals is typically only observed in rather complex metal alloys, for instance i-AlPdMn or d-AlNiCo, and strongly depends on the specific chemical composition. One way for forming monoatomic quasicrystalline structures is to use the surface of the quasicrystals as templates for adsorbed monolayers. Here we report a real space investigation of the phase behavior of micron-sized colloidal particles adsorbed onto a quasicrystalline decagonal substrate created by interfering five laser beams. For intermediate substrate strength a remarkably stable phase is found revealing likewise crystalline and quasicrystalline characteristics. It can be described by the Archimedean (3.3.3.4.4) tiling which is intersected by double rows of triangular tiles arranged in a Fibonacci sequence. The results on this model system open a route to identify the primordial parameters for the formation of pseudomorphic monoatomic quasicrystals.

CPP 21.13 Wed 16:00 Poster A

Metal salt-nanoparticle formation in supercritical water investigated by molecular dynamics simulation — •Norbert Lümmen and Bjørn Kvamme — University in Bergen, Institute for Physics and Technology, Allégaten 55, N-5007 Bergen, Norway

Nanoparticle formation of $FeCl_2$ and $MnCl_2$ from single ions in water at supercritical conditions was investigated by molecular dynamics (MD) simulations. The water-water interaction was modelled by the rigid SPC/E water model while the water-ion and ion-ion interaction was treated by a combination of Coulomb and Lennard-Jones potentials. The temperature was controlled by a heat bath thermostat using the Nosé-Hoover mechanism. The system density was chosen to match a system pressure around 25 MPa. Simulations at different heat bath temperature and system density were carried out while keeping the water to ion ratio constant.

Our results show that initial particle formation takes place within a few tens of picoseconds after the jump from ambient to supercritical conditions. Nucleation, surface growth and growth by cluster-cluster-collisions is observed. We present results on the time development of distributions of cluster sizes, cluster compositions, and cluster temperatures as well as radial distribution functions and nucleation rates.

CPP 21.14 Wed 16:00 Poster A

Low-dimensional nanoparticle chains formed via a dewetting water layer — •Leonid Govor[1], Günter Reiter[2], Gottfried H. Bauer[1], and Jürgen Parisi[1] — [1]Institute of Physics, University of Oldenburg, D-26111 Oldenburg, Germany — [2]Institut de Chemie des Surfaces et Interfaces, CNRS, 68057 Mulhouse Cedex, France

We report on self-assembly of nanoparticles (diameter 6 nm) into low-dimensional close-packed arrays. This was achieved on substrates coated with a nitrocellulose (NC) thin layer by spreading of a hexane solution containing nanoparticles, hexadecylamine, and water. In a first step, the solution film transforms into a bilayer containing a hexane layer located onto a water film. The hexane layer dewets the water layer and the latter dewets the NC covered substrate. Dewetting of the water layer leads to the formation of water droplets. Finally, the particles follow the motion of the contact line of the dewetting water layer and thus assemble into close-packed arrays at the periphery of the water droplets.

CPP 21.15 Wed 16:00 Poster A

The microSAXS/WAXS beamline at PETRA III — •Stephan V. Roth, Ralph Döhrmann, Rainer Gehrke, Ulrich Hahn, Horst Schulte-Schrepping, Michael Lohmann, Heinz Graafsma, Ralf Röhlsberger, Hermann Franz, and Edgar Weckert — HASYLAB at DESY, Notkestr. 85, D-22607 Hamburg, Germany

Due to its outstanding brilliance, the third generation synchrotron radiation (SR) source PETRA III at DESY, being currently under construction, offers ideal conditions for combining micro- and nanofocused x-ray beams with small- and wide-angle x-ray scattering (SAXS/WAXS). From mid 2009 on, the microfocusSAXS/WAXS beamline P03 will be operational at PETRA III. The beamline layout combines high resolution in both real and reciprocal space with beam sizes ranging from 40μm to 100nm. The low divergence offered by the high-β undulator allows for installing ultraSAXS geometries in combination with such small beams. We present the detailed layout of the μSAXS/WAXS beamline [1]. Strong emphasis is put on the future improvements of the various experimental scanning techniques, such as nano- and microbeam GISAXS [2], nanoWAXS [3] and micro/nanoSAXS tomography [4].

[1] S.V. Roth et al., HASYLAB Annual report 2007 (2007)

[2] S.V. Roth et al., Appl. Phys. Lett 88, 021910 (2006), ibid. 91, 091915 (2007)

[3] S.V. Roth et al., Macromolecules 36, 1585 (2003)

[4] C. Schroer et al., Appl. Phys. Lett. 88, 164102 (2006)

CPP 21.16 Wed 16:00 Poster A

Microstructured surfaces for templating colloidal particle assembly — •Melanie Pretzl[1], Anne Horn[1], Arnaud Chiche[1], Ute Zettel[1], Alexandra Schweikart[1], Conghua Lu[2], and Andreas Fery[1] — [1]Department of Physical Chemistry, University Bayreuth, 95440 Bayreuth — [2]Max Planck Institute of Colloids and Surfaces, Wissenschaftspark Golm, 14476 Potsdam

Surfaces with patterned assemblies of colloidal particles are of interest for various tasks like controlling wetting, optical properties (optical bandgap materials), electronic properties (wire formation) or combinatorial chemistry (catalytic activity of Particles, Synthesis in hollow capsules).We present two complementary approaches for creating such surfaces which are complementary. Chemical patterning can be achieved by means of microcontact printing. We apply this technique to create surfaces which are patterned in their charge density and show that in this way the immobilization of charged Microcapsules and Micro-balloons (gas filled microcapsules) can be directed. These entities can serve as micro-reactors or sensors.Controlled wrinkling offers an alternate approach with which periodic, topographically structured surfaces can be created. We demonstrate that these surfaces, when dipped into colloidal suspensions, direct particle adsorption. The wrinkling approach is lithography free and periods as low as 150 nm can be achieved, such that assembly of nanoparticles is feasible. We show first examples of ordered assemblies of gold nanoparticles and viruses that were created using this approach and discuss their potential.

CPP 21.17 Wed 16:00 Poster A

Structural Anisotropies in Filled Elastomers — •Gerald Johannes Schneider[1] and Dietmar Göritz[2] — [1]Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich — [2]Institut für Physik, Universität Regensburg, 93040 Regensburg

Nano composites consisting of an elastomer and a filler such as silica play a major role in our daily life. In general the macroscopic properties of the composite material depend on the type of silica, the filler content, and the silanization, i. e. on the interaction between the surface of the filler and the polymer matrix. Possibly a dependence on the direction of an applied external force can be found. Thus, in order to understand the macroscopic properties an investigation of the filler structure at a length scale of a few nanometers is of great interest. Scattering methods, in particular small angle X-ray scattering experiments are very suitable to study the structure and potential anisotropies of silica at the nanoscale. In our contribution we show the influence of the elastomer, the silane and the filler content on the anisotropy of the silica. We found a systematic increase of the anisotropy with increasing filler content. The influence of the silane is weak and the dependence on the elastomer is negligible.

CPP 21.18 Wed 16:00 Poster A

Evaluation of USAXS data obtained from colloidal crystals in latex films — •Rainer Gehrke — HASYLAB at DESY, Notkestrasse 85, D-22607 Hamburg, Germany

Compressed films of spherical core-shell particles with a rigid thermoplastic core (polystyrene) and a soft elastomeric shell (polymethyl methacrylate-polyethylacrylate) show a regular arrangement of the spheres. Close to the film surface the particles are ordered in an fcc lattice with the (111) net-planes parallel to the surface while in the bulk crystal-like domains with no preferred orientation are formed. USAXS measurement were performed by varying the angle between the incident beam and the surface normal stepwise from 0 degree (perpendicular incidence) to almost 90 degrees (grazing incidence) using 0.15 nm wavelength and a two-dimensional detector. Data evaluation allows separation of the scattering contributions from bulk and crystal-like top and bottom layers. The fraction of crystal-like ordered material can be estimated as well as the quality of its spatial and orientational ordering.

CPP 21.19 Wed 16:00 Poster A

The solvation energy of non–trivially shaped objects in simple liquids: testing morphology by integral equations — •Florian Pesth and Martin Oettel — Institute of Physics, Johannes Gutenberg-University, 55099 Mainz

For a given solvent, the grand potential in a finite volume in general depends in a complex way on the shape of the container, or alternatively, the solvation energy of a large solute depends in a similarly complex way on the shape of the molecule. A morphological theorem states [1], that if some physical restrictions are imposed on the container or the solute, the grand potential depends on only four quantities, namely the volume, the surface area, the integrated mean curvature and the Euler characteristic of the container or the solute. On the other hand, one may calculate solvation free energies microscopically by combining integral equation methods with density functional theory. In a first test, we compare the insertion free energies from the morphological and the microscopic route for dumbbell–shaped objects with special attention to line contributions arising from the curvature terms. This appears to be relevant for applications of this morphological theorem to the configuration dependent solvation energy of macromolecules [2].

[1] P.-M. König, R. Roth, and K. R. Mecke, Phys. Rev. Lett. 93, 160601 (2004)

[2] R. Roth, Y. Harano, and M. Kinoshita, Phys. Rev. Lett. 97, 078101 (2006)

CPP 21.20 Wed 16:00 Poster A

Influence of temperature and pH on thermoresponsive PNIPAM films — •Anna Burmistrova[1], Matthias Karg[1], Thomas Hellweg[2], and Regine von Klitzing[1] — [1]TU Berlin, Institut für Chemie, Stranski-Laboratorium, Str. d. 17. Juni 124, 10623 Berlin, Germany — [2]Universität Bayreuth, Physikalische Chemie 2, Universitätsstr. 30, 95440 Bayreuth, Germany

During the last decades microgels made of N-isopropylacrylamide (NIPAM) have attracted much interest and were studied by several techniques like microscopy and light scattering. These polymer particles show a thermoresponsive behaviour and can be classified as "smart" materials. By copolymerisation with organic acids such as acrylic acid (AAc) the temperature of the volume phase transition as well as the swelling ratio can be influenced. Moreover charged copolymers are more sensitive to changes in pH and ionic strength. Depending on the way of preparation one can achieve particles with rather low polydispersities which makes them more interesting for applications like surface coatings and sensor design. Characterisation of coated surfaces with poly-NIPAM-co-AAc microgels has been done using Atomic Force Microscopy (AFM) and ellipsometry. While AFM allows to obtain information about the particle size and arrangement, ellipsometry focuses on the overall film thickness. In order to study the films under various conditions such as temperature and solvent composition we employed liquid cells which allowed to study the surfaces under solution. The results show that the way of preparation and external stimuli like pH and temperature influences strongly the structure of the films.

CPP 21.21 Wed 16:00 Poster A

NMR Investigation of the Aggregation of Dye Molecules — Richard Szopko, Klaus Huber, and •Claudia Schmidt — Department Chemie, Universität Paderborn, Warburger Str. 100, 33098 Paderborn, Germany

The azodyes "Rot 2G" (red) and "Gelb GA" (yellow) are anionic direct dyes. A mixture of these dyes is used to produce orange hued paper. However, in the presence of alkaline-earth ions, such as Mg^{2+}, aggregates are formed, which interfere with the dyeing process. Time-resolved static light scattering, observed within 15–20 minutes after mixing the two dye solutions, has shown the formation of short aggregates with a contour length of 250–300 nm in the presence of Na$_2$SO$_4$, whereas substituting Na$^+$ ions with Mg^{2+} ions leads to a nearly tenfold increase of the contour length [1]. NMR spectroscopy revealed that even in dilute aqueous solutions of the pure dye Gelb GA aggregation occurs. The aggregation as a function of temperature and concentration has been investigated using high resolution NMR measurements of proton chemical shifts and pulsed gradient stimulated echo diffusion experiments.

[1] S. E. Inglés, A. Katzenstein, W. Schlenker, K. Huber, Langmuir, 16, 3010 (2000).

CPP 21.22 Wed 16:00 Poster A

decontamination with sugar surfactant based bicontinuous microemulsions — •Stefan Wellert[1], Thomas Hellweg[1], Christian Groetsch[2], Michael Dolle[2], Hans-Juergen Altmann[2], and Andre Richardt[2] — [1]University Bayreuth, PCI, Universitaetsstrasse 30, D-95440 Bayreuth — [2]Bundeswehr Scientific Institute (NBC-Protection), Humboldtstr, D-29633 Munster

Bicontinuous microemulsions are continuously connected interwoven domains of oil and water. In a fishlike phase diagram, this type of microemulsion structure is located in the single phase region, very close to the fishtail point, where the three-, two- and one phase region meet.

Bicontinuous microemulsions are formed by the highest amounts of oil and water and the lowest necessary amount of surfactant. We study the bicontinuous region of a quaternary system water/rapeseed methyl ester/sugar surfactant/pentanol, which is environmental compatible and hence, a promising candidate for a modern decontamination medium.

We present results from studies of the phase behavior of quaternary systems. Moreover, the influence of an additional active component like oxidizing agents and enzymes is discussed.

CPP 21.23 Wed 16:00 Poster A

Mixture of polymers and dilute colloids — •Maryam Naderian and Matthias Fuchs — University of Konstanz

Equilibrium structure and thermodynamics of a mixture of non-adsorbing polymers and dispersed particles in *Protein Limit*, where the Proteins are much larger than colloids, are very interesting. Employing a macromolecular liquid state approach leads to an integral equation method (PRISM) for polyatomic fluids, applicable for any polymer to colloid size ratio. Ideal polymers are described using a Gaussian form factor. By numerical solution of the Ornstein-Zernike equation we investigate thermodynamic and structural properties and thermodynamic consistency for the infinitely dilute regime.

CPP 21.24 Wed 16:00 Poster A

Plasma Electrochemistry in Ionic Liquids: Deposition of Copper-Nanoparticles — •Mareike Brettholle[1], Oliver Höfft[1], Sebastian Mathes[2], Sherif Zein El Abedin[1], and Frank Endres[1] — [1]Institut für Metallurgie, TU Clausthal, 38678 Clausthal-

Zellerfeld, Germany — [2]Institut für Physik und Physikalische Technologien, TU Clausthal, 38678 Clausthal-Zellerfeld, Germany

Ionic liquids are a highly interesting group of solvents for electrochemical processes - mainly due to the combination of their high electrical conductivity, their electrochemical stability and their ability to dissolve a wide range of compounds [1]. Due to their low vapour pressure low pressure plasmas can easily be applied. The idea is to use the free electrons of the plasma to reduce the dissolved metal atoms in the liquid and generate this way the metal particles. In ionic liquids this principle was utilized recently by Meiss et al. [2]. Here we present our results using an argon plasma as electrode for the electrochemical deposition of copper nanoparticles (5-100 nm) from a Cu solution in 1-butyl-1-methylpyrrolidinium bis(trifluoromethylsulfonyl)amide [BMP]Tf2N and 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)amide [EMIm]Tf2N. XPS, REM, EDX and Dynamic light scattering (DLS) were used to characterise the particles. [1] F. Endres, S. Zein El Abedin , Phys. Chem. Chem. Phys., 8 (2006) 2101; [2] S. A. Meiss, M. Rohnke, L. Kienle, S. Zein El Abedin, F. Endres and Jürgen Janek, Chem. Phys. Chem., 8 (2007) 50

CPP 21.25 Wed 16:00 Poster A

Stimuli-sensitive micelles from amphiphilic diblock copolymers — •Kordelia Troll[1], Amit Kulkarni[1], Christine M. Papadakis[1], Weinan Wang[1], Peter Müller-Buschbaum[1], Achille M. Bivigou Koumba[2], and André Laschewsky[2] — [1]Physikdepartment E13, TU München — [2]Institut für Chemie, Universität Potsdam

Amphiphilic diblock copolymers from a hydrophilic, thermosensitive block, poly(N-isopropyl acrylamide) (PNIPAM), and a hydrophobic block, polystyrene, are expected to form micelles in aqueous solution, which are swollen below the lower critical solution temperature (LCST) and collapsed above. We focus on the conformational change of the micellar shell as a function of temperature and the PNIPAM volume fraction.

Two diblock copolymers with different PNIPAM volume fractions were studied at low polymer concentrations in aqueous solution. The temperature behavior was investigated using microcalorimetry and dynamic light scattering. The polymer with a high PNIPAM volume fraction (0.80) form micelles and show a reversible collapse at the expected LCST of ∼31°C. The spherical shape of the micelles was confirmed using TEM. The polymer with the low PNIPAM volume fraction (0.29) could not directly be dissolved in water. Aqueous solutions were therefore prepared via dialysis from organic solvents. The size of the aggregates was found to depend strongly on the organic solvent, and no collapse could be detected.

CPP 21.26 Wed 16:00 Poster A

Nanorod-coated PNIPAM microgels: thermoresponsive optical properties — •Matthias Karg[1], Isabel Pastoriza-Santos[2], Jorge Pérez-Juste[2], Luis M. Liz-Marzán[2], and Thomas Hellweg[3] — [1]TU Berlin, Stranski-Laboratorium, Strasse des 17. Juni 124, 10623 Berlin, Germany — [2]Universidade de Vigo, Grupo de Quimica Fisica, 36310 Vigo, Spain — [3]Universität Bayreuth, Physikalische Chemie I, Universitätsstrasse 30, 95440 Bayreuth

Highly-charged, thermoresponsive poly-(N-isopropylacrylamide) microgels were covered with polyelectrolyte-coated gold nanorods [1]. The surface coverage of these hybrid particles was varied by changing the ratio of nanorods to microgel and determined from electron microscopy images. Temperature dependent UV-VIS measurements were done to investigate the optical behavior during the collapse of the microgel core. The results show red-shifts of the longitudinal plasmon band due to increasing electronic interactions between the gold nanorods when the polymer cores decrease in size. Further observed effects are an increase in the band width and a decrease of the amplitude of the longitudinal band. These properties strongly depend on the surface coverage and are therefore tuneable, which makes them interesting for applications such as optical filters. [1] M. Karg, I. Pastoriza-Santos, J. Pérez-Juste, T. Hellweg, L. M. Liz-Marzán, Small, 2007, 3, 1222-1229

CPP 21.27 Wed 16:00 Poster A

Hydrodynamics in colloidal suspensions: From highly charged to electrostatically screened particles — •Fabian Westermeier[1], Tina Autenrieth[1], Christian Gutt[1], Aymeric Robert[2], and Gerhard Grübel[1] — [1]Hasylab/DESY, Hamburg, Germany — [2]SLAC/Stanford University, Menlo Park, USA

We studied the dynamic behaviour of charge-stabilised colloidal suspensions. For these systems the direct particle interactions, for which the experimental data can be described by the RMSA model, are well understood. For the indirect particle interactions which are mediated by the solvent and described by the hydrodynamic function several theories have been developed and experimentally tested within the last years, but there is no universally valid theoretical model that is applicable over the whole range of volume fractions.

Therefore we undertook a systematic study where the interaction strength between the particles was altered by varying both the volume fraction of the colloids and the concentration of added electrolyte screening the electrostatic interactions. The combined use of dynamic light scattering (DLS), Small Angle X-ray Scattering (SAXS) and X-ray Photon Correlation Spectroscopy (XPCS) allowed us the determination of the hydrodynamic function free from any modeling.

CPP 21.28 Wed 16:00 Poster A

From gas–liquid to liquid crystalline phase behavior via anisotropic attraction: A computer simulation study — •Wen-Ze Ouyang and Reinhard Hentschke — Bergische Universität Wuppertal

The phase behavior of a continuum molecular model for self-assembling semiflexible equilibrium polymers is studied via Monte Carlo simulation and molecular dynamics. We investigate the transfer from ordinary gas–liquid coexistence to the appearance of liquid crystallinity driven by excluded volume interaction between rodlike aggregates. The transfer between the two types of phase behavior is governed by a tunable anisotropic attractive interaction between monomer particles. The relation to dipolar fluid models, which are also known to form reversible chains, is discussed.

CPP 21.29 Wed 16:00 Poster A

Geometric Order Parameters for Point Patterns — •Sebastian Bittner and Klaus Mecke — Institut für Theoretische Physik Universität Erlangen-Nürnberg, Staudtstrasse 7, 91058 Erlangen, Germany

Higher correlations are important to characterise hexatic phases in colloidal systems or non-Gaussian fluctuations in fluids beyond the two-point structure function. A hybrid technique of two-point correlation functions and Minkowski functions of point patterns offer the possibility to measure higher correlations in a statistically robust way.

The geometrical idea of the morphological technique is simple: a ring of outer radius R and inner radius $r < R$ is attached at each point of the pattern, which will overlap mutually. The morphology of the coverage is then analysed geometrically for all reasonable values of r and R by measuring its area, boundary length and Euler characteristic. For $r = 0$ one recovers the standard Minkowski functions of point patterns whereas for $r \to R$ the measures reduce to the two-point characteristics.

We present an algorithm for computing the morphological functions of the coverage and snapshots from visualisations of the rings. Finally, we apply this hybrid method on various point patterns in physics and biology, e.g. on colloidal configurations.

CPP 22: POSTERS Micro- and Nanofluidics

Time: Wednesday 16:00–18:30 Location: Poster A

CPP 22.1 Wed 16:00 Poster A

Kinetic Monte Carlo modeling of the fingering instability of dewetting fronts in nanoparticle suspensions — •Ioan Vancea[1], Christopher Martin[2], Matthew Blunt[2], Emmanuelle Pauliac-Vaujour[2], Philip Moriarty[2], and Uwe Thiele[1,3] — [1]Max-Planck-Institut fur Physik komplexer Systeme, Noethnitzer Str. 38, D-01187, Germany — [2]School of Physics & Astronomy, The University of Nottingham, University Park, Nottingham, NG7 2RD, UK — [3]School of Mathematics, Loughborough University, Loughborough, Leicestershire, LE11 3TU, UK

We use a kinetic Monte Carlo simulation of a 2D Lattice Gas Model to show that for a nanoparticle solution that dewets by evaporation the particles induce a strong fingering instability of the dewetting fronts. We analyze the influence of parameters, such as nanoparticle concentration, mobility, chemical potential on the characteristics of the fingering.

Furthermore we discus in detail the role played by nanopaticle-nanoparticle and liquid-nanoparticle interaction strength and distinguish parameter regions where hydrodynamic processes and liquid-particle demixing processes dominate the structure formation.

We acknowledge support by the European Union via the FP6 Marie Curie scheme [Grant MRTN-CT-2004005728 (PATTERNS)].

CPP 22.2 Wed 16:00 Poster A

Vibration dynamics of a bubble in contact with solid surface — Sergey V. Shklyaev[1] and •Arthur V. Straube[2] — [1]Theoretical Physics Department, Perm State University, Bukirev 15, 614990 Perm, Russia — [2]Department of Physics, University of Potsdam, Am Neuen Palais 10, PF 601553, D-14415 Potsdam, Germany

The linear natural and forced oscillations of a bubble in a liquid ambient in contact with a solid surface are studied [1]. We consider a class of boundary conditions allowing for different behavior at the contact line, where the three phases touch. The contact line dynamics is taken into consideration with the Hocking condition, which is shown to lead to interaction of the shape and volume oscillations even within the linear theory. Resonant phenomena, mostly pronounced for the bubble with the fixed contact line or with the fixed contact angle, are found out. The limiting case of weakly compressible bubble is analyzed. The general criterion identifying whether the compressibility of a bubble can be neglected is obtained.

[1] S.V. Shklyaev, A.V. Straube, Linear oscillations of a hemispherical bubble on a solid substrate, submitted to Phys. Fluids (arXiv:0710.0212)

CPP 22.3 Wed 16:00 Poster A

Mixing on the micron-scale with rotating colloidal clusters — •Sabri Rahmouni[1], Tobias Sawetzki[1], David Marr[2], and Clemens Bechinger[1] — [1]2. Physikalisches Institut, Universität Stuttgart — [2]Chemical Engineering Department, Colorado School of Mines

Recently, the fabrication of "lab on a chip" devices has attracted considerable attention amongst physicists and chemists. In the meantime many different approaches and solutions to operate such devices have been suggested. One of the main problems is the mixing of fluid components on the micron scale, i.e. at low Reynolds numbers where no turbulence exists. We demonstrate a novel approach to overcome this problem by subjecting paramagnetic colloidal particles to magnetic fields which rotate in the sample plane. As a result, an external torque is exerted on the colloidal particles which then act as micro mixers. When analyzing the output flow of a mixing chamber, we observe that such mixers strongly enhance the mixing of the two inlets, one of them containing small, nonmagnetic tracer particles.

CPP 22.4 Wed 16:00 Poster A

Molecular Electronics using Gel-Emulsions — •Shashi Thutupalli[1], Venkatachalam Chokkalingam[1], Marcel Mayor[3], Stephan Herminghaus[1], and Ralf Seemann[1,2] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Experimental Physics, Saarland University, Saarbrücken, Germany — [3]Department of Chemistry, University of Basel, Switzerland

We use 'gel emulsions' (emulsion with a very small continuous phase volume fraction) that arrange into a foam like topology for well defined assembly of molecules across the droplet lamellae. For certain water in oil emulsions including suitable surfactants, the lamella separating the droplets can be collapsed to form a double-layer membrane by controlling the volume fraction of the continuous phase. A hydrophobic conducting molecule might then insert into the membrane with its hydrophilic head groups immersed into the droplets while the orientation of the molecule is well known. The water droplets sandwiching these molecules can then serve as electrodes to apply a voltage across the membrane via the molecules. When the gel-emulsion flows along a network of microfluidic channels we can induce precise rearrangements of the foam like droplet topology. Thus, we expect to build various electronic circuits. As a first approach towards this, water droplets in dodecane, with monoolein as surfactant, are produced. A voltage sensitive fluorescent dye (eg. Di-4-Anepps) is inserted in the membrane and switching of the fluorescent peak is demonstrated.

CPP 22.5 Wed 16:00 Poster A

Topology transitions of monodisperse emulsions in microchannels — •Enkhtuul Surenjav[1], Martin Brinkmann[1], Craig Priest[1], Stephan Herminghaus[1], and Ralf Seemann[1,2] — [1]MPIDS, D-37073, Göttingen, Germany — [2]Saarland University, D-66041, Saarbrücken, Germany

In the confinement of a micro-channel, foam-like emulsions appear in a variety of periodic patterns, we call topologies. Transitions between certain topologies in a flowing emulsion can be induced through variations of the channel geometry. Such a 'passive' manipulation of the droplets by means of the confinement allows to position, sort, exchange, compile and redistribute droplets. These rearrangements are studied for various geometries as a function of volume fraction and droplet size. Based on numerical and analytical result we predict mechanical instabilities in straight channels and present a phase diagram for the different droplet topologies. Furthermore, we quantify the impact of a bend in the channel on the exchange of droplet positions. In combination with a technique to coalesce targeted pairs of droplets, a controlled interchange of neighboring droplets can be used to perform multi-step reactions. The transition between a bamboo and a zigzag structure demonstrates that topology transitions are inherently hysteretic at large volume fractions of the dispersed phase. 'Passive' reorganizations based on fixed channel geometries can be supplemented by 'active' manipulation of an incorporated ferrofluid phase. A ferromagnetic continuous phase facilitates reorganization of liquid compartments on demand using an electromagnetic trigger.

CPP 22.6 Wed 16:00 Poster A

Separation of Model Emulsions on Chemically Patterned Surfaces: Confinement, Hysteresis & Droplet Coalescence — •Pagra Truman, Petra Uhlmann, and Manfred Stamm — Leibniz-Institut für Polymerforschung, Hohe Str. 6, 01069 Dresden, Germany

Chemically patterned surfaces can be used to drive liquid flow along surfaces in microfluidic systems. In this work we investigate the separation of model emulsions consisting of an aqueous and a non-polar component on step gradient surfaces with one hydrophilic and one hydrophobic side. The separation is driven by the strong affinity of the aqueous component to the hydrophilic side.

Analysing the separation process in detail we identify droplet coalescence as a key phenomena during separation. Thus droplet coalescence in the presence of hydrophobic and hydrophilic surfaces in confinement and on open systems is studied. Surprisingly we find that the impact of surface wettability on droplet coalescence in confinement is opposite to the case of an open system. Introducing a simple theoretical model taking into account surface energy hysteresis we are able to explain such behaviour.

CPP 22.7 Wed 16:00 Poster A

Two-dimensional gas-liquid two-phase flow in a microfluidic device — •Yasutaka Iwashita[1], Ralf Seemann[1,2], Christian Bahr[1], and Stephan Herminghaus[1] — [1]MPI for Dynamics and Self-Organization, 37073 Göttingen, Germany — [2]Experimental Physics, Saarland University, 66041 Saarbrücken, Germany

Monodisperse emulsions with a high volume fraction of the dispersed phase can be produced using step emulsification [1]: A quasi 2D-liquid stream of a dispersed phase surrounded by a continuous phase in a shallow channel is transformed into droplets at a topographic step by a Rayleigh-Plateau-type instability.

Here we replace the dispersed liquid by gas and study the gas-liquid two-phase flow in a similar microfluidic device. Due to the compressibility and lower viscosity of gas (more than 100 times smaller than liquid) the dynamics of the quasi 2D, two-phase flow is different from that of liquids. By observing the flow we found three characteristic flow structures: (i) gas-liquid co-flow at high pressure (or large flow rate) of gas, (ii) bubble generation at the T-junction of the shallow channel and (iii) liquid one-phase flow when the gas pressure is lower than the liquid pressure at the T-junction. We will show how these flow structures depend on the conditions (height of the shallow channel, interfacial tension, etc.), and explain the findings with a "simple" theoretical analysis.

[1] C. Priest, S. Herminghaus and R. Seemann, Appl. Phys. Lett. 88, 024106 (2006)

CPP 22.8 Wed 16:00 Poster A

Recirculation flows and friction in confined gel emulsions — •Audrey Steinberger[1], Shashi Thutupalli[1], Ralf Seemann[1,2], and Stephan Herminghaus[1] — [1]MPI for Dynamics and Self-organization, D-37073 Göttingen — [2]Experimental Physics, Saarland University, D-66041 Saarbrücken

Emulsions with a high dispersed phase volume fraction, the so-called gel-emulsions, are not only a promising tool for handling liquids in microfluidic processes but also a convenient model system to study friction between membranes, as the arrangement of monodisperse droplets is defined and can be manipulated by the geometry of the microchannel in which they are flowing. Recirculation flows -controlling the mixing- inside the droplets are induced by the friction at the interfaces. We study experimentally those recirculation flows, using microparticle image velocimetry (μ-PIV), as a function of the arrangement of the droplets and the dispersed phase volume fraction, in order to investigate the friction properties of emulsions in the limit where the thickness of the continuous phase lamellas becomes very small, and possibly reduces to a surfactant bilayer.

CPP 22.9 Wed 16:00 Poster A

Thin dewetting polymer films: Fingering and the effect of interfaces — •Ludovic Marquant, Frank Müller, Julia Mainka, Oliver Bäumchen, and Karin Jacobs — Saarland University, Experimental Physics, D-66041 Saarbrücken, Germany

The dynamics of supported polymer thin films is studied along two aspects, which are the behaviour of films in bulk conditions (h> 100 nm) and the deviation from the bulk behaviour for smaller film thicknesses. First, we investigate the dynamics of the last stage of dewetting of a polymer melt from a hydrophobized substrate, where fingers are initiated by amplified fluctuations created by the growth of the rim (liquid moving front), analogue to the Rayleigh-Plateau-Instability. Film thickness and slippage influence the occurrence of the fingers structure. We demonstrate, backed by theoretical support, that slippage acts on the geometry of bulges, which become more asymmetric as the slip length increases. The system we use is a 100 nm polystyrene film prepared on top of differently hydrophobized Si wafer. Furthermore, we investigate the dynamics of the polymer at interfaces regarding the change of the glass transition temperature as we depart from bulk conditions. For molecules smaller than 300 kg/mol, it has been shown that the shift of Tg is not due to the geometrical finite size effect because the shift is independent of molecular weight. This phenomenon, studied by NMR, is explained by an enhanced molecular mobility at the free polymer interface. As NMR takes place in liquids and therefore affects the surface tension of polystyrene, we investigate in situ ellipsometry measurements of Tg with various liquids surrounding the film.

CPP 22.10 Wed 16:00 Poster A

Probing slippage of thin polymer films on smooth hydrophobic surfaces — •Oliver Bäumchen, Renate Fetzer, and Karin Jacobs — Saarland University, Experimental Physics, D-66123 Saarbrücken, Germany

We study the boundary conditions at the solid/liquid interface of thin film flow of highly viscous Newtonian liquids. To induce flow, we make use of the dewetting process. In our system, polystyrene melts below the entanglement length dewet after annealing above their glass transition temperature from smooth hydrophobic substrates, silicon wafers covered by octadecyltrichlorosilane (OTS), dodecyltrichlorosilane (DTS) brushes, and thin teflon (AF1600) films. By investigating the radii of the growing holes, we find that the dewetting velocity at a certain temperature strongly depends on the type of substrate. Identifying viscous flow and slippage contribution allows us to extract the slip length. The numbers for the slip length are consistent with results obtained from atomic force microscopy analysis of the shape of the rims that surround each hole. They exhibit either an oscillatory or a monotonically decaying rim profile. A recently developed Stokes model for a thin liquid film dewetting from a solid substrate [1], which is not restricted to a certain range of slip lengths, is used to determine slip length as well as the viscosity of the polymer melt. The slip length on the silane brushes is found to be about one order of magnitude larger on DTS than on OTS and decreases with increasing temperature, whereas on AF1600 we find a nearly vanishing contribution of slippage. [1] R. Fetzer et al., Langmuir 23 (2007) 10559.

CPP 22.11 Wed 16:00 Poster A

Lattice Boltzman and DPD Electrohydrodyamics simulations — Jens Smiatek[1], Friederike Schmid[1], •Marcello Sega[2], and Christian Holm[2] — [1]Fakultät für Physik, Universität Bielefeld, Universitätsstraße 25, D-33615 Bielefeld, Germany — [2]Frankfurt Institute for Advanced Studies, Ruth-Moufang Str. 1, D-60438 Frankfurt am Main, Germany

In the framework of the solution of coupled Navier-Stokes / Molecular Dynamics simulations of Electrohydrodynamic systems, we present the results of a comparison between Lattice Boltzmann and Dissipative Particle Dynamics.

The two methods, respectively based on the solution of the Boltzmann equation on a lattice, and on a momentum-conserving Galilean-invariant particle based thermostat, have been recently implemented into the ESPResSo simulation package. Convergence of physical observables and relative limits and strengths of the two approaches are evaluated, as well as their computational efficiency.

The benchmark system is that of an electroosmotic flow in a slit pore, where explicit ions are taken into account, with full periodic electrostatic treatment and hydrodynamic interactions.

CPP 22.12 Wed 16:00 Poster A

Water structure and slippage at hydrophobic and hydrophilic surfaces — •Christian Sendner[1], Jiri Janecek[2], and Roland Netz[1] — [1]Physik Department, Technische Universität München — [2]Institute of Physical and Applied Chemistry, Brno University of Technology, Czech Republic

Via Monte Carlo and Molecular Dynamics simulations, we probe the structure and slippage of water films at hydrophobic and hydrophilic surfaces. At nonpolar, hydrophobic surfaces, a depletion of the water density is observed which is set in relation to the wetting properties. At hydrophilic surfaces, achieved with polar hydroxyl groups on top, we examine the interfacial water structure dependent on the density, spatial distribution and angular orientation of the polar groups. In non-equilibrium simulations the slip length of sheared water layers between two hydrophobic surfaces is examined as well as the structural changes of interfacial water at hydrophilic surfaces under the influence of shearing.

CPP 22.13 Wed 16:00 Poster A

Quasistationary dynamics of droplets on chemically structured substrates — Fabian Dörfler[1,2], •Markus Rauscher[1,2], and Siegfried Dietrich[1,2] — [1]Max-Planck-Institut für Metallforschung, Stuttgart, Germany — [2]ITAP, Universität Stuttgart, Stuttgart, Germany

With open microfluidic systems in mind, we study the dynamics of droplets on chemical channels (i.e., hydrophilic stripes on otherwise hydrophobic substrates) in the quasistatic limit using the software Surface Evolver. In particular, we investigate the free energy landscape of droplets on symmetric Y-junctions in the capillary model. We find an energetic minimum right at the junction. There is a maximum in the energy landscape between two branches but no local minimum which might indicate the splitting of droplets. In addition, we find, that moving a droplet into a junction and back into a channel can result in a metastable elongated droplet shape.

We also investigate methods to include the substrate potential (i.e., the effect of long-ranged intermolecular interactions) into the Surface Evolver in order to apply this software to nanoscale droplets.

CPP 22.14 Wed 16:00 Poster A

Optical diffraction reveals microscopic properties of the superhydrophobic state. — •Helmut Rathgen and Frieder Mugele — Physics of Complex Fluids, University of Twente, The Netherlands

We study the microscopic liquid–gas menisci formed at the texture of a superhydrophobic surface, making use of the inherent optical diffraction of the material. By measuring the angle dependence of the diffracted intensity, and comparing the experimental data to theoretical optics calculations with varying curvature of the menisci, we effectively solve the inverse diffraction problem and are able to measure the shape of the menisci with nanometer resolution. We study the shape of the menisci as a function of hydrostatic pressure. Next, driving the menisci in an ultrasound field, and measuring time–resolved diffraction intensities, we observe their nanometer scale oscillations. By comparing to unsteady Stokes flow theory, we find that the frequency response of the collectively oscillating menisci is governed by strong hydrodynamic interaction.

CPP 22.15 Wed 16:00 Poster A

Single Molecule Diffusion on Chemically patterned Substrates — •Martin Pumpa and Frank Cichos — Molecular Nanophotonics Group, University Leipzig

Molecular dynamics at solid/liquid interfaces is defined by the strength of the interaction of the liquid with the solid surface. This interfacial region extendes serveral 10 nm into the liquid, where modified structure and dynamics appear i.e. in the form of liquid layering. Thus control of the surface properties of a solid substrate provides a route to control the interfacial molecular dynamics in liquid films. Within this contribution, we present first experimental results on a controlled manipulation of single molecule diffusion by chemically patterning glass surfaces. Using micro-contact printing, we prepare a hydrophilic/hydrophobic pattern on the surface. Typical dimensions of the structure of this pattern are on the order of a few micrometers. These surfaces are either covered by an ultrathin liquid film or mounted in a surface forces apparatus, where the liquid covering the pattern is confined down to a film thickness of a few 10 nanometers. To study molecular dynamics, we employ single molecule tracking of dye molecules dissolved in the liquid. The diffusion of these dye molecules is observed by fluorescence wide field microscopy. First indications of anisotropic diffusion due to the pattern structure are reported.

CPP 22.16 Wed 16:00 Poster A

Colloids dragged through a polymer solution — •Christof Gutsche[1], Friedrich Kremer[1], Matthias Krüger[2], Markus Rauscher[2], Rudolf Weeber[3], and Jens Harting[3] — [1]Institut für Experimentalphysik I, Universität Leipzig — [2]Max-Planck-Institut für Metallforschung, Stuttgart and Institut für Theoretische und Angewandte Physik, Universität Stuttgart — [3]Institut für Computerphysik, Universität Stuttgart

We present micro-rheological measurements of the drag force on colloids pulled through a solution of lambda-DNA [1] (used here as a monodisperse model polymer) with an optical tweezer [2,3]. The experiments show a drag force which is larger than expected from the Stokes formula and the independently measured viscosity of the DNA solution. We attribute this to the accumulation of DNA in front of the colloid and the reduced DNA density behind the colloid. This hypothesis is corroborated by a simple drift-diffusion model for the DNA molecules, which reproduces the experimental data surprisingly well, as well as by corresponding Brownian dynamics simulations.

[1] Gutsche C, Kremer F, Krüger M, Rauscher M, Weeber R, Harting J, arXiv:0709.4142 [2] Gutsche C, Keyser UF, Kegler K, et al. Phys. Rev. E 76 (3): 031403 (2007) [3] Gutsche C, Salomo M, Kim YW, et al. MICROFLUIDICS AND NANOFLUIDICS 2 (5): 381-386 (2006)

CPP 22.17 Wed 16:00 Poster A

On particle based velocimetry: Brownian particle near walls — •Laura Almenar[1,2] and Markus Rauscher[1,2] — [1]Max-Planck-Institut für Metallforschung, Stuttgart, Germany — [2]ITAP, Universität Stuttgart, Stuttgart, Germany

Motivated by particle based velocimetry techniques, in particular by double focus correlation spectroscopy experiments, we study the dynamics of Brownian particles in shear flow in the vicinity of planar walls. The experiments are designed to measure hydrodynamic slip in polar liquids. However, wall effects such as the fact that the particles cannot penetrate into the wall, the electrostatic double layer force, and the reduced particle mobility in the vicinity of the wall have to be taken into account in the data analysis in order to avoid spurious slip. We model the dynamics of the Brownian particles by a drift-diffusion equation taking into account the impermeability of the wall, the electrostatic double layer force, and the reduced mobility of the particles in the vicinity of the wall. The latter turns out to be irrelevant for the experimental system.

We use analytical as well as numerical tools to simulate the experiments and to quantify the spurious slip that one would measure if the data was analyzed in a naive way. Here, we find qualitative agreement with the experiment. It turns out that for a more careful analysis of experimental data one needs more detailed information on the electrostatic particle-wall interaction.

CPP 22.18 Wed 16:00 Poster A

Thermal fluctuation of single DNA-molecules and their dynamic in shear flow — Katrin Günther, •Kristin Laube, and Michael Mertig — Max-Bergmann-Zentrum für Biomaterialien, Budapester Str. 27, D-01069 Dresden, Germany

We investigate thermal fluctuations and dynamic behaviour of single λ-DNA-molecules tethered in a microfluidic cell in the dependence of cation concentration and shear rate. By the use of endspecifically attached fluorescent quantum dots instead of fluorescent dyes we do not change natural mechanical properties of the DNA and we are able to track a particular segment of the molecule. From thermal fluctuations we determine persistence lengths and therewith the 3D distribution of end-to-end-distance by simulations that take the tethering surface into account. In shear flow with different $\dot{\gamma}$ we specify fractional extensions and the amplitude of fluctuations indicating changes in the molecule's morphology. For smaller shear rates we verify theoretically predicted cyclic motion of the free end of the DNA-molecule.

CPP 22.19 Wed 16:00 Poster A

Native UV laser induced fluorescence detection for single cell analysis in a hybrid PDMS-Quartz microfluidic chip — •Dominik Greif, Alexandra Ros, and Dario Anselmetti — Experimental Biophysics & Applied Nanoscience, Bielefeld University, Universitaetsstr. 25, 33615 Bielefeld, Germany

Single cell analysis promises individual expression studies, which are not limited by ensemble averaging effects. Label free detectors based on UV laser induced autofluorescence (UV-LIF) of aromatic amino acids are a valuable extension of the single cell approach.

Here, we present an extension of our previous studies on single cell analysis with native label-free UV-LIF detection [2], in order to improve separation efficiency and detection sensitivity. We reduced the background fluorescence by the fabrication of new PDMS-Quartz-Window-chips (PQW-chips) by at least 75 percent. These PQW-chips integrate fused silica windows in the PDMS-microdevice at the point of detection. Furthermore, the fluorescence intensity of Trp was investigated for different pH values of the separation buffer. Based on these improvements we exemplarily present single cell protein electropherograms from spodoptera frugiperda (Sf9) cells.

[1] W. Hellmich, D. Greif, C. Pelargus, D. Anselmetti, A. Ros, J. Chromatogr. A 1130 (2006) 195. [2] W. Hellmich, C. Pelargus, K. Leffhalm, A. Ros, D. Anselmetti, Electrophoresis 26 (2005) 3689.

CPP 22.20 Wed 16:00 Poster A

Dynamics of nano-droplets on structured surfaces — •Ali Moosavi[1,2], Markus Rauscher[1,2], and Siegfried Dietrich[1,2] — [1]Max-Planck-Institut für Metallforschung, Stuttgart, Germany — [2]ITAP, Universität Stuttgart, Germany

Nanodroplets residing near topographical or chemical steps on solid substrates exhibit a disjoining pressure induced dynamics. Our nanoscale hydrodynamic calculations reveal that non-volatile droplets are attracted or repelled from steps depending mainly on the long-ranged component of the intermolecular interactions. Since the equilibrium contact angle depends on the balance between both long- and short-ranged interactions, in some cases droplets are attracted by the less wettable part of the substrate. This can also lead to energetic barriers for droplets crossing chemical steps from the less wettable side to the more wettable side.

CPP 22.21 Wed 16:00 Poster A

Lattice Boltzmann simulation of non ideal fluids — •Bin Wu, Fathollah Varnik, and Dierk Raabe — Max-Planck Institut für Eisenforschung, Max-Planck Straβe 1,40237 Düsseldorf, Germany

The basic idea of the Lattice Boltzmann(LB) Method is that the liquid approaches *local* equilibrium on each lattice site via collisions.The lattice Boltzmann dynamics is given by$f_{\sigma i}\left(x+\epsilon e_{i\alpha},t+\epsilon\right)-f_{\sigma i}\left(x,t\right)=-\frac{1}{\tau}\left[f_{\sigma i}\left(x,t\right)-f_{\sigma i}^{eq}\left(x,t\right)\right]$ with $\sum f_i e_{i\alpha}e_{i\beta}=P_{\alpha\beta}+nu_\alpha u_\beta$.

For a liquid-gas system,the equilibrium properties can be described by the free energy, $\Psi=\int_V(\psi_b(n)+\frac{\kappa}{2}(\partial_\alpha n)^2)dV+\int_S\psi_c(n)dS$.Minimizing the free energy gives $P_{\alpha\beta}=\kappa\partial_\alpha n\partial_\beta n+[n\partial_n\psi_b(n)-\psi_b(n)-\frac{\kappa}{2}(\partial_\alpha n)^2-\kappa n\bigtriangleup n]\delta_{\alpha\beta}$.

The free energy enters the LB algorithm via the pressure tensor, $P_{\alpha\beta}$, which is so called free energy LB approach.

The free energy LB method can deal with Navier-Stokes level hydrodynamics at low Mach numbers. We simulate a droplet's motion on a step-gradient substrate.Owing to different Laplace pressure, the droplet is driven to move on the substrate.Simulation of the droplets' coalescence on substrates is also done by us and we fit the function between the width of bridge-neck and time.We find liquid droplet instability (evaporation) depends on the size of system.

CPP 22.22 Wed 16:00 Poster A

Thermally Excited Capillary Waves on n-Alkanes: Photon Correlation Spectroscopy Studies — •Matthias Wolff and

Patrick Huber — Saarland University, Saarbruecken, Germany

Quasi-elastic light scattering from thermally excited capillary waves is a powerful method to study the surface hydrodynamics of liquids. We have designed a photon correlation spectroscopy setup in order to investigate this scattering and to relate it to the fundamental structural and thermodynamical properties of liquid surfaces. First measurements on the surface freezing effect in n-alkanes (n-eicosane, n-tetracosane) and how it affects the surface rheology are presented.

CPP 22.23 Wed 16:00 Poster A

Capillary Rise and Flow of Complex Liquids in Nanopores — •Simon Grüner and Patrick Huber — Saarland University

We present measurements on the capillary rise (spontaneous imbibition) and pressure driven flow (forced imbibition) of liquids into silica monoliths (namely porous Vycor) permeated by tortuous pores with radii of 5nm. The flow properties are studied as a function of the complexity of the building blocks of the liquids (water, n-alkanes and liquid crystals), as a function of shear rate and as a function of temperature in the case of the liquid crystal. This work has been supported within the DFG priority program 1164, Nano- & Microfluidics (Grant No. Hu 850/2).

CPP 22.24 Wed 16:00 Poster A

Surface scattering characterization of the fluid/substrate interface in a fluidic experiment — •J.-F. Moulin and P. Mueller-Buschbaum — TU Muenchen, Physik-Department, LS E13, James-Franck-Str.1, 85747 Garching (Germany)

We will present the results of Grazing Incidence X-Ray Scattering (GISAXS) performed on fluidic channels. Scattering methods such as Grazing incidence x-ray scattering (GISAXS) provide a wealth of information about the interfacial structure: with such an experimental technique both the in-plane ordering and the out of plane correlations are detected and quantitatively characterized in a non invasive/non destructive manner. Up to now this technique has never been used to characterize samples under flow. We have thus designed a new setup to perform GISAXS during a fluidic experiment where a solution is run over a substrate [1]. Together with state of the art GISAXS synchrotron beamlines such as BW4 at Hasylab (Hamburg, Germany) this setup makes it possible to map the structure of the liquid/solid interface of a fluidic channel at spots separated by c.a. 50 microns along the flow direction.

We will here present results obtained on detection of gold nanoparticles at the fluid/substrate interface as well as on the way these particles form a thin film under flow and how the structure of this film evolves with time.

[1]Flow at interfaces: a new device for x-ray surface scattering investigations, J-.F. Moulin, S .V. Roth, P. Müller-Buschbaum accepted for publication in Review of Scientific Instruments (2007)

CPP 23: Single Molecules (joint session BP/CPP)

Time: Wednesday 14:00–17:15 Location: C 243

See BP for the program of the Session

CPP 24: Semiflexible Polymers and Networks (joint session BP/CPP)

Time: Wednesday 17:30–19:30 Location: PC 203

See BP for the program of the Session

CPP 25: Polyelectrolytes

Time: Wednesday 14:30–16:00 Location: C 230

CPP 25.1 Wed 14:30 C 230

Effect of preparation parameters on the D2O/H2O uptake of polyelectrolyte multilayers — •Samuel Dodoo[1], Roland Steitz[2], and Regine von Klitzing[1] — [1]Stranski-Laboratorium für Physikalische & Theoretische Chemie, Institut für Chemie, TU Berlin, Strasse des 17. Juni 124, D-10623 Berlin — [2]Hahn-Meitner Institut, Glienicker Strasse 100, D-14109 Berlin

Polyelectrolyte multilayers (PEM) present a novel material of increasing interest. Their preparation via the layer-by-layer adsorption method1 offers a wide range of applications. We have investigated PEM of poly(styrene sulfonate) (PSS) and poly(diallyldimethyl ammoniumchloride) (PDADMAC) prepared at different NaCl concentrations, against water of different isotopes by neutron reflectometry2,3. The study addresses the effect of ionic strength and polymer charge on the water uptake by the multilayers. Increasing ionic strength increases thickness and swelling of the multilayers. The PEM swelled more in D2O than in H2O but this could not be attributed to replacement of H by D at the polymer. Two types of water were observed, "void water" about 10 vol-% which goes to fill the voids in the multilayers and "free water" about 40 vol-% which directly contributes to swelling of the multilayers. Measurements of effect of type of ions (Hoffmeister effect) are underway.

[1] Decher, G Science 1997, 277, 1232. [2] Steitz, R.; Leiner, V.; Siebrecht, R.; v. Klitzing, R. Colloids and Surfaces A 2000, 163, 63-70. [3] Steitz, R.; Leiner, V.; Tauer, K.; Khrenov, V.; v. Klitzing, R. Applied Physics A 2002, 74, S519-S521.

CPP 25.2 Wed 14:45 C 230

Conformational changes in polyelectrolyte polymer brushes - A strategy for locally controlled surface properties — •Rosa Poetes[1], Ullrich Steiner[1], Tim Kelby[2], Ron Oren[2], Feng Zhou[2], and Wilhelm Huck[2] — [1]Cavendish Laboratory, University of Cambridge, Cambridge, UK — [2]Melville Laboratory, University of Cambridge, Cambridge, UK

Stimuli-responsive polymer brushes are promising systems for local triggering of surface properties. Conformational states of polymer brushes in the liquid environment can be monitored using spectroscopic ellipsometry. We hope to achieve local switching of surface properties using stimuli-responsive polyelectrolyte polymer brushes. Binary polymer brushes with responsive and non-responsive components are particularly adapted for such applications.

Temperature induced conformational changes of Poly[N-isopropylacrylamide] (PNIPAM) in water were observed and characterised to show the applicability of the technique. Studies of patterned binary brush systems containing PNIPAM and Poly[oligo(ethylene glycol) methacrylate] (POEGMA) demonstrated the possibility of following localised conformational changes using imaging ellipsometry.

Conformational changes in polyelectrolyte polymer brushes are being studied in response to electric fields. Current work is focusing on the characterisation of polyelectrolyte polymer brushes in the liquid environment. The effects of electric fields on poly[2-(methacryloyloxy)ethyl trimethylammonium chloride] (PMETAC) in water are currently being investigated.

CPP 25.3 Wed 15:00 C 230

Small-angle x-ray scattering studies on lignosulfonate, a complex polyelectrolyte — •Ulla Vainio[1,3], Rolf Andreas Lauten[2], and Ritva Serimaa[3] — [1]HASYLAB at DESY, Notkestr. 85, D-22603 Hamburg, Germany — [2]Borregaard Lignotech, P.O. Box 162, NO-1701 Sarpsborg, Norway — [3]Department of Physical Sciences, P.O.Box 64, FI-00014 University of Helsinki, Finland

Lignosulfonate is a colloidal polyelectrolyte produced during sulfite pulping process of plants. Plant cell walls consist mostly of cellulose, hemicelluloses and lignin. During pulping lignin is made soluble and removed from the cell walls as lignosulfonate. Various uses have been invented for this byproduct of the pulping process, but even more could be possible once the behaviour of lignosulfonate in solution can be correlated to its structure.

Lignosulfonate particles of mass weighted molar mass 18 000 g/mol were studied in water and salt solutions using small-angle x-ray scattering and rheology. The concentration of the polyelectrolyte was varied from semidilute to concentrated.

Combined with molecular mass distribution obtained from gel permeation chromatography the model shape of an average lignosulfonate particles was discovered to be a flat ellipsoid by fitting different models to SAXS data. At water solutions below 0.1 mass fraction positions of the correlation peak observed in SAXS patterns scaled with concentration of lignosulfonate through a scaling law with exponent 0.28. Selfassociation of lignosulfonate particles was observed at higher concentrations from the SAXS data.

CPP 25.4 Wed 15:15 C 230

Challenging scaling laws of flexible polyelectrolyte solutions with effective renormalization concepts — •Stephan A. Baeurle[1] and Evgenij A. Nogovitsin[2] — [1]Institute of Physical & Theoretical Chemistry, University of Regensburg, D-93053 Regensburg, Germany — [2]Institute of Solution Chemistry, Russian Academy of Sciences, 153045 Ivanovo, Russia

Recasting a many-particle problem in a field-theoretic formalism is nowadays a well-established theoretical tool used by scientists across a wide spectrum of research areas, ranging from polymer physics to molecular electronic structure theory. It has shown to provide useful results in many complex situations, where the physics of the system involves many degrees of freedom and a multitude of different length-scales, generally rendering its numerical treatment on a detailed level computationally intractable. To reduce the computational burden, field-theoretic methodologies usually take advantage of the mean field approximation, which is known to give reliable information about the system in the high concentration regime, where the interactions are highly screened. However, it is well-established that the ranges of interest in most technological applications, lie in the intermediate to low concentration regimes, where fluctuations beyond the mean field level of approximation become important and dominate the overall physical behavior. In this talk we introduce a new renormalized self-consistent field theory for flexible polyelectrolyte chains, in which the monomers interact via a pair potential of screened Coulomb type, and derive suitable thermodynamic expressions for all concentration regimes.

CPP 25.5 Wed 15:30 C 230

Swelling of PEM with different charge densities at solid support in humid nitrogen atmosphere: A neutron reflectometry study — •Ralf Köhler[1,2], Ingo Dönch[2], André Laschewsky[3], Andreas Fery[4], and Rumen Krastev[2] — [1]HMI Berlin, Abt. SF1, Berlin — [2]MPI KGF, Abt. GF, Potsdam — [3]Fraunhofer IAP, Abt. Wasserbasierte Systeme, Potsdam — [4]Universität Bayreuth, Phys. Chemie II, Bayreuth, Germany

Polyelectrolyte Multilayers (PEM) are composites of self-assembled (layered) polyions of alternating charges. They are interesting materials for technical application and fundamental research with a high potential for appliance in medical, biotechnological and pharmaceutical purposes. NR maid be expected to be the perfect tool for measuring of swelling behaviour of PEM (here PSS/PDADMAC) because both, thickness change and water content can be obtained simultaneously. The samples were prepared in Layer-by-Layer technique (spraying) applying PDADMAC with different charge densities (100%, 89% and 75%). It was found that the water uptake is almost linear with the relative humidity of surrounding vapour. The swelling of the PEM depends nonlinearly from the water content of the multilayers. Significant dependence of the swelling and/or water uptake on the charge density was not observed on ultra-thin PEM. Further experiments were addressed to the swelling behaviour by variation of the initial PEM thickness. No intense thickness dependence was observed but a well pronounced non equal distribution of the polymer chains (respectively water uptake) normal to the surface was documented.

CPP 25.6 Wed 15:45 C 230

Wrinkling for measuring charge density effects in polyelectrolyte multilayers and as a novel approach towards templating — •Ingo Doench[1], Conghua Lu[1], Patrick Ott[2], André Laschewsky[3], and Andreas Fery[1,4] — [1]Max Planck Institute of Colloids and Interfaces, Potsdam, Germany — [2]Universität Potsdam, Germany — [3]Fraunhofer Institute for Applied Polymer Research, Potsdam, Germany — [4]University of Bayreuth, Germany

Polyelectrolyte Multilayers find various applications as coatings or semi-permeable membranes. Their mechanical properties are relevant for stability as well as in general for their deformation properties (pressure sensing). Still, classical indentation tests for determining mechanical properties of solid-supported films face serious problems due to substrate effects when the film thickness is below a micron. Therefore, we use an alternate approach in which we investigate wrinkling of these films and derive elastic constants from the measurement of the wrinkle period. We are able to change the charge density of the polycation for film preparation and find that this .allows tuning the mechanical properties of the multilayers. Furthermore, humidity has strong effects on the multilayers and we find that the degree of softening / swelling of the multilayers by increasing humidity can be determined by the charge density as well. Apart from the possibility to determine elastic constants of thin films, wrinkling provides a simple pathway to lithography-free topographical patterning on the micron- and sub-micron-scale. We present first results for templating of colloidal particle-deposition and discuss perspectives.

CPP 26: Micro and Nano Fluidics I: Liquids at structured materials

Time: Wednesday 14:00–16:00 Location: C 264

Invited Talk CPP 26.1 Wed 14:00 C 264

The Capillary Rise of Liquids in Nanopores — •Patrick Huber — Faculty of Physics, Saarland University, D-66041 Saarbruecken

Liquid flow driven by capillary forces is one of the most intriguing transport mechanisms in nature and technology. It is governed by a fascinating interplay of interfacial, inertia, viscous drag as well as gravity forces which liquids encounter upon invasion into geometries with often complex topologies, such as capillary networks of trees or interconnected pores and fractures in soils and ice. Whereas a detailed understanding of this phenomenon has been achieved on macroscopic scales, it is poorly explored on the meso- and nanoscale, where predictions regarding its mechanisms are hampered due to a possible breakdown of continuum hydrodynamics, conflicting reports with respect to the conservation of the fluidity and capillarity of liquids upon spatial confinement. Here we present optical and gravimetrical measurements on the capillary rise of liquids as a function of their complexity (water, chain-like hydrocarbons and rod-like liquid crystals) in networks of silica capillaries with 2.5 nm and 5 nm radii (monolithic mesoporous Vycor). We find classical Lucas-Washburn square-root-of-time invasion dynamics over the entire capillary rise time investigated (up to several hours). We demonstrate that conserved macroscopic capillary rise hydrodynamics are intimately related to the capillary condensation/evaporation hysteresis characteristic of the thermodynamic state of spatially nanoconfined liquids.

This work has been supported within the DFG priority program 1164, Nano- & Microfluidics (Hu850/2).

CPP 26.2 Wed 14:30 C 264

Simulation of fluid flow in hydrophobic rough microchannels — •Jens Harting and Christian Kunert — Institute for Computational Physics, Pfaffenwaldring 27, D-70569 Stuttgart

Surface roughness becomes relevant if typical length scales of the system are comparable to the scale of the variations as it is the case in microfluidic setups. Here, an apparent boundary slip is often detected which can have its origin in the misleading assumption of perfectly smooth boundaries. We investigate the problem by means of lattice Boltzmann (LB) simulations and introduce an “effective no-slip plane” at an intermediate position between peaks and valleys of the surface. Our simulations show good agreement with analytical results for sinusoidal boundaries, but can be extended to arbitrary geometries and experimentally obtained surface data which cannot be treated analytically. We find that the detected apparent slip is independent of the detailed boundary shape, but only given by the distribution of surface heights. Further, we show that the slip diverges as the amplitude of the roughness increases which highlights the importance of a proper treatment of surface variations in very confined geometries. At last, we extend out work to rough hydrophobic surfaces and show that the coupling of both effects can lead to non-linear effects.

CPP 26.3 Wed 14:45 C 264

Morphological clues to wet granular pile stability — •Mario Scheel[1], Marco Di Michiel[2], Martin Brinkmann[1], Ralf Seemann[1,3], and Stephan Herminghaus[1] — [1]MPI for Dynamics and Self-Organization, Bunsenstr. 10, D-37073 Göttingen — [2]European Synchrotron Radiation Facility, BP 220, F-38043 Grenoble Cedex — [3]Experimental Physics, Saarland University, D-66041 Saarbrücken

When a dry granulate is mixed with a wetting liquid, the macroscopic stiffness of the latter is increased dramatically by virtue of the surface tension of the liquid. This macroscopic mechanic behavior is constant in a large range of the liquid content. Only if nearly all pores are filled with liquid, the stiffness weakens. Using X - ray micro tomography we explore the liquid morphologies that form within the granular pile, as function of liquid content, packing density and grain shape. We can clearly separate air, liquid and grains from each other, which allows to identify the emerging liquid morphologies. Capillary bridges were found for small liquid contents. If more liquid is added, the capillary bridges grow in size and eventually merge into larger liquid cluster. As even more liquid is added, the liquid cluster grow in size and merge with surrounding clusters. For randomly close packed grains this 'building principle' is still valid for large liquid contents and always results in a ramified liquid structure. This 'building principle' was verified numerically by minimizing the surface energy of particular cluster morphologies. The experimental observed constancy of the mechanic behavior follows from the ramified liquid structure.

CPP 26.4 Wed 15:00 C 264

Liquid morphologies in random assemblies of spherical beads — •Martin Brinkmann[1], Mario Scheel[1], Daniel Hornung[1], Marcus Schwamberger[1], Ralf Seemann[1,2], and Stephan Herminghaus[1] — [1]MPI for Dynamics and Self-Organization, 37073 Göttingen — [2]Saarland University, D-66041

Small amounts of wetting liquids mixed into a random assembly of spherical glass beads are present in the form of capillary bridges between adjacent beads. At higher liquid content these bridges coalesce into larger liquid structures that eventually percolate the whole assembly. Inspired by recent X-ray microtomography data we examine the liquid morphologies in local triangular configurations of spheres where two pairs of spheres are in mutual contact while the remaining pair forms a small gap. Using numerical minimizations of the interfacial energy we predict the appearance of certain liquid morphologies as controlled by their volume, respectively, Laplace pressure, contact angle, and gap separation. The morphology diagram can be quantitatively compared to wetting experiments using isolated triangular configurations of spherical beads. Based on these results we propose a simple model to describe the consecutive coalescence of capillary bridges. This model allows to predict the percolation transition of liquid structures in a pile of beads solely based on the contact angle and the local packing geometry.

CPP 26.5 Wed 15:15 C 264

Phase behavior of fluids between thermally corrugated walls — •Gerrit Günther and Martin Schoen — Stranski-Laboratorium für Physikalische und Theoretische Chemie, Sekreteriat C7, Technische Universität Berlin, Straße des 17. Juni 115, D-10623 Berlin, Germany

To investigate the effect of flexible walls on the phase behavior of confined fluids we use the grand canonical ensemble Monte Carlo method (GCEMC). Consider a Lennard-Jones(12,6) fluid between two plane parallel walls which itself consist of single wall particles in a face centered cubic (fcc) (100) order. Wall and fluid particles are of the same type thus interacting via Lennard-Jones(12,6) potenials as well. The wall particles are not fixed to their lattice sites but bound to them by harmonic potentials. The softness of the wall is controlled via the force constant of this harmonic potential. Starting with a sufficiently high force constant the wall resembles a rigid fcc structure. By softening the wall its particles are able to react to thermal fluctuations in the fluid to a greater extent. Fluid and wall particles are then more evenly distributed in space. The structural changes lead to a shift of phase transition in confinement.

CPP 26.6 Wed 15:30 C 264

Dewetting dynamics in triangular grooves: A possible way to measure the slip length — •Krishnacharya Khare[1], Martin Brinkmann[1], Bruce M. Law[2], Stephan Herminghaus[1], and Ralf Seemann[1,3] — [1]Max-Planck Institute for Dynamics and Self-Organization, D-37073 Göttingen — [2]Kansas State University, Manhattan, KS-66506 — [3]Saarland University, D-66041 Saarbrücken

Static wetting morphologies of liquid in triangular grooves and their dynamics are studied experimentally and theoretically. For contact angles smaller than 90° minus half the opening angle of the groove, the liquid forms filaments with negative mean curvature extended along the entire length of the groove. For larger contact angles, liquid either forms elongated filaments of finite length and positive mean curvature or drop-like morphologies. Electrowetting is used to vary the contact angle and to switch between different wetting morphologies. In this way, liquid filaments can be pulled out of a large feeding drop forming elongated filaments in prefabricated surface grooves. When being quenched from the filling to the non-filling regime, the liquid filaments become unstable and break into isolated droplets with a preferred distance. This preferred droplet distance compares favorably with the linear stability model assuming the instability to be driven by the local variation of the Laplace pressure with filament width. Dynamics of the instability is studied via in situ scanning force microscopy at elevated temperature. From the measured time constant of the instability, we derived the slip length for the system which is in good agreement with the dewetting experiments on plane substrates.

CPP 26.7 Wed 15:45 C 264

Intrusion of fluids into nanogrooves — Holger Bohlen[1], Andrew O. Parry[2], Enrique Diaz-Herrera[3], and •Martin Schoen[1] — [1]Stranski-Lab. f. Physikal. und Theor. Chemie, Technische Universität Berlin, GERMANY — [2]Dept. of Mathematics, Imperial College, London, UK — [3]Dept. de Fisica, UNAM, Mexico City, Mexico

We study the shape of gas-liquid interfaces forming inside rectangular nanogrooves. On account of purely repulsive fluid-substrate interactions the confining walls are dry (i.e., wet by vapor) and a liquid-vapor interface intrudes into the nanogrooves to a distance determined by the pressure. By means of Monte Carlo simulations in the grand canonical ensemble (GCEMC) we obtain the density $\rho(z)$ along the midline $(x = 0)$ of the nanogroove for various geometries (i.e., depths D and widths L) of the nanogroove. We analyze the density profiles with the aid of an analytic expression which we obtain through a transfer-matrix treatment of an one-dimensional effective interface Hamiltonian. Besides geometrical parameters such as D and L the resulting analytic expression depends on temperature T, densities of coexisting gas and liquid phases in the bulk $\rho_{\mathrm{x}}^{\mathrm{g,l}}$ and the interfacial tension γ. The latter three quantities are determined in independent molecular dynamics simulations of planar gas-liquid interfaces. Our results indicate that the analytic formula provides an excellent representation of $\rho(z)$ as long as L is sufficiently small. At larger L the meniscus of the intruding liquid flattens. Under these conditions the transfer-matrix analysis is no longer adequate and the agreement between GCEMC data and the analytic treatment is less satisfactory.

CPP 27: Micro and Nano Fluidics II: Slipping + soft objects in flow

Time: Thursday 14:00–16:15 Location: C 264

CPP 27.1 Thu 14:00 C 264

Motion of a cylindrical droplet under an external body force — Cem Servantie and •Marcus Müller — Institut für Theoretische Physik, Georg-August Universität, Göttingen

We study the rolling and sliding motion of droplets on a corrugated substrate by Molecular Dynamics simulations. Droplets are driven by an external body force (gravity), and we investigate the velocity profile and dissipation mechanisms in the steady state. The cylindrical geometry allows us to consider a large range of droplet sizes.

The velocity of small droplets with a large contact angle is dominated by the friction at the substrate and the velocity of the center of mass scales like the square root of the droplet size. For large droplets or small contact angles, however, viscous dissipation of the flow inside the volume of the droplet dictates the center of mass velocity that scales linearly with the size.

We derive a simple analytical description predicting the dependence of the center of mass velocity on droplet size and the slip length at the substrate. In the limit of vanishing droplet velocity we quantitatively compare our simulation results to the predictions and good agreement without adjustable parameters is found.

CPP 27.2 Thu 14:15 C 264

Flow of thin polymer films on mesoporous silicon surfaces — •Matthias Lessel, Oliver Bäumchen, and Karin Jacobs — Saarland University, Experimental Physics, D-66123 Saarbrücken, Germany

The nature of boundary conditions of fluids at the interface of solid surfaces has become more and more important in recent years due to applications in lab-on-a-chip devices. Reducing the scale of fluidic systems leads to a stronger influence of this interface, which can be described by a parameter called slip length. It can be interpreted as the length below the solid/liquid interfaces where the velocity profile of the liquid extrapolates to zero. Our system consists of thin polystyrene films on top of hydrophobized Si wafers, which are heated above the glass transition temperature to induce dewetting as a driving force for Newtonian flow. The slip length can be extracted by analyzing the growth of a dewetting hole using optical microscopy or, with the help of a Stokes model for thin liquid films, from rim profiles of holes imaged by AFM. In recent experiments we study the influence of structured surfaces on the dewetting dynamics. For this we are using hydrophobized mesoporous Si substrates instead of a smooth Si wafer bearing in mind that the pore diameter and porosity of this material is alterable by parameters of the fabrication process. Moreover they can be probed by spectroscopic ellipsometry using a fit based on a Bruggeman model.

CPP 27.3 Thu 14:30 C 264

Dewetting dynamics of thin polymer films on viscoelastic substrates — •Konstantina Kostourou[1], Dirk Peschka[2], Andreas Münch[3], Barbara Wagner[4], Stephan Herminghaus[1], and Ralf Seemann[1,5] — [1]MPIDS, D-37073 Göttingen — [2]Humboldt-University, D-12489 Berlin — [3]University of Nottingham, Nottingham, NG7 2RD, UK — [4]Weierstrass Institute, D-10117 Berlin — [5]Saarland University, D-66041 Saarbrücken

The dewetting of thin liquid polystyrene (PS) films on viscoelastic substrates (PDMS and molten PMMA) is studied both experimentally and theoretically. The dewetting dynamics is found to be slower for smaller substrate elastic moduli. To explore how the dynamics is influenced by the viscoelasticity of the substrate we investigate the shape of the dewetting rim profile and the deformation of the underlying substrate. In case of PMMA substrates we remove the PS using a selective solvent and image the deformation directly on the frozen PMMA. The deformation of rubbery PDMS substrates is reversible. We therefore, lift off the PS from the substrate and image its deformation, which is frozen into the "bottom side"of the dewetting profiles. These techniques even allow to image the deformation of the substrate at the three phase contact line, which is pulled upwards. By quantifying the substrate deformation caused by PS droplets we can derive the elastic modulus of the PDMS substrates in agreement with bulk measurements. We find characteristic rim shapes and deformations of the substrate depending on the elastic modulus and the viscosity of the underlying substrate.

CPP 27.4 Thu 14:45 C 264

Flows driven by wettability gradients: A lattice Boltzmann study — •Fathollah Varnik and Dierk Raabe — Max-Planck Institut für Eisenforschung, Düsseldorf, Germany

Guided motion of liquids is studied via lattice Boltzmann computer simulations. The focus of the work is on basic issues related to driving forces generated via a step-wise (abrupt) change in wetting properties of the substrate along a given spatial direction. We first give approximate analytic expressions for forces driving the liquid motion. These theoretical estimates show qualitatively different dependence of wetting gradient induced forces on contact angle and liquid volume in the case of an open substrate as opposed to a planar channel. These results are then examined via lattice Boltzmann computer simulations. Furthermore, we also investigate effects of a wetting gradient on internal droplet dynamics and the resulting dissipation losses.

CPP 27.5 Thu 15:00 C 264

Motion of an elastic capsule in time dependent shear flow — •Steffen Kessler, Reimar Finken, and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart

The motion of an elastic three-dimensional micro-capsule in a time dependent shear flow is studied numerically using a spectral method. The shape of the capsule and the hydrodynamic flow field are expanded into smooth basis functions. Analytic expressions for the derivative of the basis functions permit the evaluation of elastic and hydrodynamic stresses and bending forces at specified grid points in the membrane. Compared to methods employing a triangulation scheme, this method has the advantage that the resulting capsule shapes are automatically smooth, and few modes are needed to describe the deformation accurately. Better stability properties compared to simple boundary integral methods follow from this strategy, which has been tested successfully recently in linear shear flow. This code is used to study the response of capsules to a modulated shear flow. We examine both a purely oscillating shear rate and a modulated shear rate around a constant value. In the latter case, we focus on the question whether dynamical phase transitions can be induced by small modulations. Computations are performed for capsules both with spherical and ellipsoidal unstressed reference shape, different elastic parameters, and different viscosity contrasts.

CPP 27.6 Thu 15:15 C 264

Long ranged hydrodynamic repulsion of polymers at interfaces — •Christian Sendner and Roland Netz — Physik Department, Technische Universität München

We consider the influence of a no slip boundary on polymers in external fields or shear flow in the zero Reynolds number regime. Due to the interplay between thermal fluctuations and hydrodynamic interactions, which leads to a preferred orientation of the polymer with respect to the surface, polymers are repelled from the interface with a force that decays with the inverse square of the surface separation. On the basis of a Fokker-Planck analysis, we give scaling relations for this repulsion in terms of length of the polymer, shear strength or external force and temperature. Brownian Dynamic simulations including hydrodynamic interactions confirm these scaling laws. This repulsive force can be used in microfluidic applications to control adsorption and desorption of polymers.

CPP 27.7 Thu 15:30 C 264

Cross-Streamline Migration of Semiflexible Actin Filaments in Microflow — •Dagmar Steinhauser, Heather M Evans, and Thomas Pfohl — Max-Planck-Institut für Dynamik und Selbstorganisation, Göttingen

Actin filaments, aside from their biological roles in cellular motility and mechanical stability, also provide an ideal system with which to study, more generally, the properties of semi-flexible polymers. Our experiments investigate the behavior of single actin filaments flowing inside symmetric microchannels with a Poiseuille velocity profile. Fluorescence microscopy using stroboscopic laser light illumination is utilized in order to visualize the moving actin filaments. The dimensions (width and depth) of the channels are in the same order of magnitude as the persistence length as well as the contour length of the filaments. A detailed analysis of the center-of-mass probability distribution along a cross-section of the channel is reported. Depletion layers, found at the walls, can be explained by migration due to hydrodynamic interactions with the walls. In addition, the conformation of the actin filaments in flow depends on the shear stress, which increases towards the walls for Poiseuille flow. The resulting spatially-varying diffusivity leads to a striking migration of filaments away from the center and consequently to a minimum in the center-of-mass distribution at the channel center. Analyzing the change in diffusivity from the measured conformations, the Fokker-Planck equation can be solved and the center-of-mass distributions can be described quantitatively for different velocities.

CPP 27.8 Thu 15:45 C 264

Fluctuating vesicles in hydrodynamic Stokes flow — •Reimar Finken and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart

The behaviour of soft objects in hydrodynamic flow has received increasing attention in recent years, both theoretically and experimentally. An important and intriguing aspect is the interaction of the flow with thermal fluctuations out of thermal equilibrium. Thermal noise becomes particularly important near dynamic phase transitions, where the motion is sensitive to external forces. As a paradigmatic model system we study the stochastic motion of a vesicle in a planar shear flow at finite temperature. In the absence of thermal noise, this system exhibits a rich dynamical behaviour including tank-treading, tumbling, and breathing regimes. We consider the stochastic motion of quasi-spherical three dimensional vesicles and develop Langevin type equations of motion for the deformation amplitudes. Near the phase transitions a separation of time scales between the ellipsoidal modes and the higher order modes allows us to treat the higher modes as a bath and study the remaining degrees of freedom using a Fokker-Planck equation. We pay particular attention to the vesicle motion near the "triple point", where the three dynamic regimes meet. This work was funded by the DFG Priority Program SPP 1164 "Nano- and Microfluidics".

CPP 27.9 Thu 16:00 C 264

Hydrodynamic lift forces on solute particles in a nanotube forest — •Vladimir Lobaskin and Roland Netz — Physik Department T37, TU München, 85747 Garching

We apply theory and hybrid Langevin dynamics – lattice Boltzmann simulations to study shear-induced molecular transport in polymer solutions and colloidal dispersios close to an interface modified by a grafted inclined hard posts (carbon nanotube forest) or brush of semiflexible polymer segments. We show that the excluded volume interactions of particles and polymer chains with the posts lead to appearance of residual hydrodynamic size-dependent lift forces, which can promote a depletion of the solute from the forest or its accumulation at the surface and serve as a basis of sseparation techniques.

CPP 28: Micro and Nano Fluidics III: Migration and flow

Time: Thursday 16:30–18:30 Location: C 264

Invited Talk CPP 28.1 Thu 16:30 C 264

Mixing in passive and active microflows — •Arthur V. Straube — Department of Physics, University of Potsdam, Am Neuen Palais 10, PF 601553, D-14415 Potsdam, Germany

Recent progress and numerous applications in medicine, chemistry and biotechnology have witnessed great interest in understanding the fundamental aspects of mixing at small scales. Because of nonturbulent nature of microflows, mixing of small amounts of even passive liquids is a highly nontrivial task. For active flows, where the different liquid substances can additionally react, this problem becomes especially challenging. In this talk we start with the most important achievements of the mixing problem in passive flows and then proceed to the mixing-induced phenomena in active flows.

CPP 28.2 Thu 17:00 C 264

Colloidal Particles Operating Microfluidic Devices — •Tobias Sawetzki[1], Sabri Rahmouni[1], Stefan Bleil[1], David W.M. Marr[2], and Clemens Bechinger[1] — [1]2. Physikalisches Institut, Universität Stuttgart — [2]Chemical Engineering Department, Colorado School of Mines

The miniaturization of microfluidic devices has raised the interest of researchers in biology, chemistry, engineering and physics. Nevertheless, the future goal of a fully functional small and mobile device, the 'lab on the chip', has proven to be quite difficult to reach. In our approach we use paramagnetic colloidal particles as *in situ* building blocks for different functionalities such as pumping or mixing of liquids in channel structures on the micron scale. Once arranged by optical tweezers, the colloidal particles are driven by an external magnetic field which rotates in the sample plane and thus exerts a torque on the colloidal clusters. We demonstrate how this approach allows us to create pumps, valves, T-junctions and mixers. In contrast to other approaches, our concept is quite insensitive to the character of the liquid and the channel material and can be easily scaled up or down thus making it a versatile approach for creating microfluidic devices.

CPP 28.3 Thu 17:15 C 264

Positive and negative diffusive-like migration of particles using ion specific effects in microchannels — •Lyderic Bocquet[1], Benjamin Abecassis[2], Cecile Cottin-Bizonne[2], Christophe Ybert[2], and Armand Ajdari[3] — [1]University of Lyon and Technical University Munich — [2]University of Lyon — [3]ESPCI, Paris - Saint-Gobain

Developing versatile methods for driving and manipulating macromolecules or biological cells in microchannels is a key challenge for lab-on-a-chip devices. State of the art approaches for particles' manipulation usually require external fields or specifically designed channel geometries. Here we present a passive and very simple method leading to a tunable and efficient migration of particles in the absence of any external field. Using this method the particles are shown to exhibit a diffusive-like motion which is strongly amplified compared to their bare diffusion process. Moreover both spreading and focusing of the particle assembly can be achieved on demand, corresponding to positive or negative diffusive-like migration. While focusing is a priori conflicting with the second law of thermodynamics, it is obtained in the present mechanism by slaving the particle's dynamics to a fast carrier specie, here a dilute salt, via a chemotaxis-like transport phenomenon, diffusio-phoresis. As a proof of principle, both homogeneization and focusing of a colloidal solution in a microchannel are demonstrated, illustrating the potential of this versatile method for microfluidic applications.

CPP 28.4 Thu 17:30 C 264

X-ray optics with microfluidics: Stabilization of gas bubbles by surface ordering and freezing — •Yasutaka Iwashita[1], Christian Bahr[1], Ralf Seemann[1,2], and Stephan Herminghaus[1] — [1]MPI for Dynamics and Self-Organization, D-37073 Göttingen — [2]Experimental Physics, Saarland University, D-66041 Saarbrücken

Compound refractive lenses (CRL), which are composed of many lenses of small radii in a row embedded in a solid medium, have been developed as X-ray lenses (A. Snigirev et al. [1]). CRL has numerous advantages as X-ray optics: It is robust, easy to align and to operate, and can be used for hard X-rays.

To broaden the possibilities and functions of CRL, we propose a "dynamic CRL": This is composed of gas bubbles in a liquid as lenses, where the bubbles are generated and flowing consecutively in a microfluidic device. Due to the continuous renewal of the materials, this system leads to a high stability against high X-ray intensities. Furthermore, the variation of bubble shape controlled via flow parameters allows in-situ optimization of the optical properties of the system.

Here we study the stabilization of gas-liquid foam in microfluidic devices by surface freezing of n-alkanes and surface ordering of liquid crystals. These systems have great advantages for dynamic CRL:(i) X-ray transmission is high and (ii) gas bubbles can be stabilized without surfactants. As a result, we succeeded in stabilizing gas-liquid foam by surface freezing and ordering, and in controlling the foam structure.

[1] A. Snigirev, V. Kohn, I. Snigireva and B. Lengeler, Nature 384(6604), 49(1996)

CPP 28.5 Thu 17:45 C 264

Droplet-Based Emulsion Microfluidics for Monodisperse Silica Particle Synthesis — •Venkatachalam Chokkalingam[1], Boris Weidenhof[2], Wilhelm F. Maier[2], Stephan Herminghaus[1], and Ralf Seemann[1,3] — [1]Max Planck Institute for Dynamics and Self-Organization, Goettingen, Germany. — [2]Technical Chemistry, Saarland University, Saarbrücken, Germany. — [3]Experimental Physics, Saarland University, Saarbrücken, Germany.

We explore the possibility to produce silica particles from sol-gel chemistry by means of droplet based microfluidics. Aqueous droplets containing tetramethoxysilane (TMOS), solution (A), and ammonia, solution (B), are formed using two individual production units. The droplet production is synchronized at a Y-junction to form regular pairs of droplets containing the solutions A and B, respectively. The sol-gel reaction is started by merging the individual droplets using either electrocoalescence or a geometrical constriction. Mixing within the coalesced droplets proceeds quite efficiently and the gelation time of the sol-gel solution is adjusted to be within few seconds such, that the gel is fully developed when the gel particles are collected outside the microfluidic device for subsequent drying and heat treatment. The resulting silica particles have a diameter of a few micrometers, only. Since the sol-gel process can be used to produce mixed oxides with tailored porosity and pore size, this controlled monodispersed particle production is of potential interest for a broad range of applications in heterogeneous catalysis. Moreover, different volumetric combinations of any two chemicals are a first step towards combinatorial chemistry.

CPP 28.6 Thu 18:00 C 264

Vortex formation in travelling wave-driven micropumps — •Richard Stein[1], Magnus Jäger[2], Andreas Münch[3], Alexander Mielke[3], Michael Böttcher[2], Michael Stuke[4], and Claus Duschl[1] — [1]Fraunhofer Institute for Biomedical Engineering (IBMT), Am Mühlenberg 13, 14476 Potsdam, Germany — [2]Saarland University, Faculty Clinical Medicine, Department Medical Technology, Am Mühlenberg 13, 14476 Potsdam, Germany — [3]Weierstraß Institute for Applied Analysis and Stochastics (WIAS), Mohrenstraße 39, 10117 Berlin, Germany — [4]Max Planck Institute for Biophysical Chemistry, Am Faßberg 11, 37077 Göttingen, Germany

Electrothermally driven flows in microfluidic channel systems with integrated electrodes currently attract increased interest due to their potential biomedical applications, e.g. for switchable accumulation of viruses. Recently, an elaborate experimental study of the electrothermal pumping reported on the formation of vortices at the edges of the electrode field [1]. The vortices appeared to be quite robust and may hold great promise for applications, e.g. as a tool for the separation, accumulation and analysis of biological micro- and nanoparticles in microdevices, provided their formation can be controlled reliably.

In our talk, we introduce a 3D model for the fluid flow in microchannels extending the model of [2]. The approach uses the relevant electro-, thermo- and hydrodynamic mechanisms and is systematically derived by asymptotic techniques. Finally, the flow is numerically evaluated.

[1] M. Felten et al., Phys. Fluids 2006, 18, 051707.

[2] A. González et al., J. Fluid Mech. 2006, 564, 415-433.

CPP 28.7 Thu 18:15 C 264

Fluid flow induced by temperature waves - a thermomechanical pumping mechanism for microfluidics — Franz M. Weinert[1], •Jonas A. Kraus[2], Thomas Franosch[2], and Dieter Braun[1] — [1]Applied Physics and Center for NanoScience (CeNS), Department of Physics, Ludwig-Maximilians-Universität München, Amalienstrasse 54, D-80799 München, Germany — [2]Arnold Sommerfeld Center for Theoretical Physics (ASC) and Center for NanoScience (CeNS), Department of Physics, Ludwig-Maximilians-Universität München, Theresienstrasse 37, D-80333 München, Germany

Recently, flow at the scale of millimeters and below has attracted significant attention, stimulated by the rapid advances to manipulate and to control small-scale devices. Here, conventional pumping encounters major difficulties and a challenge of the field of microfluidics is to provide adequate tools for fluid manipulation at the microscale.

Here we propose a new mechanism that allows to generate net fluid flow by optical control. The thermal expansion of a fluid combined with a temperature-dependent viscosity introduces nonlinearities in the Navier-Stokes equations unrelated to the convective momentum current. With a suitable set-up we demonstrate that nonsteady heating can be employed to induce non-trivial flow patterns at small scales. This novel thermo-mechanical effect is investigated for a thin fluid chamber by a numerical solution of the Navier-Stokes equations and analytically by a perturbation expansion. A demonstration experiment confirms the basic mechanism and quantitatively validates our theoretical analysis.

CPP 29: Polymerphysics I

Time: Thursday 9:30–12:45 Location: C 130

CPP 29.1 Thu 9:30 C 130

The physical resolution limit for replica molding — •Ovidiu D. Gordan[1], Bo N. J. Persson[2], Claudia M. Cesa[1], Dirk Mayer[3], Bernd Hoffmann[1], Sabine Dieluweit[1], and Rudolf Merkel[1] — [1]IBN-4, FZ-Jülich, 52425, Jülich, Germany — [2]IFF, FZ-Jülich, 52425, Jülich, Germany — [3]IBN-2, FZ-Jülich, 52425, Jülich, Germany

The key element of the fast evolution in the information technology is the ability to replicate patterns at increasingly lower scales. Besides photolithography, in the last decade, soft lithography[1] developed as a cheaper microfabrication alternative. This technique also allows to imprint micro-structures in polymers. Therefore today micropatterned elastomer surfaces are widely used in micro-fluidics[2] and micro-contact printing. Moreover, it enables emerging techniques in biotechnology, where very soft microstructures are employed, to mimic physiological conditions for living cells. However, up to now the general understanding of pattern preservation during the molding process was limited to the rule of thumb "the harder the better".

This study shows the analytical dependence of the molding fidelity of the elastomer stiffness, surface tensions and dimensions of the topographic features.

[1] Y. Xia and G. M. Whitesides, Annu. Rev. Mater. Sci. 28, 153 (1998).

[2] G. M. Whitesides, Nature 442, 368 (2006)

CPP 29.2 Thu 9:45 C 130

Changing the fracture properties of Polypropylene by blending — •Stefan Fischer[1], Dirk Doser[1], Tobias Diesner[2], Bernhard Rieger[2], and Othmar Marti[1] — [1]Institute of Experimental Physics, Ulm University, Albert-Einstein-Allee 11, 89069 Ulm, Germany — [2]Wacker-Lehrstuhl für makromolekulare Chemie, TU München, Lichtenbergstraße 4, 85747 Garching, Germany

Isotactic Polypropylene is among the most widely used plastics. Still it suffers from brittleness at ambient conditions. By enhancing it's fracture properties it could substitute other structures stabilizing solids while introducing it's own advantages like low weight and ductility to high ranges. Therefore in industrial polymers different additives are used to soften the polymer, reducing the brittleness. Still the polymers tend to break easily.

Our research has shown, that blending commercially available Polypropylene with high molecular one we can access new ranges in mechanical stability under certain conditions. The high molecular weight iPP seems to facilitate and propagate the reorientation of crystalline material while suppressing the evolution of cracks. This prevents the fracture at low elongations and allows high stresses and elongations until failure.

We will show the results of tensile tests, SAXS (Small Angle X-Ray Scattering), WAXS (Wide Angle X-Ray Scattering), DSC (Differential Scanning Calorimetry) and AFM (Atomic Force Microscopy) measurements. The effect of high molecular Polypropylene will be discussed, the problems still appearing at ambient conditions will be addressed.

CPP 29.3 Thu 10:00 C 130

On the creation of dielectric interphases in composites containing nano- and micro- particles. — •Béatrice Hallouet[1], Pauline Desclaux[1], Bernd Wetzel[2], Alois K. Schlarb[2], and Rolf Pelster[1] — [1]Fachrichtung 7.2 Experimentalphysik, Universität des Saarlandes Campus E 2.6 D-66 123 Saarbrücken Germany — [2]Institut für Verbundswerkstoffe GmbH (IVW) Erwin-Schrödinger-Straße, Geb.

58 D-67 663 Kaiserslautern Germany

We investigate composites consisting of magnetic particles (Fe3O4) in a polymer matrix (an epoxy resin) using broadband dielectric spectroscopy in a frequency range between 50 Hz and 1 GHz. Especially, we compare systems containing nano-particles (mean diameter between 20 and 30 nm) and micro-particles (mean diameter about 5 μm). Temperature-dependent measurements allow us to characterize a molecular relaxation of the matrix material, that is modified by the presence of the dispersed particles. For a model-free and non ambiguous analysis of these effects we use the spectral representation of Bergman [1]. We discuss the results in terms of modified interactions at the interfaces of the particles and check whether they depend on the microstructure of the composites and/or on the surface-to-volume ratio of the particles.

[1] B. Hallouet, B. Wetzel, and R. Pelster, "On the dielectric and magnetic properties of nanocomposites " , JNM in press.

CPP 29.4 Thu 10:15 C 130

Free volume in two untreated, presure-densified, and CO2 gas exposed polymers — Günter Dlubek[1], Jürgen Pionteck[2], •Muhammad Qasim Shaikh[3,4], Liane Häussler[2], Stefan Thränert[3], Essmat Sayd Hassan[3], and Reinhard Krause-Rehberg[3] — [1]ITA Institut für Innovative Technologien, Köthen/Halle, Wiesenring 4, D-06120 Lieskau (Halle/S.), Germany — [2]Leibniz-Institut für Polymerforschung Dresden e.V., Hohe Strasse 6, D-01069 Dresden, Germany — [3]Martin-Luther-Universität Halle-Wittenberg, Fachbereich Physik, D-06099 Halle/S., Germany — [4]Technische Fakultät, Lehrstuhl für Materialverbunde, Christian-Albrecht Universität, Kaiser Str.2, D-24143, Kiel, Germany

Changes in the microstructure of the free volume and its temperature dependence in ethylene-norbornene copolymer and bisphenol-A polycarbonate due to densification under pressure and swelling with CO2 gas have been examined using positron annihilation lifetime spectroscopy (PALS) and were compared with pressure-volume-temperature (PVT) experiments from Dresden. From the PALS spectra analyzed with the new routine LT9.0 the size distribution of subnanometre holes and its mean and mean dispersion were calculated. Above Tg, the dispersion mirrors the thermal fluctuations in the free volume. PALS data show that the mean hole size and its dispersion in the glassy state is decreased due to densification and increased due to swelling.

CPP 29.5 Thu 10:30 C 130

Generalized mode-Grüneisen-parameters as a universal measure for the chemically induced glass transition in reactive systems — •Ulrich Müller[1], Martine Philipp[1], Jan Kristian Krüger[1], Roland Sanctuary[1], Wulff Possart[2], Bartosz Zielinski[1], Jörg Baller[1], Ravindrakumar Bactavatchalou[1], Patrick Alnot[3], and Christelle Vergnat[1] — [1]Université du Luxembourg, LPM, Campus Limpertsberg, L-1511 Luxembourg — [2]Universität des Saarlandes, ASPG, 66041 Saarbrücken — [3]Université Henri Poincaré - Nancy I, Nancy, France

A fundamental understanding of the glass transition is still lacking and so the controversy about the nature of the glass transition, being it a kinetic or intrinsic transition, is going on. The investigation of an isothermal cure of reactive systems by means of generalized mode-Grüneisen-parameters (gMGP) offers an alternative access to this problem. In contrast to the MGP known from solid state physics being sensitive to changes of elastic anharmonicity (3rd order elasticity), gMGP probe in addition 2nd order elasticity modified by structural changes during the curing process. Using epoxies and polyurethanes as model systems and combining Brillouin spectroscopy with high resolution refractometry the temporal evolution of the related gMGP indicate indeed the onset of chemical freezing. The comparison with caloric data suggests that there is a rough coincidence of the gGMP anomaly and the vanishing excess heat capacity with respect to the heat capacity of the glassy state.

break

CPP 29.6 Thu 11:00 C 130

MAO is a polymer! - Analysis of polymeric methylaluminoxane via small angle neutron scattering and neutron spin echo spectroscopy — Aizhen Niu[1], •Jörg Stellbrink[1], Jürgen Allgaier[1], Dieter Richter[1], Geoffrey W. Coates[2], and Lewis J. Fetters[2] — [1]IFF, Forschungszentrum Jülich, D-52425 Jülich — [2]Cornell University, Ithaca, New York 14853, USA

Since its discovery as a crucial co-catalyst in metallocene and post-metallocene olefin polymerizations methylaluminoxane (MAO) has retained commercial and academic status. In spite of continued interest the MAO structure remains until now ambiguously defined.

Here we present a combined SLS/DLS/SANS study on the structural properties of MAO in toluene solutions ($\phi/\phi^* \leq 0.6$). In dilute solution the main structure assayed is a linear polymer chain consisting of [-Al(CH_3)-O-] monomer units with a M_w of 20 kg/mol, $R_g \approx 46\AA$ and a negative second virial coefficient A_2. The latter fortifies the recognized state of play that toluene is a poor MAO solvent. With increasing concentration SANS data reveal the (reversible) formation of interchain branching due to a change from 3 to 4 in the coordination number of the Al-atoms in the polymer backbone [1].

Moreover, preliminary analysis of neutron spin echo (NSE) experiments reveals a dynamical stiffness of MAO chains. Zimm dynamics typical for polymer solutions in a good solvents are crucially retarded indicating a large internal rotational barrier of MAO chains.

[1] J. Stellbrink et al., *Macromolecules*, **40**, 4972, 2007.

CPP 29.7 Thu 11:15 C 130

Tomographic Techniques in Small-Angle X-Ray Scattering (SAXS) and Grazing-Incidence SAXS (GISAXS) — •Jan M. Feldkamp[1], Christian G. Schroer[1], Marion Kuhlmann[2], Stephan V. Roth[2], Andreas Timmann[2], Rainer Gehrke[2], Norbert Stribeck[3], and Armando Almendarez-Camarillo[3] — [1]Institute for Structural Physics, TU Dresden, D-01062 Dresden, Germany — [2]HASYLAB at DESY, Notkestr. 85, D-22607 Hamburg, Germany — [3]Institute of Technical and Molecular Chemistry, Hamburg University, Bundesstrasse 45, D-20146 Hamburg, Germany

Small-Angle X-Ray Scattering (SAXS) has become a standard technique for the investigation of nano-structured materials. The emerging technique of Grazing Incidence Small-Angle X-Ray Scattering (GISAXS) enables one to study the nano-structure at the surface of materials and in thin films. These measurements provide valuable information to scientists from various fields, including material science, chemistry, polymer science, and biology.

In many cases the structure of a specimen is not homogeneous on a macroscopic scale. For these kinds of samples, scanning tomography provides additional real-space information. Using SAXS-tomography, the distribution of the nano-structure can be studied at each location on a virtual section through the sample. GISAXS-tomography allows one to map the distribution of the nano-structure on surfaces and in thin films.

In this presentation, these tomographic techniques are used to determine the structure of inhomogeneous polymer samples.

CPP 29.8 Thu 11:30 C 130

SANS observation of the relaxation of a hyperbranched polymer in a linear matrix after a large step strain deformation — •Louisa Dahbi[1], Wim Pyckhout-Hintzen[1], Juergen Allgaier[1], Dieter Richter[1], Ekkehard Straube[2], Nikos Hadjichristidis[3], Hermis Iatrou[3], and Melissa Sharp[4] — [1]Forschungszentrum Juelich, IFF, D-52425 Jülich, Germany — [2]M-L University Halle, D-0 6122 Halle, Germany — [3]University of Athens, Polymer Group, Greece — [4]GKSS, IMR, D-21502 Geesthacht, Germany

The feasibility of well defined branched model polymer and the recent advances in the tube model theory gave rise to a better understanding of the dynamic and rheology of branched polymers. Our study aims to focus on the relaxation of a non-linearly stretched hyperbranched polymer blended with linear chains of different length, constituting the matrix, so as to study the effects of this latter on the time dependence of the relaxation process of the hyperbranched arms. The relaxation was investigated with quenched SANS experiments using our elongational stretching rheometer which decouples microscopic and laboratory time scales. Hyperbranched as well as linear polymers used for this study are constituted by polyisoprene. Both systems (short and long matrix) were submitted to identical relaxation times so as to quantify and conclude on the influence of the matrix length on the time dependence of the relaxation process of the hyperbranched arms. The relaxation of the short matrix taking place concurrently is expected to accelerate the relaxation of the hyperbranched itself. A link to a former work on linear polymer and well entangled H-shaped is presented.

CPP 29.9 Thu 11:45 C 130

Characterisation of structural changes during deformation and relaxation of semi-crystalline polymers by simultane-

ous online SAXS and WAXS measurements — •Konrad Schneider[1], Andreas Schöne[1], Andreas Timmann[2], and Manfred Stamm[1] — [1]Leibniz Institut für Polymerforschung Dresden e.V., Hohe Strasse 6, 01069 Dresden, Germany — [2]DESY, Hasylab, Notkestr. 85, 22607 Hamburg, Germany

Time resolved small and wide angle x-ray scattering using synchrotron radiation allows to follow up structural changes during deformation and relaxation of semi-crystalline polymers. On the example of polyolefins the changes of the structure in the crystalline and in the amorphous domains were followed during the three characteristic stages of the load-displacement curves: The elastic stage and the plastic range composed of the stage of the lowering load in the force-displacement-curve (yielding) and the strain hardening.

It is found that most rigorous changes are observed during yielding. There are found changes on a scale of seconds during relaxation, while the structural changes during relaxation in the other regions are much less pronounced.

CPP 29.10 Thu 12:00 C 130

Structure investigations of thermo-sensitive triblock copolymers — •Amit Kulkarni[1], Kordelia Troll[1], Charles Darko[1], Christine M. Papadakis[1], Weinan Wang[1], Peter Müller-Buschbaum[1], Achille M. Bivigou Koumba[2], and André Laschewsky[2] — [1]Physikdepartment E13, TU München — [2]Institute für Chemie, Universität Potsdam

Thermo-sensitive triblock copolymers consisting of a hydrophilic block, poly(N-isopropylacrylamide) (PNIPAM), and hydrophobic polystyrene end blocks, are expected to form physically cross-linked micellar gels in aqueous solution, which are swollen below the lower critical solution temperature (LCST) and collapsed above. They are of interest for a number of applications. We focus on the conformational change of the micellar shell as a function of temperature and the PNIPAM volume fraction. Three triblock copolymers with different PNIPAM volume fractions and three triblock copolymers having deuterated polystyrene blocks were studied by small angle X-ray scattering, small angle neutron scattering and dynamic light scattering with respect to the core-shell structure and swelling-deswelling of the shell. The non-deuterated triblock copolymers show the LCST at 31°C with micelles size of around 22 nm below collapse temperature and 17nm above.

CPP 29.11 Thu 12:15 C 130

The relation between craze structure and molecular weight in PS as revealed by μSAXS experiments — •Nikolaos E. Zafeiropoulos[1], Richard J. Davies[2], and Manfred Stamm[1] — [1]Leibniz Institut für Polymerforschung Dresden, Hohe strasse 6, 01069 Dresden — [2]European Synchrotron Radiation Facility, BP 220, F-38043 Grenoble Cedex, France

The phenomenon of crazing in polymers has received considerable attention in the past as it plays a pivotal role in determining the performance of polymers under load. One aspect of particular interest has been the interconnection between molecular structure, craze characteristics and macromechanical properties. It is generally accepted that the mean craze fibril diameter, the mean craze fibril spacing and the orientation of the craze fibril with respect to the tensile load direction control the craze stability. The fibril volume fraction is independent of molecular weight (MW) under test conditions at temperatures significantly below the glass transition temperature. In addition, little changes in crazing are expected for MWs above the critical molecular weight of entanglement. Three different grades of polystyrene (PS) with different molecular weights have been systematically investigated in situ with synchrotron radiation microfocus SAXS. The results suggest that there are different mechanisms operating in PS samples with low and very high molecular weights, compared to those of medium-high molecular weight. Previously it was thought that, above the critical molecular weight of entanglement, the effect of molecular weight on PS's mechanical behaviour at room temperature was negligible.

CPP 29.12 Thu 12:30 C 130

Structural levels of organization in spider silk as studied by time-resolved polarized Rheo-FTIR spectroscopy — •Periklis Papadopoulos, Jan Sölter, Immanuel Weidner, and Friedrich Kremer — Universität Leipzig, Germany

The employment of polarized FTIR spectroscopy in combination with mechanical measurements is unique in unraveling the effects of external fields on the different moieties of spider silk under both equilibrium and non-equilibrium conditions. This allows us to construct quantitative structural models for the major (dragline) and minor ampullate spider silk and explain the differences between their respective mechanical properties. Both silks are semi-crystalline with β-sheeted crystals interconnected by pre-strained amorphous chains. The frequency shift of several absorption bands, in combination with a simple quantum mechanical model, allows tracing the microscopic force on the crystals and its distribution[1]. Thus, the structural model delivers the experimentally observed stress-strain dependence for both major and minor ampullate silk[2]. The former has a significantly higher degree of pre-strain, explaining its higher modulus, the lower extensibility and the effect of supercontraction, whereas the latter exhibits some degree of strain-induced crystallization. The very high toughness in both cases is attributed to the breaking of hydrogen bonds in the crystals.

[1] Papadopoulos, P.; Sölter, J. and Kremer, F. *Eur. Phys. J. E: Soft Matter* (2007) *in press*

[2] Papadopoulos, P.; Sölter, J. and Kremer, F. *Biophys. J.* (2007) *submitted*

CPP 30: Polymerphysics II

Time: Thursday 14:00–17:00 Location: C 130

CPP 30.1 Thu 14:00 C 130

Study of rubber network structure by low field ^{1}H double-quantum NMR experiments — •Juan Lopez Valentin and Kay Saalwachter — Martin-Luther-Universität Halle-Wittenberg, Institut für Physik; Friedemann-Bach-Platz 6, D-06108 Halle (Germany)

Elastic properties of rubber are closely related with the network structure, and Solid-state nuclear magnetic resonance (NMR) is a successful tool to obtain this local information. Proton double-quantum (DQ) is one of the most recent and versatile approach towards the measurement of weak residual dipolar couplings (the NMR observable) associated with "NMR submolecules" (related to the Kuhn segments). It provides in the same experiment not only quantitative information on semi-local chain order (thus cross-link density) and its distribution, but also about chain dynamics [1].

Based on this methodology, natural rubber networks, which were vulcanized with different cure systems (sulphur and organic peroxide), were studied. Important variations in the quantity of non-coupled network defects (which are not elastically active), crosslink distribution as well as chain dynamics were found according to the different vulcanization reactions. They could partially explain the variation in the elastic properties of these samples. Note that we never observe any influence of Gaussian chain statistics on network chain dynamics. Cooperativity between polymer chains reduces and homogenise the conformational space that ultimately governs the chain entropy.

[1] K. Saalwachter. Prog. NMR Spectrosc., 2007, 51, 1-35.

CPP 30.2 Thu 14:15 C 130

Structure and Dynamics of silicone networks as investigated by ^{1}H low field double-quantum NMR — •Walter Chassé and Kay Saalwachter — Martin-Luther-Universität Halle-Wittenberg, Institut für Physik, Friedemann-Bach-Platz 6, D-06108 Halle, Germany

The existence of cross-links and other topological restrictions lead to non-isotropic fast segmental fluctuations, and therefore some residual dipolar couplings persist, which are directly related to the crosslink density. Based on this principle, we have used static ^{1}H double-quantum NMR spectroscopy to measure quantitatively these residual dipolar couplings and their distribution[1].

Usually the easiest method to study network structure (crosslink density) is the swelling experiment based on Flory-Rehner-Theory. In this view we have compared the molecular weight between cross-links MC obtained from DQ-NMR with results of as well performed swelling experiments for PDMS networks with different topologies. Independently of this, the crosslink density can also be taken from ^{1}H MAS experiments. With these results, we obtained information not only about the network structure of the rubber but also about the validity of the model used to analyze the DQ-NMR data, thermodynamics of swelling (polymer solvent interaction parameter χ), and the influence of network heterogeinities in that process. In conclusion we could show that DQ-NMR in combination with swelling experiments is a powerful method to characterize structure and dynamics of rubber.

[1] K. Saalwächter, Prog. in NMR Spectr., 2007, 51, 1-35.

CPP 30.3 Thu 14:30 C 130

Dynamics in polymer networks containing liquid crystal — •Rachid Hadji[1,2,3], Silke Rathgeber[1], Amina Négadi[2], and Ulrich Maschke[3] — [1]Max-Planck-Institute for Polymer Research, Polymer Physics, 55128 Mainz, Germany. — [2]Université Aboubakr Belkaïd, Laboratoire de Recherche sur les Macromolécules, 13000 Tlemcen, Algeria. — [3]Université des Sciences et Technologies de Lille, Laboratoire de Chimie Macromoléculaire, 59655 Villeneuve d'Ascq Cedex, France.

Polymer networks filled with liquid crystal are of interest due to their actuatoric properties but also due to their possible optical applications. Their anisotropic optical properties allow the switching from a transparent to an opaque state by alignment in an external electrical field. Changing the temperature through the disorder/order transition of the liquid crystal leads to a deswelling/swelling of the network which can be used for actuatoric applications. We studied the molecular dynamics of polymer networks containing different amounts of liquid crystal with dielectric spectroscopy (DS) and mechanical spectroscopy at the nematic-isotropic transition of the liquid crystal. We also followed the phase transitions of the systems by dynamic scanning calorimetry. The networks under investigation were poly(n-butyl acrylate) networks filled with the commercial liquid crystals 5CB and E7, respectively. We were able to follow the dynamical changes occuring in the polymeric matrix as well as in the liquid crystalline solvent at the nematic-isotropic transition. In addition we studied the effect of the degree of sterical hindrance by changing the crosslink density.

CPP 30.4 Thu 14:45 C 130

Topological aspects in random copolymer globules — •Daniel Bölinger, Hsiao-Ping Hsu, and Peter Virnau — Institute of Physics, Johannes Gutenberg-University, 55099 Mainz

Although globular homopolymers display an abundance of knots [1], little is known about the topology and the degree of entanglement in copolymer globules. To this end we investigated globular structures which were generated with numerical simulations of the HP model using the nPERMis algorithm [2]. In this talk we will highlight structural and topological differences between homopolymer and random copolymer globules and demonstrate that entanglements are greatly reduced in copolymer structures. These results also shed some light on the longstanding controversy why only few knots have been observed in experimentally determined protein structures.

[1] P. Virnau, Y. Kantor, and M. Kardar, J. Am. Chem. Soc 127, 15102 (2005).

[2] H.P. Hsu, V. Mehra, W. Nadler and P. Grasberger, J. Chem. Phys. 118, 441 (2003).

CPP 30.5 Thu 15:00 C 130

Effects of molecular shape and flexibility on the permitivity ratio of a model polymer network — •Henning Hörstermann and Reinhard Hentschke — Bergische Universität, Wuppertal, Germany

Sorption and diffusion of binary mixtures of small molecules in randomly crosslinked amorphous model polymer networks is studied via computer simulation. Three types of molecules identical in volume but different in shape and flexibility (compact, linear-stiff, and linear-flexible) are combined into binary mixtures (compact/linear-stiff) and (linear-stiff/linear-flexible). The relative effects of shape and flexibility on separation factor and diffusion coefficient inside random polymer networks are studied using a Molecular Dynamics/Gibbs-Ensemble Monte Carlo hybrid technique. In addition the effects of temperature, pressure, and network strand length are considered. We find that the compact molecules are preferentially absorbed into the network at all strand lengths and temperatures considered. Flexibility only leads to minor preferential sorption under most conditions. Diffusion coefficients of the competing species inside the network are found to agree within the error bars.

Additionally, the relation between connectivity ratio and network shrinkage is studied over a wide range of temperatures and pressures. The simulation results are compared to a mean-field Flory–Huggins lattice model.

CPP 30.6 Thu 15:15 C 130

On the statistics of Gaussian two and three-dimensional networks: Fluctuations of junctions and collapse driven by structure. — •Michael Lang[1,2], Sergey Panyukov[3], Michael Rubinstein[2], and Jens-Uwe Sommer[1] — [1]Leibniz-Institute for polymer Research, Hohe Str. 6, 01069 Dresden, Germany — [2]Department of Chemistry, University of North Carolina, 27599 Chapel Hill, N.C., USA — [3]P. N. Lebedev Physics Institute, Russian Academy of Sciences, Moscow, Russian Federation

We investigate ideal Gaussian networks both analytically and with computer simulations using the Bond Fluctuation model with and without excluded volume interactions. The focus of this study is on fluctuations and the collapse of networks with different connectivity and dimensionality.

We show that the size of a perfect square 2D network made from n^2 Gaussian chains with N monomers each is $R_g \sim N_1/2 \cdot log(n)$. Thus, fluctuations in two-dimensional networks diverge logarithmically with the size of these films while fluctuations of three-dimensional networks with cubic structure is $\sim N^{1/2}$ and do not increase with their size. We study the cross-over between two and three-dimensional networks by following the dependence of junction fluctuations on the thickness of films.

The results of model systems are compared with more realistic networks in order to understand the effect of disorder on the properties of the network and fluctuations of network junctions.

break

CPP 30.7 Thu 15:45 C 130

Influence of Electric Fields on the Phase Behavior of Concentrated Block Copolymer Solutions — •Heiko G. Schoberth[1], Kristin Schmidt[2], and Alexander Böker[1] — [1]Physikalische Chemie II, Universität Bayreuth, 95440 Bayreuth, Germany — [2]Materials Research Laboratory, University of California, Santa Barbara, USA

We investigate the influence of the electric field on the phase behavior of diblock copolymer morphologies in concentrated solutions using Synchrotron SAXS. We observe a decrease of the order-disorder-transition temperature and phase separation with increasing electric field strength. This shift is found in T_{ODT} even at moderate field strengths and follows a linear dependence.

Furthermore we can also induce an order-order-transition. We synthesized different block copolymers with compositions close to the predicted phase boundaries. Due to the lower free energy of aligned anisotropic microdomain structures parallel to the electric field, we can induce a transition from the metastable hexagonally perforated lamellae to the lamellae phase under strong electric fields. In addition for an isotropic cubic gyroid phase, which cannot be aligned, a transition to aligned cylinders is found.

CPP 30.8 Thu 16:00 C 130

Multiscale Simulations of Polybutadiene Solutions — •Thomas Strauch, Peter Virnau, and Wolfgang Paul — Johannes Gutenberg-Universität Mainz

Polymer processing relies in general on detailed knowledge of the polymer solvent phase diagram. Computer simulations have become a powerful tool to investigate complex systems and particularly their phase behavior. However, it is often impossible to treat the polymer solvent mixture in complete chemical detail within simulations. To avoid this problem, one can coarsen the fully atomistic model. We present a new, systematic coarse-graining procedure applied to the Polybutadiene(1,4)-Butane solution. For the polymeric component, the procedure uses an equation of state known from atomistic simulations or experiment to validate the choice of the coarse grained potentials. Furthermore structural quantities are compared with results from chemically detailed simulations or experiments. The solvent's nonbonded potential can be determined by mapping the critical point of the model system onto the experimental critical point of the substance. To investigate the phase diagram of the polymer solution, a potential for the interaction between the two components is chosen by using Lorentz-Berthelot mixing rules. In addition to the systematic coarse-graining procedure, results for the phase behavior of the Polybutadiene(1,4)-Butane solution obtained by grand canonical

Monte Carlo simulations will be shown.

CPP 30.9 Thu 16:15 C 130

Calculation of the segmental order parameter for a polymer chain in good solvent — •Zoryana Usatenko[1,2] and Jens-Uwe Sommer[1] — [1]Leibniz Institute for Polymer Research Dresden e.V.,01069 Dresden,Germany — [2]Institute for Condensed Matter Physics, NAS Ukraine,79011 Lviv,Ukraine

We have calculated the segmental tensor order parameter of flexible polymer chains in weak good solvent. This quantity is directly observable in multi-quantum NMR experiments. We have used the Edwards model for polymer chains and have applied direct perturbation expansion with respect to excluded volume interactions in one loop order. The obtained results indicate that the distribution of the tensor order parameter is not homogeneous along the chain as expected for ideal Gaussian statistics. Overall segmental order is lower as compared to Gaussian chains and decays towards the chain ends [1]. These results are in agreement with computer simulation studies on single chains with fixed ends in good solvent. The overall reduction of the tensor order parameter has been also observed in NMR experiments on swollen polymer networks [2].

[1] Z.Usatenko, J.-U.Sommer, Macromolecular theory and simulations, 2007 (in press).

[2] K. Saalwächter and J.-U. Sommer, Macromol.Rapid Commun.28, 1455 (2007).

CPP 30.10 Thu 16:30 C 130

From simple liquid to polymer dynamics: a field cycling NMR study on linear polymer melts of different molecular weights — •Axel Herrmann, Sobiroh Kariyo, Catalin Gainaru, Harald Schick, Julia Hintermeyer, Alexander Brodin, Vladimir N. Novikov, and Ernst A. Rössler — Universität Bayreuth, Experimentalphysik II, 95440 Bayreuth

We utilize fast field cycling NMR relaxometry to investigate the crossover from glassy dynamics through Rouse to reptation behavior in a series of polybutadienes (PB) and polydimethylsiloxanes (PDMS) with molecular weights M ranging from the low M (simple liquid dynamics) to the high M limit (reptation dynamics). The dispersion data $T_1(\omega)$ are transformed into the susceptibility $\chi''(\omega) \propto \omega/T_1$ and master curves are constructed for each M. By extracting the polymer spectra through subtracting the glass spectrum from the total spectra and comparing them to Rouse theory, we are able to determine the Rouse unit M_R and entanglement weight M_e. These characteristic molecular weights also show up in the M dependence of the dynamic order parameter S, a measure of the relative correlation loss due to polymer dynamics, and the glass transition temperature T_g. Thus, the glass process is specifically modified by the polymer dynamics. We find similar results for the samples of PDMS. For partially deuterated PB our approach yields the common polymer dynamics although the values of S are different. Hence in order to provide a coherent interpretation of NMR dispersion data of polymers, the contribution of the glass dynamics has to be taken explicitly into account.

CPP 30.11 Thu 16:45 C 130

Dynamics of n-alkyl-cyanobiphenyl and cyano-n-alkylbenzoate molecules in a surface layer adsorbed onto aerosil — Stefan Frunza[1], Ligia Frunza[1], and •Andreas Schönhals[2] — [1]National Institute of Materials Physics, R-077125 Magurele, Romania — [2]Federal Institute of Materials Research and Testing, D-12205 Berlin, Germany

Composites prepared from aerosil and n-alkyl-cyanobiphenyl (nCB, n=2 - 8) or cyano-n-alkylbenzoate (CPnB; n= 4 - 7) molecules are investigated by dielectric spectroscopy (10 mHz to 1 GHz) in a large temperature range. The selected high silica density allows the observation of the behavior of a thin layer (with nearly a one or two-monolayer structure) adsorbed on the silica particles. For the composites one relaxation process is observed at frequencies much lower than that of the processes found for the corresponding bulk. It is assigned to the dynamics of molecules in a surface layer. The temperature dependence of its relaxation rates obeys the Vogel/Fulcher/Tammann law, characteristic for glassy dynamics liquids. For both systems they vary continuously with the length of alkyl chain. This is discussed in detail in the frame work of quasi two-dimensional character of glassy dynamics of molecules adsorbed on a surface.

CPP 31: Thin Films

Time: Thursday 9:30–11:00 Location: C 264

CPP 31.1 Thu 9:30 C 264

Cylindrical phase of diblock copolymers in thin films — •Rosa Marianne Breuer and Barbara Drossel — Institut für Festkörperphysik, Hochschulstr. 6, 64289 Darmstadt

Diblock copolymers are polymers in which two chains of different monomers are covalently bound to one another. Because of their different chemical nature the blocks have a tendency to phase separate, but a macroscopic phase separation is prohibited by the chemical bond connecting the different blocks. Therefore such molecules have a tendency to separate on a microscopic scale forming a variety of ordered structures, called microphases. We investigate the microphases of diblock copolymers confined in a thin film with walls attracting one of the monomer types. We focus on the possible structures of copolymers that form cylindrical phases in the bulk. We employ both self-consistent field theory and strong segregation theory to obtain the concentration profile minimizing the free energy of the system and to compare the free energy of possible morphologies. We present a phase diagram showing the possible microphases for a diblock copolymer with fixed volume fraction and fixed segregation parameter in dependence of the film thickness and the affinity of the walls. We study the effects of numerical inaccuracies on the appearance of different morphologies and their free energies.

CPP 31.2 Thu 9:45 C 264

3-Dimensional Control over lamella orientation in thick block copolymer films — •Violetta Olszowka, Larisa Tsarkova, and Alexander Böker — Physikalische Chemie II, Universität Bayreuth, Germany

We present a novel route to produce thick films with long-ranged 3D ordered upstanding lamellae and a perfectly ordered nano-striped surface pattern. Thick lamella polystyrene-b-*poly*(2-vinyl pyridine) diblock copolymer films are exposed simultaneously to a selective solvent vapor and to an in-plane electric field. The orientation of the lamellae was studied by combined scanning force microscopy, grazing incidence small angle x-ray scattering and transmission electron microscopy measurements. The lamellae orientation perpendicular to the film plane upon long-term selective solvent annealing was detected in a narrow window of the film thickness (about 17-22 lamella distances). In thicker and thinner films, lamellae were perfectly aligned parallel to the film plane due to the surface fields effects. Theoretical model is proposed to account for the thickness- and annealing time dependent reorientation of lamella domains. The observed phenomena presumably initiates in the interior of the film when the concentration fluctuations due to selective swelling overcome the suppression by the surface fields.

CPP 31.3 Thu 10:00 C 264

Phase behaviour of ultra-thin polymer films grafted on Micro-Cantilever-Sensors (MCS) — •Sebastian Lenz[1], Sebastian K. Nett[1,2], Mine Memesa[1], Rüdiger Berger[1], Jochen S. Gutmann[1,2], Andreas Timmann[3], and Stephan V. Roth[3] — [1]Max-Planck Institute for Polymer Research, Ackermannweg 10, D-55128 Mainz (Germany) — [2]Institute for Physical Chemistry, Johannes Gutenberg University, Jakob-Welder-Weg 10, D-55099 Mainz (Germany) — [3]HASYLAB at DESY, Notkestr. 85, D-22603 Hamburg (Germany)

Phase behaviour of polymer films plays an important role to tailor surface properties of materials. Using a polymer blend mixture with a lower miscibility gap, we anticipate a phase transition from a one phase towards a two phase system upon changing temperature. As a suitable system a polymer blend composed of polystyrene (PS) and poly-vinyl-methyl-ether (PVME) [1] is chosen.

During phase transition, we want to correlate structural changes in the grafted polymer layer to surface stress induced curvature changes of the MCS over time. To study structural features in the nanometre scale and due to the small sample size of a polymer-coated cantilever we have to use recently developed characterization techniques. A combination of micro-focused Grazing Incident Small Angle Scattering (GISAXS) [2] and micro-focused X-Ray reflectivity was chosen to obtain structural information of the systems.

[1] Tanaka et al., Macromolecules 28, (1995) 934-938.
[2] S.V. Roth et al., Rrv. Sci. Instr. 77, (2006) 085106.

CPP 31.4 Thu 10:15 C 264

Solvent content in thin spin-coated polymer films — •Jan Perlich[1], Volker Körstgens[1], Ezzeldin Metwalli[1], Leander Schulz[1], Robert Georgii[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department LS E13, James-Franck-Str. 1, 85748 Garching (Germany) — [2]Forschungsneutronenquelle Heinz Maier-Leibnitz, TU München, Lichtenbergstr. 1, 85747 Garching (Germany)

The detection of remaining solvent in thin polymer films is important due to its effect on chain mobility and film homogeneity. It is essential for swelling experiments to define the initial state with respect to the amount of solvent included inside the film directly after preparation. Moreover, it gives an estimate on possible aging effects caused by the reduction of the solvent content. The investigation focuses on a well controlled model system, which consists of protonated polystyrene (PS) with different molecular weights, spin-coated out of protonated or deuterated solvent onto silicon substrates. Directly after spin-coating the thin films were investigated with neutron reflectometry at the MIRA instrument of the research neutron source FRM-II. A narrow qz range around the critical edge was probed with high resolution. Due to the high sensitivity of the position of the critical edge on the ratio of protonated PS and deuterated solvent, the exact position of the critical edge enables to determine the solvent content. Two different key parameters are addressed: the molecular weight of PS and the film thickness. In addition, annealing of the as-prepared films is discussed. We acknowledge financial support by project MU 1487/4-2.

CPP 31.5 Thu 10:30 C 264

Temperature dependent swelling behavior of PNIPAM based block copolymer films — •Weinan Wang[1], Peter Müller-Buschbaum[1], Kordelia Troll[1], Amit Kulkarni[1], Christine Papadakis[1], Achille M. Bivigou Koumba[2], and Andre Laschewsky[2] — [1]TU München, Physik - Department E13, James-Franck-Str. 1, D-85747 Garching — [2]Potsdam Universität, Inst. Chemie, Karl-Liebknecht-Str. 24-25, D-14476 Potsdam-Golm

PNIPAM is one of the prominent stimuli-sensitive hydrogels because it has a relatively low collapse transition temperature at 32°C. To introduce an internal ordering and increase the mechanical stability in the films, the homopolymer is typically replaced by PNIPAM based block copolymers. We focus on how the internal structures depend on the temperature in the swollen state and how the transition temperature depends on the initial film thickness. The films are freshly made by spin coating. For the investigation of the morphologies of the films at different temperatures in the swollen state, especially the changes of internal structures, grazing incidence small angle X-ray scattering (GISAXS) and transmission X-ray scattering are performed. To detect the possible shift of the transition temperature with film thickness, in-situ ellipsometry is applied. It is observed that both the size and the ordering of internal structures are changed at the transition temperature. The transition temperatures of the films depend strongly on the initial film thickness and are significantly different from those of the bulk materials. In addition, atomic force microscopy (AFM) and X-ray reflectivity are also used for characterization.

CPP 31.6 Thu 10:45 C 264

Glass transition and miscibility of polymer blends in ultrathin films — •Dongshan Zhou[1,2], Heiko Huth[1], Alexander Minakov[1], and Christoph Schick[1] — [1]Inst. Phys., Univ. Rostock, Germany — [2]School. Chem. & Chemical Eng., Nanjing Univ., China

Glass transition and polymer blend miscibility in ultra-thin films is critical for their use as materials. Calorimetric studies can provide important information on finite size and interfacial effects on the phase separation. Here we use the recently developed differential alternating current chip calorimeter to study glass transition and miscibility of blend composed of equal mass ratio of polystyrene and poly(2,6-dimethyl-p-phenylene oxide)confined in thin film (5 ˜ 320 nm). The step of heat capacity during the glass transition is well indentified even for the thinest film of c.a. 4.5 nm, showing the performance of the calorimeter to measure the change of heat capacity in the level of picoJ/K[H. Huth, J. Polym. Sci. B Polym. Phys. 2006, 44, 2996]. Despite the remarkable change of thickness (from below 1/2 Rg to 13.5 Rg), both the glass transition temperature and the temperature range of the transition keep unchanged in the frequency range available. The independence of the Tg with thickness in this work is in consistence with calorimetric measurements in thin films of single component polymers, but contrary to previous work on the same polymer blends based on ellipsometry [J. H. Kim, Macromolecules, 2002, 35,311]. In the system under investigation we see only one glass transition, arguments on whether the miscibility is changed or not due to the confinement will be available after investigation on a wider range of compositions.

CPP 32: Colloid Dynamics

Time: Thursday 11:15–12:30 Location: C 264

CPP 32.1 Thu 11:15 C 264

Directed motion of colloidal particles by external magnetic fields — •Christian Kreidler, Larysa Baraban, Ina Seuffert, Paul Leiderer, and Artur Erbe — Universität Konstanz. FB Physik, Germany

Directed motion of microscopic particles can be used in many biological systems to transport molecules in a controlled way. Existing techniques, e.g. laser tweezers, work well under certain conditions. Here we demonstrate a concept of micro engines, which is based on the usage of asymmetrically catalytic colloidal particles. A chemical reaction is used to generate movement of the magnetic particles in suspension. Specially designed magnetic properties of colloids help to achieve their directed motion on the long time scale. The strength of the external magnetic field influences the velocity of the particles. Increasing its amplitude we can change the direction of the motion from antiparallel to parallel to the magnetic field. In principle, the technique can work even without direct optical access to the system. We present the time dependence of the mean square displacement for these particles as a proof of our concept. Further experiments concentrate on binding biological material to the moving particles in order to demonstrate the ability of the particles to serve as "transporters" for molecules.

CPP 32.2 Thu 11:30 C 264

Persistent correlations of constrained colloidal motion — •Jonas A. Kraus[1], Thomas Franosch[1], Sylvia Jeney[2], Branimir Lukić[2], and László Forró[2] — [1]Arnold Sommerfeld Center for Theoretical Physics and Center for NanoScience (CeNS), Department of Physics, Ludwig-Maximilians-Universität München, Theresienstrasse 37, D-80333 München, Germany — [2]Institut de Physique de la Matierère Complexe, Ecole Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland

The dynamic behavior of a single colloidal particle in water confined by an optical trap and a plane surface is investigated at time scales where the inertia of the surrounding fluid plays a significant role. First, we quantify the influence of the confinement created by the harmonic potential of the optical trap on the particle's velocity autocorrelation (VACF). In particular, we observe a regime of anti-correlation which cannot be explained by the harmonic restoring force and the particle's inertia alone. For intermediates times unconstrained bulk behavior is recovered and we give first direct experimental evidence for the celebrated power-law long-time tails.

Second, the particle is brought close to a surface and we observe how the subtle interplay of surface confinement and hydrodynamic backflow changes the decay of the particle's VACF from a slow $t^{-3/2}$ to a much faster power-law $t^{-5/2}$. We compare our data to a recently developed theory by Felderhof [1] which we have extended by a harmonic trapping force.

[1] B.U. Felderhof, J. Phys. Chem. B 109, 21406 (2005).

CPP 32.3 Thu 11:45 C 264

Critical dynamics of ballistic and Brownian particles in a heterogeneous environment — •Felix Höfling, Tobias Munk, Erwin Frey, and Thomas Franosch — Arnold Sommerfeld Center for Theoretical Physics (ASC) and Center for NanoScience (CeNS), Department of Physics, Ludwig-Maximilians-Universität München, Theresienstraße 37, 80333 München

Transport of tagged ions, macromolecules, or nanoparticles in heterogeneous environments is strongly hindered by the presence of a variety of differently sized components. Three major transport phenomena are observed: normal diffusion, immobilization or localization, and anomalous transport. It will be shown that all aspects may be unified into the concept of transport in a disordered, heterogeneous medium with a percolation transition [1].

We have investigated Lorentz models with ballistic and Brownian tracer particles by means of large-scale computer simulations. It is demonstrated that in the immediate vicinity of the localization transition, universality holds at large time scales. The scaling function describing the crossover from anomalous transport to diffusive motion is found to vary extremely slowly and spans at least 5 decades in time. To extract the scaling function, one has to allow for the universal corrections to scaling. Our findings suggest that apparent power laws with varying exponents generically occur and dominate experimentally accessible time windows as soon as the heterogeneities cover a decade in length scale.

[1] Höfling, Franosch & Frey, Phys. Rev. Lett. 96, 165901 (2006)

CPP 32.4 Thu 12:00 C 264

Dumbbell diffusion in a spatially periodic potential — •Jochen Bammert and Walter Zimmermann — Theoretische Physik I, Universität Bayreuth, D-95440 Bayreuth

We present a numerical investigation of the Brownian motion and diffusion of a dumbbell in a two-dimensional periodic potential. Its dynamics is described by a Langevin model including the hydrodynamic interaction. With increasing values of the amplitude of the potential we find along the modulated spatial directions a reduction of the diffusion and a reduction of hydrodynamic interaction effects on the dumbbell mobility. For modulation amplitudes in the range of the thermal energy the dumbbell diffusion exhibits a pronounced local maximum at a wavelength of about 3/2 of the dumbbell extension. This is especially emphasized for stiff springs connecting the two beads.

CPP 32.5 Thu 12:15 C 264

The dynamics of several small rotating dumbbells in a fluid — •Steffen Schreiber and Walter Zimmermann — Lehrstuhl Theoretische Physik I, Universität Bayreuth, 95440 Bayreuth, Germany

Dumbbells in a fluid carrying a magnetic moment may be set in rotation by an external rotating magnetic field. The hydrodynamic interaction between two or three rotating dumbbells causes a motion of the centers of mass of the dumbbells, which follow circular trajectories. The period of the circular motion of the centers of mass depends on the rotation frequency of the external magnetic flield. Transitions of three and more hydrodynamically interacting dumbbells to more complex dynamics are explored.

CPP 33: Molecular Structure

Time: Thursday 15:00–16:45 Location: C 230

CPP 33.1 Thu 15:00 C 230

The structure of liquids studied by soft x-ray emission (XES) and absorption (XAS) spectroscopy — •M. Blum[1], O. Fuchs[1], M. Weigand[1], F. Maier[1], E. Umbach[1,2], L. Weinhardt[3], M. Bär[3], C. Heske[3], M. Zharnikov[4], Y. Zubavichus[4], M. Grunze[4], and J.D. Denlinger[5] — [1]Universität Würzburg, Experimentelle Physik — [2]Forschungszentrum Karlsruhe — [3]University of Nevada, Las Vegas — [4]Angew. Physikal. Chemie, Uni Heidelberg — [5]ALS, Berkeley

Recently, soft x-ray XES and XAS techniques have been employed to probe the electronic structure of liquids. Such experiments represent a technically challenging task, since they require a third-generation synchrotron source and a liquid cell with a thin window separating the liquid from ultra-high vacuum. XES is particularly elaborate in this respect, since it requires a high-efficiency grating spectrometer. With our flow-through liquid cell and a novel high-transmission, high-resolution x-ray spectrometer we have investigated the electronic structure of various liquids including H_2O, D_2O, NaOH, NaOD, acetic acid, amino acids, and various other aqueous solutions under well-defined and reproducible conditions. We will present 2-dimensional resonant inelastic x-ray scattering (RIXS) maps of these liquids, which give unprecedentedly detailed information on the electronic structure. The XES spectra of water show effects that can be correlated with molecular dynamics on the time scale of the core hole lifetime. Moreover, the maps of the aqueous solutions reveal subtle changes in the electronic structure which can be attributed to the influence of the hydration shell and the pH-value.

CPP 33.2 Thu 15:15 C 230

Dipole switching in extended molecular systems: Explicitly time-dependent configuration interaction simulations — •Tillmann Klamroth and Pascal Krause — Institut für Chemie, Theoretische Chemie, Universität Potsdam

We perform laser-driven charge transfer simulations for Li-$(\mathrm{Ph})_n$-CN ($n = 1, 2, 3$) using the TD-CIS (Time-Dependent Configuration Interaction Singles)[1] approach. These molecules serve as systematically extendable model systems. The selectivity, and thus controllability, of an ultra-short laser-induced electronic excitation as a function of the molecular size is investigated. For example, such control may be needed if a small electronic molecular switch is embedded in a larger molecular device.

Using the TD-CIS method within the fixed nuclei approximation, ultra-short π-pulses are employed in order to induce a charge transfer transition. We show that for certain pulse widths the selectivity is lost mainly due to multi-photon transitions and dynamic polarizations of the molecules. The latter processes depends systematically on the molecular size, i.e. it gets more important for larger molecules.

[1] T. Klamroth, Phys. Rev. B 68, 245421 (2003); P. Krause, T. Klamroth, P. Saalfrank, J. Chem. Phys. 123, 074105 (2005); T. Klamroth, J. Chem. Phys.124, 144310 (2006).

CPP 33.3 Thu 15:30 C 230

"Phase"-Transitions in Amorphous Water — •Katrin Winkel[1], Michael S. Elsaesser[2], Erwin Mayer[1], and Thomas Loerting[1,2] — [1]Institute of General, Inorganic and Theoretical Chemistry, University of Innsbruck — [2]Institute of Physical Chemistry, University of Innsbruck

An understanding of the anomalies of water is closely linked to an understanding of the phase diagram of the metastable non-crystalline states of ice. Three distinct structural states of amorphous water are known, they are called low- (LDA), high- (HDA) and very high density amorphous ice (VHDA). In our present work decompression of VHDA from 1.1 GPa to 0.02 GPa at 140 K is studied by means of dilatometry and powder X-ray diffraction of quench-recovered states. It is shown that the three amorphous states of ice are reversibly connected to each other. However, while the downstroke VHDA–>e-HDA transition is apparently continuous, the e-HDA–>LDA transition takes place quasi-discontinuously. That is, two amorphous-amorphous transitions of a distinct nature are observed for the first time in a one-component system - a first-order like transition (e-HDA–>LDA) and a transition which is not first-order like but possibly of higher-order (VHDA–>e-HDA). VHDA and e-HDA are established as the most stable and limiting states in the course of the transition. We interpret our results as evidence disfavouring the hypothesis of multiple first-order liquid-liquid transitions (and the option of a third critical point), but favouring a single first-order liquid-liquid transition (and the option of a second critical point).

CPP 33.4 Thu 15:45 C 230

Effect of compression rate on re-crystallization of hexagonal ice — •Marion Bauer[1], Erwin Mayer[1], and Thomas Loerting[2] — [1]Institute of General, Inorganic and Theoretical Chemistry, University of Innsbruck — [2]Institute of Physical Chemistry, University of Innsbruck

We studied the re-crystallization kinetics of ice upon compression under isothermal conditions (170 - 230 K) and characterized the recovered phases by powder X-ray diffraction at 80 K. A competition between crystallization to the thermodynamically stable and a metastable phase was found. The Ice Ih –> Ice II and the Ice Ih –> Ice III transitions are the two competing parallel reactions in the pressure range 0.2 - 0.4 GPa. Stable Ice II is formed at compression rates up to 0.01 GPa/min, predominantly metastable Ice III is formed at compression-rates exceeding 0.1 GPa/min and mixtures of Ice II and Ice III are formed at compression-rates in-between. That is, Ice Ih has two energetically similar ways of adapting the hydrogen bonded network as a reaction to the application of external pressure. Similarly, high density amorphous ice (HDA) shows two parallel ways of crystallization upon heating under isobaric conditions [1]. For both the compression-rate dependent case observed here and the heating-rate dependent case observed earlier [1], the stable ice polymorph shows a slower, albeit earlier growth compared to the metastable polymorph.

[1] Salzmann, Mayer, Hallbrucker, PCCP 6, 5156-5165 (2004).

CPP 33.5 Thu 16:00 C 230

Mixed Quantum-Classical Simulations of Optical Spectra: Pheophorbide-a Butanediamine Dendrimers in Ethanol — •Hui Zhu, Volkhard May, Steffen Hackbarth, and Beate Röder — Institut für physik, Humboldt-Universität zu Berlin, Newtonstraße 15, D-12489 Berlin, Germany

Linear absorbance and time-resolved luminescence spectra are calculated in combining an improved exciton model with classical path approximation npT-ensemble MD simulations [1,2]. The exciton model includes an excitonic coupling based on ab initio electronic structure calculations, single pheophorbide-a excitation energy fluctuations due to solvent dynamics and structure fluctuations of the whole dendrimeric complex, and a separate account for intra chromophore vibrations. All computed spectra are compared with measured data and reproduce the observed trends when increasing the number of included pheophorbide-a molecules from 4 to 32.

[1] H. Zhu, V. May, B. Röder, M. E. Madjet, and Th. Renger, Chem. Phys. Lett. 444 , 118(2007).

[2] H. Zhu, V. May, B. Röder, and Th. Renger, J. Chem. Phys. (submitted).

CPP 33.6 Thu 16:15 C 230

Exact Born-Oppenheimer decomposition of the many-body wavefunction for the complete system of electrons and nuclei — •ALI ABEDI[1], NEEPA T.MAITRA[2], and E.K.U GROSS[1] — [1]Institut fuer Theoretische Physik, Freie Universitaet Berlin, Arnimallee 14, D-14195 Berlin, Germany — [2]Department of Physics and Astronomy, Hunter College of the City University of New York, USA.

We propose a new set of equations to treat non-adiabatic couplings between electrons and nuclei. The key idea behind the equations is to rewrite the many-body wave-function as a Born-Oppenheimer-type product of the nuclear and electronic wave-function. From the variational principle, we deduce formally exact equations for them. The electronic back-reaction term in the nuclear equation is rigorously contained in a time-dependent vector potential. We illustrate the formalism by performing calculations on one-dimensional diatomic molecule for which the many-body Schr\"odinger equation can be solved numerically.

CPP 33.7 Thu 16:30 C 230

Exact and approximate forces in the diffusion Monte Carlo method — •A. Badinski and R. J. Needs — Theory of Condensed Matter Group, Cavendish Laboratory, J. J. Thomson Avenue, Cambridge CB3 0HE, United Kingdom

The problem of calculating accurate inter-atomic forces within the diffusion Monte Carlo (DMC) method has been a long-standing issue[1-3]. The DMC method is highly successful for calculating ground-state total energies of many-electron systems, but there is still a lack of an accurate and efficient way of calculating forces. Therefore, DMC calculations are usually performed using geometries obtained from either density-functional theory or conventional quantum chemistry methods, or from experiment. In this talk, we present exact expressions for DMC forces and give a practical scheme of estimating them[4]. Equilibrium geometries are derived from DMC forces and compared with those obtained from DMC potential energy curves. Results for four small molecules show that the equilibrium bond lengths obtained from the force and energy calculations are in very good agreement.

[1] C. Filippi, C. J. Umrigar, Phys. Rev. B **61**, 16291 (2000)
[2] R. Assaraf, M. Caffarel, J. Chem. Phys. **119**, 10536 (2003)
[3] A. Badinski, R. J. Needs, Phys. Rev. E **76**, 036707 (2007)
[4] A. Badinski, R. J. Needs, Phys. Rev. B (accepted for publication)

CPP 34: POSTERS Polymerphysics

Time: Thursday 17:00–19:30 Location: Poster A

CPP 34.1 Thu 17:00 Poster A

About the Generalized Cauchy Relation in Non-Equilibrium Amorphous Materials — •Martine Philipp[1], Christelle Vergnat[1], Ulrich Müller[1], Ravi Bactavatchalou[1], Wulff Possart[2], Roland Sanctuary[1], Jörg Baller[1], Bartosz Zielinski[1], Patrick Alnot[3], and Jan Krüger[1] — [1]LPM, Université du Luxembourg, L-1115 Luxembourg — [2]Universität des Saarlandes, Saarbrücken, Germany — [3]Université Nancy, France

From solid state physics it is known that Cauchy relations (CR) increase the symmetry of the elastic tensor compared to the actual point symmetry. These CR hold true only under severe conditions concerning local symmetry and harmonicity of the elastic interaction potential. Since amorphous materials show no translational invariance the existence of CRs is not expected for these materials. Nevertheless, the authors have found for amorphous solids and high frequency clamped liquids a generalized CR (gCR) under the form of a linear transformation c11=3c44+A, with A being a constant. Once A is known, one of the two elastic constants can be predicted by knowing the other. This surprising result means that for amorphous materials the independency of the two elastic constants is strongly reduced. In the current presentation we discuss to which extent thermodynamic non-equilibrium violates the gCR. For that purpose the interdependency of c11 and c44 of reactive polymers is studied in the course of the curing process by Brillouin spectroscopy. Special attention is paid to accompanying transition phenomena like gelation and chemically induced freezing. An attempt is made to interpret the parameter A.

CPP 34.2 Thu 17:00 Poster A

cellular polyethylene-naphthalate piezo- and ferroelectrets: foaming in supercritical carbon dioxide, structure improvement through inflation and stretching — •PENG FANG[1], WERNER WIRGES[1], REIMUND GERHARD[1], and LARISSA ZIRKEL[2] — [1]Applied Condensed-Matter Physics, Institute of Physics, University of Potsdam, Am Neuen Palais 10, 14469 Potsdam, Germany — [2]Institute of Polymer Materials, Friedrich-Alexander University Erlangen-Nürnberg, Martensstrasse 7, 91058 Erlangen, Germany

Cellular polymer films can be used as ferroelectrets in many transducer applications. Here, we propose a preparation process for cellular polyethylene-naphthalate (PEN) films with the following steps: (1) Foaming by means of supercritical carbon dioxide (CO2), (2) controlled inflation through gas diffusion and expansion, and (3) biaxial stretching. We demonstrate and describe the cellular structure that is formed under suitable processing conditions. For the foaming process, a PEN film is saturated with supercritical CO2 at room temperature for a few hours, at a pressure as high as 100 bar, where the temperature is very critical for controlling the sample density. Additional inflation can improve the cellular geometry. Stretching may be employed in order to achieve a cellular structure with lens-like voids. Piezoelectric coefficients of up to 140 pC/N demonstrate the suitability of such cellular PEN films for transducer applications. However, high electromechanical responses are found only on samples within the proper density range and with optimal cellular structures. Their piezoelectricity is partially stable at elevated temperatures as high as 100°C.

CPP 34.3 Thu 17:00 Poster A

Röntgenabsorptionsmessungen an freien Aminosäure-Nanopartikeln — •René Lewinski, Christina Graf, Burkhard Langer, Bernhard Wassermann, Harald Bresch, Roman Flesch und Eckart Rühl — Institut für Chemie und Biochemie, Freie Universität Berlin, Takustr. 3, 14195 Berlin

Die Immobilisation von Aminosäuren auf Nanopartikeln ist ein Modell für die Wechselwirkung von Biomolekülen mit Oberflächen. Zum Verständnis der Bindungsverhältnisse in solchen Systemen wurden Nanopartikel aus reinen Aminosäuren sowie nur an der Oberfläche mit Aminosäuren funktionalisierte Nanopartikel in die Gasphase gebracht und mit Innerschalenanregung studiert. Diese wurden in einem Nanopartikelstrahl erzeugt und anschließend mittels eines aerodynamischen Linsensystems ins Hochvakuum überführt. So ist es möglich, auch geringe Substanzmengen elementspezifisch zu charakterisieren, wobei Strahlenschäden sowie die Wechselwirkung mit einem anderen Substrat ausgeschlossen werden. Zunächst erfolgte eine Untersuchung der elektronischen Struktur der reinen Aminosäuren Cystein und Methionin. Dabei wurde auch studiert, wie sich der pH-Wert bei der Partikelbildung auf die elektronische Struktur von Nanopartikeln aus aggregierten Aminosäuren auswirkt. Schließlich wurden Silicananopartikel charakterisiert, deren Oberfläche eine Submonolage Methionin gebunden ist. Die Resultate zeigen, dass die genutzte Methode zur Charakterisierung der elektronischen Struktur von kleinen Mengen an empfindlichen Biomolekülen auf Nanopartikeln gut geeignet ist.

CPP 34.4 Thu 17:00 Poster A

Structure formation upon sputtering of iron in diblock copolymer film with and without maghemite nanoparticles - an in-situ GISAXS study — •Mottakin M. Abul Kashem[1], Gunar Kaune[1], Alexander Diethert[1], Weinan Wang[1], Kai Schlage[2], Sebastian Couet[2], Ralf Röhlsberger[2], Stephan V. Roth[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department LS E13, James-Franck-Str. 1, 85747 Garching, (Germany) — [2]HASYLAB at DESY, Notkestr. 85, 22603 Hamburg (Germany)

Sputtering technique can be used to incorporate metal particle fillers into a self-assembled block copolymer film to get a nanocomposite. We have investigated the structures formed during sputtering of iron on the diblock copolymer films with and without iron oxide nanoparticles. We used cylindrical structure forming diblock copolymer polystyrene-block-poly-methyl methacrylate and maghemite nanoparticles to produce the films. The metal iron was sputtered on to the surface of nanostructured film and the structure formation was recorded and investigated with in-situ grazing incident small angle X-ray scattering (GISAXS) technique. The surface topography of the composite films before and after sputtering is investigated by atomic force microscopy (AFM). The presence of nanoparticles in the film act as a nucleation site which leads to a different type and size of structures with compared to the film without nanoparticles upon sputtering of iron. Funding by the CompInt network is acknowledged.

CPP 34.5 Thu 17:00 Poster A

Poly(N-Isopropylacrylamide) as thermo responsive coating on Microcantilever Sensors — •Sebastian K. Nett[1,2], Calvin Bradley[1], Mine Memesa[1], Yajun Cheng[1], Sebastian Lenz[1], Rüdiger Berger[1], and Jochen S. Gutmann[1,2] — [1]Max Planck Institute for Polymer Research, Ackermannweg 10, D-55128 Mainz — [2]Institute for Physical Chemistry, Johannes Gutenberg University, Jakob-Welder-Weg 10, D-55099 Mainz

Micro fabricated cantilevers proofed to be a versatile system to be used as sensors. Any stress applied to the cantilever is very precisely detectable. Our system is consisting of an array of eight microcantilever (MCS) with a width of 90 μm, a length from 500 to 1000 μm and a thickness from 1 to 10 μm. Combined with a functional layer it is possible to build a very specific sensing system. Poly(N-Isopropylacrylamide) (PNIPAM) is known to be a polymer which exhibits a coil to globule transition in water at around 32°C [1]. PNIPAM is grafted from the silicon surface of the MCS by atom transfer polymerization (ATRP). The surface layer was analyzed on the single cantilever by μ-focus GISAXS [2] and imaging ellipsometry to determine the layer thickness. We monitored the transition by heating the coated cantilever in water. The bending was detected by the so called deflection method. At the transition temperature a change in bending is clearly observed. The reasons for the bending are discussed as a function of grafting density and layer thickness. [1] Heskins, M., et. al., J. Macromol. Sci. Chem. A2 1968, 1441. [2] Wolkenhauer, M., et. al., Applied Physics Letters 2006, 89.

CPP 34.6 Thu 17:00 Poster A

About the importance of thermodynamic properties for the understanding of nanoparticle-matrix interaction — •Bartosz Zielinski[1], Jörg Baller[1], Martine Philipp[1], Ravi Bactavatchalou[1], Ulrich Müller[1], Jan Krüger[1], Wulff Possart[2], and Roland Sanctuary[1] — [1]LPM, University of Luxembourg, Luxembourg — [2]Universität des Saarlandes, Saarbrücken, Germany

Despite the tremendous importance of thermoset-based nanocomposites there is still a huge lack of understanding concerning the relation between the desired phenomenological properties and the implementation of unexpected structures due to the nanoparticles. We will show, that from the viewpoint of phenomenology investigations of static and dynamic thermodynamic properties are amongst the most promising. Combining selected scenarios of DSC and TMDSC provide a new view into the interaction mechanisms between nanoparticles and matrix. These results give access to the interpretation of the active role of the nanoparticles on network formation. As a model system we have chosen an epoxy thermoset filled with alumina nanoparticles.

CPP 34.7 Thu 17:00 Poster A

Self-assembly of liquid crystals induced by chemically patterned substrates — •Manuel Greschek and Martin Schoen — Stranski-Laboratorium für Physikalische und Theoretische Chemie Technische Universität Berlin, Strasse des 17.Juni 135, D-10623 Berlin

We present Monte Carlo simulations for ellipsoids of revolution interacting with chemically patterned planar walls. The simulations are performed in the grand-canonical and in the isostress-isostrain ensemble. In simulations with constant stress the volume of the simulation box may change in the direction of the wall normal. Two anchoring mechanisms are investigated, namely, homeotropic alignment (symmetry axis of the particle parallel to the wall normal) across a strip of width d_{wet}, homogeneous planar alignment (symmetry axis is perpendicular to wall normal) outside this strip. The fluid particles interact via a shifted Lennard-Jones (12,6) potential modified to account for the anisotropy of the interaction. The fluid-wall interaction is modelled via a Lennard-Jones (10,4) potential and modified to account for the preferred orientation of the fluid particles. Due to larger geometric incompability stratification is more diffuse than in "simple"fluids . Molecular frustration at the junction between homeotropic and planar orienting portions of the walls decreases with increasing film thickness.

CPP 34.8 Thu 17:00 Poster A

Effective single-particle dynamics according to the Hori-type Langevin equation — •Jörg R. Silbermann[1], Sabine H. L. Klapp[1,2], and Martin Schoen[1] — [1]Stranski-Lab für Physikalische und Theoretische Chemie, Technische Universität Berlin, Strasse des 17. Juni 124, 10623 Berlin — [2]Institut für Theoretische Physik, Technische Universität Berlin, Strasse des 17. Juni 124, 10623 Berlin

We consider the dynamics of a single tagged particle of mass M in a 2D Lennard-Jones (LJ) system. Employing the Mori-Zwanzig projector operator formalism, it is possible to derive an effective equation of motion of the form of a generalized Langevin equation (GLE). The "random force" $F_0^r(t)$ appearing in the GLE is in general unknown. For a harmonic solid, however, one can derive [1] a GLE where $F_0^r(t)$ coincides with the total force $F_0^*(t)$ acting on the tagged particle in a "reference system", where the mass is changed from M to an arbitrary mass m^*. We study to what extent this GLE is still able to capture the dynamics of the tagged particle under conditions where the harmonic approximation is no longer justified. To this end we compute typical time-autocorrelation functions for the tagged particle in molecular dynamics simulations for the full LJ system and compare these with the ones obtained by solving the GLE. We find excellent agreement at low temperatures and surprisingly good reproduction of the dynamics even in the high-temperature liquid phase.

[1] K. Wada, J. Hori, Prog. Theor. Phys. **49**, 129 (1973).

CPP 34.9 Thu 17:00 Poster A

Dipolar ordering between three and two dimensions — •R. Andreea Trasca[1] and Sabine H.L. Klapp[1,2] — [1]Stranski-Laboratorium für Physicalische und Theoretische Chemie, Sekretariat C7,Technische Universität Berlin,Strasse des 17. Juni 115, D-10623 Berlin, Germany — [2]Institut für Theoretische Physik, Sekretariat PN 7-1, Facultät II für Mathematik und Naturwissenschaften, Technische Uniersität Berlin, Hardenbergstraße 36, D-10623 Berlin, Germany

We perform Monte Carlo simulations to investigate the orientational and translational ordering behavior of dipolar soft-sphere films confined between planar walls with gaps between 5 and 1.5 σ [1]. At 5 σ the dipolar film exhibits a spontaneous ferromagnetic transition similar to ones previously found at larger gaps and in bulk [2]. As the gap is decreased the ferromagnetic order vanishes, but a high degree of dipolar allignment is preserved, as antiferromagnetic stripes.

Besides the orientational ordering, the dipolar film forms layers due to soft-sphere interactions. The translational order in the plane of the layers is investigated using pair correlation functions and bond angle order parameters. As a reference we also compute the translational order of confined soft-sphere films. At very high densities, starting from the equilibrated soft-sphere configuration and random dipoles,a nontrivial change of the translational as well as the orientational structure of the dipolar soft-sphere film is observed.

1. R.A. Andreea and S.H.L. Klapp, in preparation.
2. S.H.L.Klapp and M.Schoen, J.Chem.Phys. 117, 8050 (2002).

CPP 34.10 Thu 17:00 Poster A

Surface-pattern recognition by molecular fluids — •Timo Poppmann and Martin Schoen — Stranski-Laboratorium für Physikalische und Theoretische Chemie, Technische Universität Berlin, Germany

We investigate the phase behavior of molecular, rodlike fluids confined between nonplanar substrates by means of canonical ensemble Monte Carlo(CEMC) simulations. Substrates are infinitely long in the y-direction and consist of a periodic sequence of wedge-shaped furrows of depth D and periodicity s_x in the x-direction. Moreover, the substrates stay in register in the x-direction. The interaction potentials are of the Lennard-Jones type with an anchoring orientation function g($\hat{u}$). We find a clear correlation between the preferred orientation of molecules and the fluid density in the vicinity of the substrates.

CPP 34.11 Thu 17:00 Poster A

Multimode analysis of Ni-, Pd-, and Pt- phthalocyanines — •Davoud Pouladsaz, Thiruvancheril Gopakumar, Michael Hietschold, and Michael Schreiber — Institut für Physik, Technische Universität Chemnitz

We investigate the photoelectron spectra of the first ionization of Ni-, Pd-, and Pt- phthalocyanines by a multimode analysis as the computation of vibronic coupling constants and reorganization energies with density functional theory (DFT).

CPP 34.12 Thu 17:00 Poster A

Structure and thermodynamics of concentrated electrolyte solutions — •Immanuel Kalcher and Joachim Dzubiella — Physics Department, TU Munich

Concentrated electrolytes are a substantial component of many molecular systems, e.g. in cell biology, nanofluidics, or clays. The prediction of their equilibrium structure and thermodynamics in bulk and confinement remains a difficult task. We address this challenge by performing extensive explicit-water molecular dynamics (MD) computer simulations of electrolytes for a wide range of salt species and concentrations (<6M). The bulk ion-ion radial distribution functions (rdfs) are calculated and then used as input in statistical mechanics approaches to predict macroscopic thermodynamics and the inhomogeneous electrolyte structure in confinement. Here we utilize the interesting observation that the water-induced short-ranged structure of the bulk electrolyte is only weakly dependent on salt concentration. By applying a simple Debye-Hueckel approach with a concentration dependent permittivity we show that the different radial distribution functions can be mapped onto each other by separating the short and long range contributions. This mapping enables us to reproduce the experimental osmotic pressures of electrolyte solutions fairly well over a range of 0-3 mol with the knowledge of only two accurate bulk rdfs. Furthermore, strong structural inhomogeneities are observed in MD simulations of concentrated electrolytes in nanometer-sized confinement and are compared to solutions of Poisson-Boltzmann based approaches.

CPP 34.13 Thu 17:00 Poster A

Influence of the nanoscale lamellar orientation of UHMW-PE surfaces on the protein adsorption — •Thomas Keller, Matthias Grosch, Erik Vater, David Trimbach, and Klaus D. Jandt — Institut für Materialwissenschaft und Werkstofftechnologie (IMT), Friedrich-Schiller-Universtität Jena, Löbdergraben 32, 07743 Jena

The here presented study shows that for thin-melt drawn films of ultra-high molecular weight polyethylene (UHMW-PE) - an implant material already in use - the lamellar crystal arrangement on the surface can be influenced on the nano-scale by processing conditions. These lamellae protrude from the film surface and therefore, such highly oriented UHMW-PE films open up the possibility to investigate the interaction of nano-topographic features with proteins and cells. The in arthroplasty most relevant protein human serum albumin (HSA) was systematically adsorbed on these UHMW-PE surfaces and analyzed by means of atomic force microscopy (AFM). Solutions of different HSA concentrations in PBS buffer were brought onto the highly ordered UHMW-PE surfaces and left for adsorption for different periods of time. By varying the concentration and time for protein adsorption, a partial to full surface coverage was achieved. On the partially HSA-covered UHMW-PE surfaces a preferential alignment of the proteins with the lamellar thickness parallel to the drawing direction was observed. Thus, new insight into the interaction of proteins with nanoscale topographic features of UHMW-PE surfaces was gained.

CPP 34.14 Thu 17:00 Poster A

Direct observation of phonon decay in two-dimensional colloidal crystals — •Julian Dietrich[1], Jörg Baumgartl[1], Hans-Hennig von Grünberg[2], and Clemens Bechinger[1] — [1]2. Physikalisches Institut, Universität Stuttgart, 70550 Stuttgart, Germany — [2]Institut für Chemie, Karl-Franzens-Universität, 8010 Graz, Austria

Lately there is growing interest in the band structures of so called phononic crystals which exhibit a phononic band gap. In a recent study it has been shown that such phononic band gaps can also be induced in colloidal crystals through anisotropic interactions including substrate-particle and particle pair interactions. In our experiment we investigate a new approach to determine the band structure of such a two-dimensional colloidal crystal directly from the phonon dynamics. Since colloidal suspensions are overdamped systems the phonons do not propagate but decay exponentially with a characteristic decay time inversely connected to the phonon band structure. We directly measure these decay times using video microscopy. Moreover, we apply a commensurate hexagonal substrate created with three interfering laser beams in order to tune the decay times. Finally, we investigate the behaviour of the decay times for vanishing substrate strengths; preliminary results indicate that hydrodynamical effects become important in the centre of the first Brillouin zone, i.e. for long wavelength phonons.

CPP 34.15 Thu 17:00 Poster A

Light-Induced Surface Relief Gratings on Novel Low-Molecular-Weight Organic Glasses Containing Azobenzene Side Groups — •Hubert Audorff[1], Lothar Kador[1], Roland Walker[2], and Hans-Werner Schmidt[2] — [1]Institute of Physics and BIMF, University of Bayreuth, 95440 Bayreuth — [2]Macromolecular Chemistry I and BIMF, University of Bayreuth, 95440 Bayreuth

A number of novel low-molecular-weight glass formers with azobenzene moieties has been synthesized to examine the formation of surface relief gratings (SRGs). In addition to birefringent volume gratings, SRGs with heights up to 650 nm were formed in holographic experiments. The amplitudes of the latter were calculated from the diffraction efficiencies and independently measured by atomic-force microscopy. The temporal evolution of the diffraction efficiencies of both types of gratings was monitored. The gradient force model is capable of explaining all the experimental results. The differences between the gratings generated with different writing polarizations can be ascribed to the varying strengths of the gradient force. The influence of the molecular end groups on the SRG formation was investigated. Temperature-dependent measurements allow the determination of the glass transition temperature. At elevated temperatures, the SRG formation rate drops due to increased fluidity of the material.

CPP 34.16 Thu 17:00 Poster A

Temperature dependent optical spectroscopy of rubrene single crystals — •Olga Krylova[1], Jens Pflaum[2], Rainer Stöhr[2], Linus Gisslen[3], Reinhard Scholz[3], and Moritz Sokolowski[1] — [1]Institut für Physikalische und Theoretische Chemie, Universität Bonn — [2]3. Physikalisches Institut, Universität Stuttgart — [3]Walter Schottky Institut, Technische Universität München

High quality rubrene crystals were grown by sublimation under streaming hydrogen. Polarized and angle-resolved fluorescence and absorption spectra were measured as a function of temperature. The fluorescence spectrum shows a strong reversible variation with temperature. The spectral changes are accompanied by a very strong (1000 fold) increase of the luminescence intensity at low T. At room temperature, the luminescence can be understood by the formation of H-aggregates of the transition dipoles due to efficient coupling in the (b,c)-crystal plane. This leads to emission from the zone boundary and hence causes a low luminescence yield and a large Stokes shift. At low temperatures, the luminescence spectrum is more reminiscent to that of a J-aggregate. This would imply that at low T, there exists a minimum of the exciton dispersion at the center of the Brillouin zone, which allows luminescent decay with high efficiency. We plan time-dependent PL measurements, which allow us assign temperature-dependent decay rates of the various PL bands, allowing estimates of the respective radiative lifetimes and the activation energies of non-radiative quenching mechanisms. Supported by DFG through the research unit 557.

CPP 34.17 Thu 17:00 Poster A

Light-induced modifications of the molecular switch 3-(4-(4-Hexylphenylazo)phenoxy)propan-1-thiol adsorbed on Au(111) studied by two photon photoemission — •Nils Heinemann[1], Oleksiy Andreyev[1], Ulrich Jung[1], Claudia Bornholdt[2], Olaf Magnussen[1], Rainer Herges[2], and Michael Bauer[1] — [1]Institut für Experimentelle und Angewandte Physik, Uni Kiel — [2]Otto-Diehls Institut für Organische Chemie, Uni Kiel

Molecular switches and their intriguing properties attract much interest in the field of molecular electronics. Whereas the reversible switching of molecules has been well studied in gases and liquids, the successful realization and sensing of molecular switching at surfaces still remains a challenging task. Quite recently, Hagen et al. reported on the observation of a photoinduced reversible switching of tetra-tert-butyl-azobenzene molecules adsorbed on a Au(111) surface by means of the two photon photoemission technique (2PPE) [1].

In this contribution we will present 2PPE results of the molecular switch 3-(4-(4-Hexylphenylazo)phenoxy)propan-1-thiol adsorbed on Au(111). A tuneable 80 MHz fs-laser system is employed to study changes in the electronic structure of the adsorbed molecule induced by laser illumination at 365 nm and 435 nm. We observe a distinct and wavelength characteristic impact on the 2PPE spectra, which also depends critically on the applied light intensity. The results will be discussed particularly in the context of a switching of the adsorbed molecule.

[1] S. Hagen et al., Chem. Phys. Lett. 444 (2007) 85-90.

CPP 34.18 Thu 17:00 Poster A

MD Simulations of Sheared Polymer Brushes with Explicit Solvent — •Andre Galuschko, Torsten Kreer, Joachim Wittmer, and Joerg Baschnagel — Institut Charles Sadron, 6 rue Boussingault, F-67083 Strasbourg Cedex, France

Polymer brushes play an important role as lubricants in many technical applications, e.g. in hard disk drives or artificial joints [1]. They are furthermore believed to be crucial for minimizing friction between synovial joints [2], such as human knees or hips.

Using Molecular Dynamics simulations of a standard coarse grained model we study the lubrication properties of short chain polymer brushes. We extend further approaches (see, e.g. Refs.[3-5]), which have been performed without explicit solvent, to new simulations, where we now account for hydrodynamic interactions via including solvent molecules. We investigate the static properties of isolated and compressed brushes, and study the response of these systems to stationary and non-stationary external shear. This is done under variation of the molecular parameters, i.e. grafting density and chain length. By comparing to previous simulation results of the same model without explicit solvent, we aim at understanding the role of hydrodynamic interactions in polymer brush lubrication.

[1] T. Moro et al., Nat. Mater. 3, 829 (2004).
[2] J. Klein, Proc. IMechE J 220, 691 (2006).
[3] G.S. Grest, Phys. Rev. Lett. 76, 4979 (1996).
[4] P.S. Doyle et al., Phys. Rev. Lett. 78, 1182 (1997).
[5] T. Kreer et al., Langmuir 17, 7804 (2001).

CPP 34.19 Thu 17:00 Poster A

Force Studies on Responsive Polymeric Brush Surfaces — •Mukesh Kumar Vyas, Konrad Schneider, Bhanu Nandan, and Manfred Stamm — Leibniz Institute of Polymer Research Dresden, Hohe Strasse 6, 01069 Dresden, Germany

Surface forces such as adhesion and friction play important roles in the manipulation, assembly, and operation of micro- and nanoscale devices. We perform atomic force microscope (AFM) based force studies on polystyrene * poly(2-vinylpyridine) (1:1) mixed polymer brushes and corresponding monobrushes in air. Adhesion and friction force behaviour of polymer brush surfaces in contact with inorganic and polymeric surfaces, was studied using silicon tips, silicon nitride tips, colloidal probe with silica particle and colloidal probe with polystyrene (PS) and poly(acrylic acid) brushes on surface. The effect of switching behaviour of chemical composition of binary brush surfaces (on treatment with suitable solvents) on the wettability, surface roughness, and hence on the adhesion and friction properties of the surfaces, was investigated. Surface roughness values for the entire polymer brushes samples were in the same range and had minimal influence on the trend obtained for the force values. Adhesion force values were in accordance with the wettability of the samples. Adhesion and friction values were correlated to wettability for most of the cases except for the silicon tip.

CPP 34.20 Thu 17:00 Poster A

Self-rolled Polymer Microtubes and Toroidal Microcavities — •Kamlesh Kumar, Valeriy Luchnikov, and Manfred Stamm — Leibniz Institute of Polymer Research Dresden, Hohe Strasse 6, 01069 Dresden, Germany

Microtubes and microtoriods of different nature find various applications in microfluidic devices, sensors, filters, wave-guides etc. In the present work, we have investigated the fabrication of microtube and microtoroids by self-rolling of thin strained bilayer polymer films, composed of polystyrene/poly (4-vinyl pyridine) and released in controllable manner from a solid substrate. The bilayer film develops strain due to unequal swelling of polymers in selective solvents and hence the film bends and scrolls in order to minimize its free energy. These tubes and toroids were characterized in detail using optical microscopy, atomic force microscopy, and scanning electron microscopy.

Inner surfaces of tubes and toroids could be functionalized using photolithography, micro-contact printing, vacuum sputtering of metals, ion beams, plasma chemical activation etc. Photolithography, electron beam lithography and direct mechanical patterning with a sharp blade were used for the structuring of the bilayer before the rolling of tube. Looped tubes with metallized hidden walls, produced by self-rolling technique, may act as micro-resonators in the corresponding frequency range. The self-rolling approach opens new broad opportunities for mesoscale engineering of the tube-based devices, since it combines highly developed planar methods of surface modification with self-organized formation of 3D micro- and nanostructures.

CPP 34.21 Thu 17:00 Poster A

Identification of dissipative and elastic contributions in force spectroscopy curves and tapping mode AFM images for polymeric model surfaces — •Klaus Schröter, Albrecht Petzold, Thomas Henze, and Thomas Thurn-Albrecht — Institut für Physik, Universität Halle-Wittenberg

The separate identification of dissipative and elastic force contributions in Atomic Force Microscopy (AFM) is discussed. We show that within a harmonic approximation the interaction of the AFM tip with the sample surface can be described by average interaction parameters which can be extracted in a simple way from measured data. The method is applied to force spectroscopy curves on hard and soft polymeric model surfaces. The understanding of the basic effects then enables a clearer interpretation of AFM images and an identification of phases in systems with hard-soft contrast as for instance on semicrystalline polymers.

CPP 34.22 Thu 17:00 Poster A

Side chain dynamics and crystallization in nanophase-separated regio-random poly(3-alkyl thiophenes) — •Shireesh Pankaj, Elke Hempel, and Mario Beiner — Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle/Saale, Germany

A series of regio-random poly(3-alkyl thiophenes-2, 5-diyl) has been investigated by differential scanning calorimetry, x-ray scattering and dynamic mechanical analysis. Samples with varying side chain lengths from $C = 4$ to $C = 12$ alkyl carbons were studied to understand details of the interplay between structure and cooperative dynamics in these nanophase-separated side chain polymers. Two glass transitions are observed for the amorphous members ($C = 4 - 8$) like in previously studied atactic poly($n-$alkyl methacrylates). In both cases, the aggregation of alkyl groups to small alkyl nanodomains with a typical dimension of about 1 nm is indicated by a prepeak in x-ray scattering data. Crystallization of alkyl groups within the alkyl nanodomains is seen for the higher thiophenes, i.e., for the decyl ($C = 10$) and dodecyl ($C = 12$) members. A special feature which is observed for the dodecyl member is that different melting peaks are seen depicting polymorphism of the crystallizable side chains. This is not observed in poly($n-$alkyl methacrylates) and poly($n-$alkyl acrylates) with similar side chain lengths. Isothermal crystallization results for these samples are presented and discussed in the light of recently developed theories of polymer crystallization.

CPP 34.23 Thu 17:00 Poster A

Optical Properties of Ink-Jet-Printable PPE-PPV/ Semiconductor Nanocrystal Hybrid Materials — •Thomas Blaudeck[1], Stephan Jahn[1], Daniel A. M. Egbe[1], Reinhard Baumann[1], and Christian von Borczyskowski[2] — [1]Institute of Print and Media Technology, TU Chemnitz, 09107 Chemnitz, Germany — [2]Optical Spectroscopy and Molecular Physics, TU Chemnitz, 09107 Chemnitz, Germany

Hybrid materials made of organic poly(p-phenylene-ethynylene-alt-poly(p-phenylene-vinylene) (PPE-PPV) and inorganic semiconductor nanocrystals are promising candidates for various applications in electronic and optoelectronic devices such as LEDs, OBDs, and transistors. Considering the high chemical structural versatility and mechanical flexibility of PPE-PPV, devices in mind have to go along with suitable low-cost production routines. In this respect, digital fabrication techniques such as ink-jet printing have gained considerable interest as they combine the demand for a high throughput with small structure sizes down to the range of several micrometers. Whilst the suitability of PPE-PPV for printing was recently proven [1], additives and impurities were found to considerably affect the optical, functional, and rheological properties of the printing formulation. Apart from some empirical data, their particular role is still poorly understood. In this study, we focus on the influence of semiconductor nanocrystals on the optical properties of a series of ink-jet printable PPE-PPV formulations and their precursors.

[1] E. Tekin et al., Journal of Materials Chemistry 16, 4294 (2006).

CPP 34.24 Thu 17:00 Poster A

Static and dynamic properties of tethered chains in different surface regimes. Monte Carlo studies. — •Radu Descas[1], Jens-Uwe Sommer[2], and Alexander Blumen[1] — [1]Theoretische Polymerphysik, Universität Freiburg, Hermann-Herder-Strasse 3, D-79104 Freiburg — [2]Leibniz-Institut für Polymerforschung Dresden, Hohe Strasse 6, D-01069 Dresden

Using MC simulations combined with scaling arguments we study the adsorption of tethered polymer chains at flat surfaces. The interplays between the grafting density σ, the excluded volume, and the strength of adsorption κ lead to different surface regimes. We suggest a $\sigma - \kappa$ phase diagram and focus on the semidilute surface regime and on the oversaturated brush regime. In these regimes we study both the static [1] and the dynamic [2] properties of the chains. Using scaling arguments and computer simulations we analyse the average extension of single chains both parallel and perpendicular to the surface. Especially for the parallel component our simulation results agree well with the scaling predictions. In the semidilute regime the dynamics is well described by a model in which the chains form adsorption blobs. In the oversaturated brush regime the system can be visualized as a brush-like state formed on top of a saturated adsorption layer. Our simulations show that in this regime the dynamics is controlled by three-dimensional blobs.

[1] R. Descas, J.-U Sommer, and A. Blumen, J. Chem. Phys. **125**, 214702 (2006).

[2] R. Descas, J.-U Sommer, and A. Blumen, in preparation.

CPP 34.25 Thu 17:00 Poster A

Hyperquenching in linear polyethylene and ultrafast calorimetry at heating and cooling rates up to 2 millions K/s — •Alexander Minakov[1,2] and Christoph Schick[1] — [1]University of Rostock, Institute of Physics, Universitätsplatz 3, 18051 Rostock, Germany — [2]A.M. Prokhorov General Physics Institute, Vavilov 38, 119991 Moscow, Russia

Ultrafast nanocalorimetry was applied for hyperquenching in ultra high molecular weight linear polyethylene (UHMWPE). We determine the quenching rate required to obtain amorphous polyethylene from the melt. UHMWPE can be strongly supercooled at high cooling rates. The peak in heat capacity cp(T) corresponding to crystallization shifts to lower temperatures with increasing cooling rate in the range 10ˆ3 - 10ˆ5 K/s. This shift attains saturation at the rate 10ˆ5 K/s. At subsequent increasing cooling rate the peak in cp(T) decreases. Crystallization can not be accomplished for 10 μs. Totally amorphous PE sample at cooling and subsequent heating rate ca. 2*10ˆ6 K/s was obtained for samples of 0.1 ng and 0.06 ng (the samples thickness was ca. 0.1 μ). Considerable superheating of the melting in UHMWPE was observed. We have performed superheating measurements for 2.5 ng and 0.06 ng samples melt-crystallized for 1 min at 96°C and 106°C in the range 2*10ˆ3 - 2*10ˆ6 K/s of the heating rate. The rate dependence of superheating increment is described by the power law with exponent 0.212.

CPP 34.26 Thu 17:00 Poster A

Thermo-optical and thermo-mechanical properties of smectic liquid-crystal — •Jörg Petzold[1], Tilo Finger[1], Ralf Stannarius[1], Patrick Beyer[2], and Rudolf Zentel[2] — [1]Otto-von-Guericke Universität Magdeburg — [2]Johannes Gutenberg-Universität Mainz

Incorporation of liquid-crystal mesogens in polymer backbones and subsequent cross-linking leads to the preparation of main chain liquid crystalline elastomers (LCE). Such compounds show unique effects because of the interaction of mesogenic and elastomer properties.

We report mechanical, x-ray and optical measurements of freely suspended filaments of such LCE. Among the interesting effects are the reversible elongation of the filaments along the smectic-isotrop phase transition (thermoelasticity) and a strain induced birefringence due to the coupling of mesogen orientation and applied stress. Elastic and optical parameters are derived from the stress-strain characteristics.

For additional information: ”Monodomain Liquid Crystal Main Chain Elastomers by Photocrosslinking” by Patrick Beyer, Eugene M. Terentjev, Rudolf Zentel

CPP 34.27 Thu 17:00 Poster A

Observation and visualization of block copolymer microdomain dynamics — •Eike-Christian Spitzner, Christian Riesch, Christian Dietz, Nicolaus Rehse, and Robert Magerle — Chemische Physik, TU Chemnitz, D-09107 Chemnitz

We investigate the microdomain dynamics in thin films of polystyrene-*block*-polybutadiene copolymers which form hexagonally ordered polystyrene cylinders in bulk. The films are swollen in chloroform vapour and observed in situ with tapping mode scanning probe microscopy. A temporal resolution of 15 s per frame is achieved. Image sequences show the dynamics of structural phase transitions and individual point defects. Phenomena such as defect annihilation, fluctuations of cylinder thickness and meandering of cylinders are of particular interest. From local Fourier transformations we obtain colour-coded maps of the cylinder orientation. With Nanotomography, consisting of consecutive steps of etching and imaging, we acquire volume images of microdomain structures.

CPP 34.28 Thu 17:00 Poster A

Modelling charge transport in polypyrrole — •Victor Rühle[1], James Kirkpatrick[1,2], Kurt Kremer[1], and Denis Andrienko[1] — [1]Max-Planck-Institut für Polymerforschung, Ackermannweg 10, 55128 Mainz, Germany — [2]Centre for Electronic Materials and Devices, Department of Physics, Imperial College London, London SW7 2BW, UK

Polypyrrole is one of the most stable and easy to synthesize conductive polymers. The charge transport in its reduced and oxidized states is however not fully understood. The main problem is to link the morphology to the conducting properties, since different time and length scales are involved: the individual electron hops occur on a quantum scale and hence strongly depend on the local structure. However, the entire path which charges follow is strongly affected by the large scale morphology.

In this work, an atomistic model to generate morphologies of PPy is first developed. Ab-initio methods are used to derive an atomistic force field for the neutral as well as the oxidized polymer. To be able to generate large scale morphologies, coarse graining of this atomistic model is then performed. Finally, both models are applied to small samples of PPy and the physical properties are compared. Once whole morphologies are generated, the charge mobility is calculated combining Marcus theory with a Master equation approach.

CPP 34.29 Thu 17:00 Poster A

Molecular dynamics of ultrathin supported polysulfone films studied by dielectric spectroscopy — Diana Labahn and •Andreas Schönhals — Federal Institute for Materials Research and Testing, Unter den Eichen 87, 12205 Berlin

Broadband dielectric spectroscopy (10 mHz to 10 MHz) was employed to study the glassy dynamics of ultra thin supported polysulfone layers. The ultra thin films were prepared between two aluminum electrodes. Glass slides, cleaned in an ultrasound alkaline bath, rinsed in pure chloroform, and dried under nitrogen flow, were used as supporting substrates. Thin polymer films were spin-coated from a chloroform solution at 3000 rpm. The film thickness from microns down to below 10 nm was adjusted by changing the concentration of the polymer in solution. After spin-coating, the samples were annealed at a temperature well above the bulk glass transition. As a main result, for carefully annealed samples no change of the glass transition temperature with the decreasing film thickness is observed in contradiction to literature results. A more detailed analysis using a derivative technique shows that the Vogel temperature increases und the fragility parameter decreases with decreasing film thickness.

CPP 34.30 Thu 17:00 Poster A

Dielectric and Gas transport Properties of Polymeric Nanocomposites based on Polyhedral Oligomeric Silsesquioxanes — Ning Hao, Martin Böhning, and •Andreas Schönhals — Federal Institute for Materials Research and Testing (BAM), 12205 Berlin, Germany

Polymer based nanocomposites continue to receive tremendous attention for different applications. They show remarkable property improvement (increased tensile properties, decreased gas permeability, decreased solvent uptake, increased thermal stability and flame retardance) when compared to conventionally scaled composites. Different polymer based nanocomposites are prepared where polycarbonate and polystyrene are used as polymer matrices. As molecular nanofiller polyhedral oligomeric silsesquioxanes (POSS) with Phenethyl substituents is used. The property structure relationships of these nanocomposites are investigated by dielectric spectroscopy, gas transport measurements (permeation, sorption) and density measurements as well. The results are discussed with regard to the phase structure of the nanocomposites. This includes the construction of phase diagrams. For the first time a correlation between dielectric and gas transport data are given.

CPP 34.31 Thu 17:00 Poster A

AFM analysis of novel Polypropylenes — •Dirk Doser[1], Stefan Fischer[1], Othmar Marti[1], Tobias Diesner[2], and Bernhard Rieger[2] — [1]Institute of Experimental Physics, University of Ulm, 89069 Ulm, Germany — [2]Wacker-Lehrstuhl für makromolekulare Stoffe, TU München

The aim of this work was to observe the complex structures of novel isotactic Polypropylenes (iPP) using tapping mode and pulsed force mode AFM. Therefore two different approaches in sample preparation were investigated. Thin film preparation on Silicon wavers with toluene solved Polypropylene served to explore the unstretched structure. The thin films were also prepared on stretchable carriers like PDMS for studying the stretched iPP. Second samples of isotactic Polypropylene microtome cuts were prepared by potassium permanganate etching. In that case some samples were stretched before preparation. The results of this measurements will be discussed.

CPP 34.32 Thu 17:00 Poster A

Micromechanics of thin films of elastomeric polypropylenes — •Mechthild Franke, Mario Zerson, Mario Jecke, Robert Magerle, and Nicolaus Rehse — Chemische Physik, TU Chemnitz, 09107 Chemnitz

Elastomeric polypropylene consists of lamellar crystals embedded in an amorphous matrix. The arrangement, distribution, and connectivity of these crystals are important factors which determine the mechanical properties of the polymer. Free standing, ~ 1 μm thick films of different elastomeric polypropylenes are produced by dip coating the polymer solution on a NaCl crystal, floating the film onto water, and depositing it on a slotted silicon substrate. A stretching device, based on a piezoelectric drive, allows stretching the free standing film stepwise up to strains of 100%. The changes in shape, orientation, and morphology of crystalline regions are observed in situ with scanning force microscopy. Caused by the induced stress new lamellae crystallize; existing ones elongate or break into blocks. Furthermore, amorphous areas are stretched a lot more than crystalline ones. Volume images of thin films obtained with SFM based Nanotomography allow to explain some of the observed rearrangements of the microstructure.

CPP 34.33 Thu 17:00 Poster A

Nanotomography of semicrystalline polypropylene using bimodal atomic force microscopy — •Christian Dietz[1], Mario Zerson[1], Christian Riesch[1], Alexander M. Gigler[2], Robert W. Stark[2], Nicolaus Rehse[1], and Robert Magerle[1] — [1]Technische Universität Chemnitz, Reichenhainer Str. 70, 09107 Chemnitz, Germany — [2]Center for Nanoscience and Dept. Earth and Environmental Sci., Ludwig-Maximilians-Universität München, Theresienstraße 41/II, 80333 München

High resolution volume images of semicrystalline polypropylene were obtained by stepwise wet-chemical etching followed by atomic force microscopy imaging of the specimen. Compositional contrast changes from crystals that are stiff to the amorphous phase which is rather soft. The dissipated energy as function of the cantilever's oscillation amplitude allows to identify dissipation processes at the nanoscale and to distinguish crystalline from amorphous regions. To enhance resolution a bimodal atomic force microscope was used where the first two flexural eigenmodes of the cantilever are mechanically excited and the cantilever deflection signal is analyzed using two lock-in amplifiers. While the amplitude of the first mode is used as an electronic feedback signal, the amplitude and phase signal of the second eigenmode are used to distinguish compositional changes of the material. This approach allows for a higher signal to noise ratio than the phase signal of the first eigenmode and it is less influenced by the sample topography.

CPP 34.34 Thu 17:00 Poster A

Influence of substrate temperature on pulsed laser deposited PMMA films — •Britta Lösekrug, Susanne Seyffarth, Andreas Meschede, and Hans-Ulrich Krebs — Institut für Materialphysik, Universität Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen

Poly(methyl methacrylate) (PMMA) thin films are important for applications e. g. as coating materials and in microelectronics. Here pulsed laser deposition (PLD) at a wavelength of 248 nm is used with low laser energy densities slightly above the deposition threshold of PMMA (between 80 and 160 mJ cm^{-2}). Under these conditions at room temperature thin films can be produced which are completely smooth and show no droplets at all [1].

In contrast, for higher substrate temperatures above the glass transition (at 110 °C) a dewetting of PMMA thin films on Si(111) substrates occurs. Additionally, an increased hardness of these PMMA films compared to films deposited at room temperature is observed. So the properties of PMMA films change with substrate temperature during deposition. It can be shown by infrared spectroscopy (FTIR) and size exclusion chromatography (SEC) that the chemical composition of the PMMA films is still intact up to 200 °C, while the chain lengths are reduced compared to the starting material. At still higher temperatures the deposited material begins to evaporate.

[1]B. Lösekrug, A. Meschede, H.U. Krebs, Appl. Surf. Sci. **254** (2007) 1312

CPP 34.35 Thu 17:00 Poster A

Are there cross-aggregates? In-situ NMR study of the t-butyllithium initiated butadiene polymerization — •Aizhen Niu[1], J. Allgaier[1], L. Willner[1], J. Stellbrink[1], D. Richter[1], R. Hartmann[2], and L. J. Fetters[3] — [1]IFF, Forschungszentrum Jülich, D-52425 Jülich — [2]INB2, Forschungszentrum Jülich, D-52425 Jülich — [3]Cornell University, Ithaca, NY 14853, USA

The anionic polymerization kinetics and mechanism are complicated by the aggregation phenomena of organolithium compounds. In our previous work, the kinetics and aggregation states were investigated under standard polymerization conditions by the combination of in situ small angle neutron scattering (SANS) and ^{1}H NMR techniques. It is clear that the measurement of kinetic orders is not a tool that can be used to assay aggregation states as has long been assumed. We found that the existence of cross-aggregates formed from initiator and the polybutadienyllithium head groups can be the reason making the initiator become more reactive than in the pure self-aggregated state. In an attempt to understand the influence of cross-aggregattion plays in anionic polymerization, the investigation on cross-aggregation of an anionic polymerization were performed by high resolution ^{1}H NMR and Li^7 NMR. The cross-aggregation in the mixture of t-butyllithium and living chains, 3-Neopentylallyllithium and in the initiation stage of real polymerization were studied. It is clear that there are cross-aggregates and they play an important role in anionic polymerization.

CPP 34.36 Thu 17:00 Poster A

Crystallization Kinetics in Nanocomposites of Semicrystalline Polymers — •Andreas Wurm[1], Alexander Minakov[1], Dirk Lellinger[2], Tetyana Skipa[2], Ingo Alig[2], Petra Pötschke[3], and Christoph Schick[1] — [1]University of Rostock, Institute of Physics, Polymerphysics, 18051 Rostock, Germany — [2]Deutsches Kunststoff-Institut, Schloßgartenstr. 6, 64289 Darmstadt, Germany — [3]Leibniz Institute of Polymer Research, Hohe Str. 6, 01069 Dresden, Germany

In order to understand the nucleation and crystallization in CNTpolymer composites simultaneous experiments with a combination of different methods are extremely useful. As an important supplement to the classical techniques for crystallization (SAXS/WAXS or DSC), measurements of the AC conductivity and permittivity are of interest for CNT-polymer composites. These experiments allow the investigation of the changes in the conductive percolation structure by crystallization. Two effects are expected to influence conductivity and dielectric properties: (i) crystallisation near the CNT and at the CNT-polymer-CNT contacts and (ii) crystallization in the bulk. Therefore a microcalorimeter was designed, which allows to measure thermal properties like heat capacity and thermal conductivity, which can be used in a X-ray beam of a synchrotron, where simultaneously SAXS and WAXS patterns on the same sample volume can be recorded. On the other hand the microcalorimeter was extended for additional dielectric relaxation spectroscopy, again at the same time on the same sample volume.

CPP 34.37 Thu 17:00 Poster A

Crosslinkable Polymer Brushes - Synthesis and Characterization — •Sebastian G. J. Emmerling, Andreas Hanewald, and Jochen S. Gutmann — Max Planck Institute for Polymer Research, Ackermannweg 10, D-55128 Mainz, Germany

Atom transfer radical polymerization (ATRP) has opened the way to macromolecular engineering of polymeric materials. In this field, molecular brushes with poly(dimethylsiloxane) (PDMS) side chains were prepared by atom transfer radical polymerization (ATRP) conditions via macromonomer method (grafting through)[1]. The properties of these molecular brushes are dominated by the PDMS side chains, giving rise to numerous applications. In most of the cases, silicones are used as coatings because of their unique surface properties. Polydimethylsiloxane (PDMS) is undoubtedly the most widely used silicone. To produce this polymer living anionic polymerization is employed. However, this method requires stringent purification and stoichiometric conditions, which is a major drawback. The wide range of applications, that illustrates the versatility of this inorganic polymer arises from its unique combination of properties such as low surface tension, low glass transition temperature, high permeability to gas, and excellent weather resistance. However, since PDMS is a fluid at room temperature, the homopolymer lacks dimensional stability. In order to produce silicone-based materials with more desirable mechanical properties, we copolymerize the macromonomer with a benzophenone crosslinker[2].

[1] Neugebauer, D., et al., Macromolecules 2005, 38, 8687.

[2] Beines, P. W., et al., Langmuir 2007, 23, 2231.

CPP 34.38 Thu 17:00 Poster A

Characterisation of empty and polymer-filled, cylindrical mesopores using small-angle X-ray scattering — •Martin Engel[1], Bernd Stühn[1], Jörg Schneider[1], Thomas Cornelius[2], and Meike Naumann[1] — [1]Technische Universität Darmstadt — [2]Gesellschaft für Schwerionenforschung mbH

With improvements in creating well-defined mesopores in the last decades their use for investigations in nanotechnology gained great attraction. They are very promising matrices offering controllable confined geometries for self-organisation processes. Before their use as matrices it is essential to characterise these systems. In current scientific literature mesoporous systems are the object of close investigations.

In our work two kinds of mesoporous systems, highly ordered 2D hexagonal cylindrical alumina on one hand and randomly distributed well defined cylindrical ion-track polycarbonate pores were investigated with small-angle X-ray scattering (SAXS) and additionally with scanning electron microscopy. The data are analysed with the help of currently accepted models modified to deal with different sample orientations. Hence important properties like opening diameter, cylinder distance, polydispersity and sample orientation, that show up in anisoptropy of the scattering image, can be characterised.

We fill this well-defined mesopores with diblock-copolymers. Static and time-resolved scattering experiments are planned to investigate structure formation in this kind of confined geometries. The influence of the confining geometry on the resulting structure and the potential of SAXS to determine these structures will be discussed.

CPP 34.39 Thu 17:00 Poster A

Immobilized fraction in crystallizable polymer nanocomposites. — •Mohamed Ismail[1], Andreas Wurm[1], Bernd Kretzschmar[2], Doris Pospiech[2], and Christoph Schick[1] — [1]University of Rostock, Institute of Physics, Universitätsplatz 3, 18051 Rostock, Germany — [2]Leibniz Institute of Polymer Research Dresden, P. O. Box 120 411, 01005 Dresden, Germany

In this contribution we demonstrate the crystallization behavior of PA 6.6 filled with different concentrations of nanoparticles (Nanofil 919) to provide a wide range of systems with different mobility. We used a temperature modulated DSC (TMDSC) technique to determine heat capacity at the glass transition of the polymer. The existence of an immobilized fraction in PA / Nanofil 919 nanocomposites was shown. We obtained crystalline fraction, C, immobilized fraction, RAF, and the mobile amorphous fraction, MA for the whole sample series. The remaining mobile amorphous fraction of the polymer part, determined from step height at glass transition *cp, seems to be independent on filler content. Also, a slight decrease in Tg was found for more than 29.2 wt.% nanoparticles. For composites with less than 29.2 wt.% nanoparticles, the Tg is independent on filler content. By annealing experiments at and below the glass transition these results were verified.

CPP 34.40 Thu 17:00 Poster A

Solidification of fast crystallizing polymers studied by differential chip nano-calorimetry — •Evgeny Zhuravlev, Saurabh Garg, Andreas Wurm, and Christoph Schick — University of Rostock, Institute of Physics, Universitätsplatz 3, 18051 Rostock, Germany

The device was developed for investigation of thermal processes during fast thermal treatments of nanosized samples. The idea of the device was taken from differential scanning calorimetry. It consists of high sensitive, low addenda heat capacity thin film sensors used as sample and reference measuring cell. Small heated area and sensitive thermopiles allow both controlled fast heating and cooling.

Electrical control circuit was slightly modified in comparison with PerkinElmer power compensated DSC. This solution gives directly changes in heat flow from/to the sample during temperature scans.

The device works in the range of scanning rates between 0.1 and 10000 K/s with nanogram samples. It positioned exactly between existing DSC and ultra-fast scanning techniques.

Scheme, main principles and working of control circuits will be presented. We show first data on In, Sn and Pb. Measurements of supercooling of Sn samples using DSC, differential power compensated fast scanning technique and ultra-fast scanning is discussed. These measurements cover 10 orders of magnitude in scanning rate. Further we present data on isothermal crystallization of iPP and nucleated iPP in a wide temperature and dynamic range.

CPP 34.41 Thu 17:00 Poster A

Theoretical study of electron transfer through polyacetylene nanowires in different contact structures — •Davoud Pouladsaz[1], Saeideh Mohammadzadeh[2], Thomas Gessner[2], Michael Schreiber[1], and Reinhard Streiter[2] — [1]Institut für Physik, Technische Universität Chemnitz — [2]Zentrum für Mikrotechnologien, Technische Universität Chemnitz

The electron transfer of polyacetylene nanowires is studied by employing the non-equilibrium Green function's technique within the density-functional-based tight-binding method. The conductance of *trans*-polyacetylene molecules, sandwiched between Au(111) surfaces in three different contact structures, is calculated for various lengths. As well, the dependence of the conductance oscillations on the length of the molecules is investigated.

CPP 34.42 Thu 17:00 Poster A

Dielectric Properties of nanocomposites based on polyethylene and layered double hydroxide — •Andreas Schönhals[1], Francis Reny Costa[2], Udo Wagenknecht[2], and Gert Heinrich[2] — [1]Federal Institute of Materials Research and Testing (BAM), Unter den Eichen 87, D-12205 Beerlin — [2]Leibniz Institute of Polymer Research, Hohe Straße 6, D-01069 Dresden

Polymer based nanocomposites continue to receive tremendous attention for different applications. They show remarkable property improvement (increased tensile properties, decreased gas permeability, decreased solvent uptake, increased thermal stability and flame retardance) when compared to conventionally scaled composites. The dielectric properties of nanocomposites based on Mg / Al layered double hydroxide (LDH) as nanofillers and polyethylene (PE) as matrix are investigated by dielectric spectroscopy (10 mHz to 10 MHz) in a large temperature range. One dielectric active relaxation processes is observed which increases in its intensity with the concentration of the incooperated LDH. It is assigned to the segmental relaxation of PE segments which fluctuate together with the surfactant. The polar surfactant used for the interaction/exfoliation enables to observe the molecular motions of the apolar PE segments located close to the LDH sheets. A quantitative analysis provides information about the amount of the interfacial region between the inorganic LDH sheets and the bulk PE matrix.

CPP 34.43 Thu 17:00 Poster A

Microstructure and anisotropic properties of Polyamide 6 films — •Astrid Naumann[1], Hussein Shanak[1], Karl-Heinz Ehses[1], Jan Lion[1], Walter Goetz[2], and Rolf Pelster[1] — [1]Universität des Saarlandes, Gebäude E2 6, 66123 Saarbrücken, Germany — [2]BASF Company, 67056 Ludwigshafen, Germany

We have studied the anisotropy and homogeneity of Polyamide films that were prepared using different stretching techniques (uniaxial, sequential biaxial, simultaneous biaxial and "double bubble"). Structural changes concerning crystallinity and orientation of crystallites are evaluated using X-ray measurements (SAXS, pole figures). We show how the microstructure correlates with the anisotropy of properties, that are sensitive to the molecular orientation (microwave permittivity and infrared absorption). We conclude with a quantitative comparison of the above industrial production techniques.

CPP 34.44 Thu 17:00 Poster A

Crystallization kinetics of monodisperse n-alkanes at high supercooling — •Sergey Adamovsky and Christoph Schick — University of Rostock, Institute of Physics, Polymer Physics Group, 18051 Rostock, Germany

Production of monodisperse n-alkanes[1] allows to study the nanoscale process of polymer crystallization by measurements on a macro scale. Because of exactly the same chain length a measurable amount of material behaves similar way. This way providing an opportunity to derive conclusions about individual crystals from the measured sample-average properties.

Mostly DSC equipment was used for calorimetric study of these materials which is limited to tens of seconds in time resolution; thus only the high temperature slow-end tail of melt crystallization was accessible.

Fast scanning calorimetric technique[2] developed in our lab was applied to study crystallization behavior of these materials. This allowed studying kinetics of crystallization from melt in a wide temperature range with crystallization halftimes from milliseconds to hours.

Results for three selected samples are presented: $C_{122}H_{146}$, $C_{162}H_{326}$ and $C_{390}H_{782}$.

[1] G. M. Brooke, S. Burnett, S. Mohammed et al., Journal of the Chemical Society-Perkin Transactions 1 (13), 1635-1645 (1996).

[2] S. Adamovsky and C. Schick, Thermochim. Acta 415, 1-7 (2004).

CPP 34.45 Thu 17:00 Poster A

Microphase separation in cross-linked polymer melts — •Abigail Klopper[1], Carsten Svaneborg[2], and Ralf Everaers[3] — [1]Max-Planck-Institut für Physik komplexer Systeme, Dresden — [2]Department of Chemistry and Interdisciplinary Nanoscience Center (iNano), University of Aarhus, Aarhus, Denmark — [3]Université de Lyon, Laboratoire de Physique, École Normale Supérieure de Lyon, Lyon, France

Highly concentrated liquids comprising long polymeric chains can undergo a process of cross-linking, invoking the formation of a disordered solid with a frozen memory of its preparation conditions. The cross-linking creates quenched connective and topological disorder which plays a role familiar from glassy systems in breaking the translational symmetry of the initial liquid state. In mixtures of different polymer species interacting with one another, it is responsible for the inhibition of a bulk phase separation and the establishment of microphases on intermediate length scales.

We pair a replica formalism with data from large-scale molecular dynamics simulations of nearly ideal cross-linked polymer systems with purely repulsive monomer interactions. By combining simulation with theory in this way, we are able to describe neutron scattering measurements in microphase-separating systems with attractive monomer interactions, without resorting to exhaustive simulation. In doing so, we uncover system-specific effects relating to the intrinsic length scales of our networks.

CPP 34.46 Thu 17:00 Poster A

Structure and dynamics of coarse grained polystyrene melts — •Dominik Fritz[1], Vagelis A. Harmandaris[1], Dirk Reith[2], Nico F. A. van der Vegt[1], and Kurt Kremer[1] — [1]Max-Planck-Institut für Polymerforschung, Ackermannweg 10, 55128 Mainz, Germany — [2]Fraunhofer-Institut für Algorithmen und Wissenschaftliches Rechnen, Schloss Birlinghoven, 53754 St. Augustin, Germany

Polymers show characteristic properties in a wide range of time scales. To access longer time scales in simulations, purely atomistic simulations are far too expensive to perform. The mesoscopic description of polymers allows to exceed the computational limitations of atomistic simulations. Following a systematic procedure one coarse grains atomistic polymer models into mesoscopic models, which cover time scales larger by several orders of magnitude. By reinserting details into systems, simulated with the mesoscopic model, we get well-equilibrated atomistic systems of high molecular weight.

In this contribution, we study coarse grained models of atactic polystyrene and compare its static and dynamic properties to atomistic simulation data. While static properties are used to develop coarse grained force fields, we look especially at aspects of the time scales in atomistic and mesoscopic simulations. We investigate mapping factors between dynamic properties, e.g. diffusion constants, in atomistic and mesoscopic melt simulations and their dependence on chain length.

CPP 34.47 Thu 17:00 Poster A

Microdomain Dynamics in Thin Films of Blockcopolymer Melts with Highly Ordered Cylinder Morphology — •Peter Fey, Christian Riesch, Sabine Rehse, Nicolaus Rehse, and Robert Magerle — Chemische Physik, TU Chemnitz, 09107 Chemnitz

We study a polystyrene-*block*-polybutadiene copolymer melt which forms cylinders in the bulk. With a shearing device based on a rubber stamp large areas of cylinders oriented parallel to the surface are produced in films of a thickness equivalent to one or two cylinder layers. After alignment, the film surface is imaged with tapping mode atomic force microscopy. It allows *in-situ* observation of the polymer melt during annealing at high temperatures ($\approx$ 100 - 120°C). The fluctuations of the orientation and width of cylinders is quantified using image processing algorithms, such as local Fourier transformations. Our goal is to achieve a better understanding of microdomain shape fluctuations in thermal equilibrium. Specimens with different degree of alignment are used to study the influence of defects on the observed dynamics.

CPP 34.48 Thu 17:00 Poster A

Logarithmic chain-exchange kinetics of diblock copolymer micelles — Reidar Lund[1,2], Lutz Willner[1], •Jörg Stellbrink[1], and Dieter Richter[1] — [1]IFF, Forschungszentrum Jülich, D-52425 Jülich — [2]Donostia International Physics Center, 20018 San Sebastián, Spain

We present a study of equilibrium chain-exchange kinetics of a well-defined model system for starlike PEP-PEO micelles in water/DMF mixtures [1, 2]. In this study we used time resolved small angle neutron scattering (TR-SANS) technique employing a particular H/D labeling scheme. This technique is perfectly suited for determination of exchange kinetics in equilibrium as, unlike other techniques,virtually no chemical or physical perturbations are imposed on the system.

The exchange kinetics crucially depends on the interfacial tension γ. By variation of γ the rate could be tuned over a wide time scale spanning from milliseconds to infinity. The results show that the kinetics follows a logarithmic time dependence [3] in sharp contrast to theory where single exponential behavior is predicted [4]. The logarithmic time dependence hints towards strongly coupled chain dynamics within the micellar cores induced by geometrical constraints. The same feature has been found for two other micellar systems confirming a general feature of exchange kinetics of block copolymer micelles.

[1] R. Lund et al., *Macromolecules*, **37**, 9984-9993, 2004.
[2] M. Laurati et al., *Phys. Rev. Letters*, **94**, 195504, 2005.
[3] R. Lund, et al., *Phys. Rev. Letters*, **96**, 068302, 2006.
[4] A. Halperin and S. Alexander, *Macromolecules*, **22**, 2403, 1989.

CPP 34.49 Thu 17:00 Poster A

Self Assembly of Block Copolymer Micelles — •Michael Ströbl, Gerald Johannes Schneider, Jörg Stellbrink, Jürgen

Allgaier, and Dieter Richter — Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich

Amphiphilic diblock copolymers play a crucial role in basic research as well as in applied science. In aqueous solution these diblock copolymers form micelles, which structure depends on the interfacial tension between the hydrophobic block and the selective solvent.

Using recently synthesized poly(alkyleneoxide)-poly(ethyleneoxide) block copolymers (PAO-PEO) the variation of the interfacial tension can now be achieved by changing the monomer of the hydrophobic block but keeping the same solvent, i.e. water. In the homologue series propyleneoxide (PPO), butyleneoxide (PBO), hexyleneoxide (PHO), and octyleneoxide (POO) the hydrophobicity increases continuously due to the growing aliphatic side group.

We present the results of static light scattering experiments and small angle neutron scattering experiments on the samples mentioned above.

CPP 34.50 Thu 17:00 Poster A

Multiple-quantum NMR study of entangled polymer melt dynamics — •Fabian Vaca Chavez and Kay Saalwachter — Martin-Luther-Universität Halle-Wittenberg, Institut für Physik; Friedemann-Bach-Platz 6, D-06108 Halle (Germany)

Entangled polymers melts exhibit a variety of dynamic processes covering a wide range of time scales, starting form the fast segmental reorientation in the picoseconds scale up to the diffusive and cooperative motions in the range of seconds. NMR is a powerful tool to study molecular dynamics due to its sensitivity to different molecular motions. In particular, multiple quantum (MQ) NMR emerged a few years ago as a new and robust tool to study polymer chain dynamics [1]. This technique yields quantitative information in particular on chain ordering, i.e., on entanglement effects and crosslink densities, and on the timescale of chain motion. In this work, we apply MQ NMR to linear poly(cis -1,4-isoprene) and poly(dimethyl siloxane) over suitable ranges of well defined molecular weight and temperature, in order to establish the dynamic regimes predicted by the tube model, and obtain in in-depth comparison of the entangled dynamics of these polymers. The data is analyzed by establishing simple scaling laws [1], and full analytical expressions based on a correlation function which explicitly includes the Rouse and reptation dynamics [2].

[1] R. Graf, A. Heuer, H.W. Spiess, *Phys. Rev. Lett.*, **80**, 5738-5741 (1998).

[2] K. Saalwachter, A. Heuer, *Macromolecules*, **39**, 3291-3303 (2006).

CPP 34.51 Thu 17:00 Poster A

Polyelectrolyte-Compression Forces between Spherical DNA Brushes — •Kati Kegler[1], Martin Konieczny[2], Gustavo Dominguez-Espinosa[1], Christof Gutsche[1], Matthias Salomo[1], Friedrich Kremer[1], and Christos N. Likos[2] — [1]Institute for Experimental Physics I, University of Leipzig, Linestr. 5, D-04103 Leipzig, Germany — [2]Institute for Theoretical Physics II: Soft Matter, Heinrich-Heine-Universität Düsseldorf, Universitätsstr. 1, D-40225 Düsseldorf, Germany

Optical tweezers are employed to measure the forces of interaction between a single pair of DNA-grafted colloids in dependence of the molecular weight of the DNA-chains, and the concentration and valence of the surrounding ionic medium [1]. The resulting forces are short-range and set in as the surface-to-surface distance between the colloidal cores reaches the value of the brush height. The measured force-distance dependence is analyzed by means of a theoretical treatment based on the compression of the chains on the surface of the opposite-lying colloid. Quantitative agreement with the experiment is obtained for all parameter combinations. [2]

[1] K. Kegler, M. Salomo, and F. Kremer, PRL 98, 058304 (2007)

[2] Kati Kegler, Martin Konieczny, Gustavo Dominguez-Espinosa,Christof Gutsche, Matthias Salomo, Friedrich Kremer, and Christos N. Likos submitted to PRL

CPP 34.52 Thu 17:00 Poster A

Static and dynamic properties of Polyelectrolytes — •Jens Smiatek and Friederike Schmid — Fakultät für Physik, Condensed Matter Theory, Universität Bielefeld, 33615 Bielefeld, Germany

We study the dynamics of charged macromolecules in salt solutions, taking full account of the electrostatic and the hydrodynamic interactions.

The polyelectrolyte is modeled by a simple coarse-grained bead-spring model which is embedded in free solution. All particles are simulated by Dissipative Particle Dynamics and we use the freely available software package ESPResSo.

Special interest is spent on the dynamic and static properties of polyelectrolytes like the structure factor and the single monomer displacement. All results will be carefully analyzed in the light of existing theories.

CPP 34.53 Thu 17:00 Poster A

Polypyrrole Nanowires Grown from Polyelectrolyte Single Molecules — •Vera Bocharova[1], Anton Kiriy[1], Hartmut Vinzelberg[2], Ingolf Moench[2], and Manfred Stamm[1] — [1]Leibniz Institute of Polymer Research Dresden, Dresden, Germany — [2]Leibniz Institute for Solid State and Materials Research, Dresden, Germany

Low-dimensional nanostructures of conductive polymers have attracted a great interest as building blocks for future miniatuarized nanoelectronic devices and highly sensitive chemical or biological sensors. We have developed a template method to grow continuous highly conductive polypyrrole (Ppy) nanovires (NWs) of variable diameter by polymerization of pyrrole from individual adsorbed polystyrene sulfonic acid (PSA) molecules. [Bocharova, V. Kiriy, A.; Vinzelberg, H.; Mönch, I.; Stamm, M. Angew. Chem. 2005, 117, 6549] The DC conductivity of individual Ppy NWs is not linearly dependent on their diameter. It is likely due to of granular structure of the NWs and a percolation-like conductivity reflecting a transition from the 1D to 2D and then to 3D-percolation networks of grains resulting into increase of the conductivity up to typical Ppy bulk conductivity. We found that the conductivity decreases with decreasing of temperature, as typical for semiconductors. The conductivity can be described using variable-range hopping model. According to this model the transition from 2D to 3D-percolation network of spherical grains was found.

CPP 34.54 Thu 17:00 Poster A

Influence of solvent and counterion on the effective charge and size of polyelectrolytes — •Ute Böhme and Ulrich Scheler — Leibniz Institute of Polymer Research Dresden, Hohe Strasse 6, D-01069 Dresden, Germany

The effective charge of polyelectrolytes in mixtures of organic solvents and water is primarily governed by the permittivity. Decreasing the dielectric constant leads to stronger charge- charge interaction on the polyelectrolyte resulting in enhanced counterion condensation and thus reduced effective charge. A combination of diffusion and electrophoresis NMR is applied to determine the effective charge of polyelectrolytes with different monovalent counterions in polar solvents adjusting permittivity by water content [1,2].

In solvents with high water fraction the charge decreases linearly with the permittivity while in mixtures with low water content the effective charge and size of the polyelectrolyte drops dramatically depending on the counterion. Reduced repulsive interactions between the charges along the chain lead to a more compact conformation of the polyelectrolyte.

[1] U. Scheler in H.S. Nalwa (ed.): Handbook of Polyelectrolytes and their applications, American Scientific Publishers (2002), Vol.2

[2] U. Böhme, U. Scheler, J. Colloid Interface Sci., 309, (2007), 231.

CPP 34.55 Thu 17:00 Poster A

Phase behavior of polyelectrolyte multilayer investigated by thin film calorimetry — •Heiko Huth[1], Renate Müller[2], Andreas Fery[3], and Christoph Schick[1] — [1]Universität Rostock Institut für Physik, Universitätsplatz 3, 18051 Rostock — [2]MPI für Kolloid- und Grenzflächenforschung, Am Mühlenberg, 14424 Potsdam — [3]Universität Bayreuth Physikalische Chemie II, Universitätsstr. 30, 95447 Bayreuth

Polyelectrolyte multilayer can be easily assembled using spraying or dipping of the different polyelectrolytes [1]. The thickness of the produced layers (nanometer range) is well controlled by the preparation conditions. Only a few methods are available for dynamic investigations, as afm for mechanical properties [2].

AC-chip calorimetry is used as a very sensitive tool for calorimetric investigations of such thin films as demonstrated for thin polymeric films [3]. To investigate the phase behavior of polyelectrolytes the humidity is used as a new parameter in addition to temperature for calorimetry. First measurements with the modified calorimeter for the PSS/PDADMAC polyelectrolyte multilayer system are shown. Further extensions of the calorimeter for better understanding of the phase behavior are discussed.

[1] Decher, G. and J.D. Hong, Phys. Chem. Chem. Phys., 1991. 95(11): 1430.

[2] Mueller, R., et al. Macromolecules, 2005. 38(23): 9766.

[3] Huth, H., Minakov, A. A., Schick, C., J. Polym. Sci. B Polym. Phys. 2006 44: 2996.

CPP 34.56 Thu 17:00 Poster A

Forces of interaction between polyacrylic acid brushes as measured by optical tweezers — •Gustavo Dominguez-Espinosa[1], Alla Synytska[2], Astrid Drechlser[2], Christof Gutsche[1], Friedrich Kremer[1], Petra Uhlmann[2], and Manfred Stamm[2] — [1]Institute of Experimental Physics I, Leipzig University, Linnéstr. 5, 04103, Leipzig, Germany — [2]Leibniz Institute of Polymer Research Dresden, Hohe Str. 6, 01069, Dresden, Germany

The forces of interaction between polyacrylic acid brushes grafted on two separated silica colloids are measured by Optical Tweezers (resolution of the forces 0.5 pN and resolution in position 3 nm). The interaction potential of the polyacrylic acid brushes is determined in dependence of the pH, ion concentration and valence of the surrounding medium. Scaling of the brush thickness with the power of the ionic strength is found in qualitative agreement with the theoretical predictions. The observed increase in the brush thickness with the increasing pH is attributed to the electrostatic repulsion caused by dissociation of the polyacrylic acid.

CPP 34.57 Thu 17:00 Poster A

Influence of preparation conditions on lateral and vertical surface structure of polyelectrolyte multilayers — •Matthias Cornelsen, Stephan Block, Manesh Gopinadhan, and Christiane A. Helm — Institut für Physik, Ernst-Moritz-Arndt Universität, Felix-Hausdorff-Str. 6, D-17487 Greifswald, Germany

Polyelectrolyte multilayers from PAH and PSS are formed at different ion concentrations and temperatures. If the electrostatic force is screened (i.e. the ion concentration exceeds 0.05 M), then the film thickness increases on the rise of both temperature and salt concentration. However, for each salt concentration there is a maximum temperature up to which stable films can be formed. If films from temperatures 40 to 5 K below this maximum temperature are compared, one finds with X-ray reflectivity that the film/air roughness increases (from 1 to 4.5 nm) on approach to the maximum temperature. Also, with AFM a surface coarsening is observed on the scale of 150 to 300 nm. Furthermore, the average distance between height maxima is measured, which changes depending on preparation conditions from 15 to 30 nm. These maxima may be attributed to coils or parts of coils of single chains.

CPP 34.58 Thu 17:00 Poster A

Water incorporation in poylectrolyte multilayers: Hofmeister effect? — •Oxana Ivanova[1], Olaf Soltwedel[1], Manesh Gopinadhan[1], Jens-Uwe Günther[1], Matthias Cornelsen[1], Roland Steitz[2], and Chrstiane A. Helm[1] — [1]Institut für Physik,Ernst-Moritz-Arndt Universität,Felix-Hausdorff-Straße 6, 17489 Greifswald,Germany — [2]Hahn-Meitner Institut, Glienicker Straße 100, D-14109 Berlin, Germany

The Hofmeister effect - the effect of salt on the hydrophobic effect - on the formation of polyelectrolyte multilayers is studied. Films are prepared while varying the preparation temperature T and the countercation (1 M XCl). For characterization, X-ray and neutron reflectivity are used. Selectively deuterated polyanion layers lead to at least two superstructure peaks. The PAH/PSS bilayer thickness is independent of the kind of salt and increases on temperature rise. Yet, at low T the amount of bound water depends strongly on the position of the cation in the Hofmeister series ($Cs^+ < Ka^+ < Na^+$). The internal roughness is 30-40 % of the bilayer thickness; it increases to up to 60% at high T. The temperature at which the roughening starts is a function of the countercation (ca. 50°C for NaCl, ca. 40°C for KCl and ca. 30°C for CsCl). It appears that the temperature effect - which is attributed to the melting of the first-shell water on temperature rise - is promoted by the countercations as predicted by the Hofmeister series. The effect is subtle; it manifests itself as an increased internal roughness, a loss of bound water and a downshift of the roughening temperature - whereas the thickness of the deposited bilayer is not affected.

CPP 35: Interfaces

Time: Friday 10:30–12:30 Location: C 130

Prize Talk CPP 35.1 Fri 10:30 C 130

Nonlinear light scattering: Bridging the gap between surface science & soft matter — •Sylvie Roke — Max-Planck Institute for Metals Research, Heisenbergstrasse 3, 70569 Stuttgart — Trägerin des Herta-Sponer-Preises

Interfaces are important locations for an enormous variety of physical, chemical and biological processes. Although surface science studies are usually performed on flat interfaces under controlled environments, in reality most interfaces are part of complex (soft matter) systems, such as cell membranes, emulsions or grains in solid materials. In the last decades it has become possible to address structural and dynamical questions relating to flat interfaces under ambient conditions, by probing them with nonlinear optical techniques. If one combines light scattering with nonlinear optical processes it is now becoming possible to go one step further: Interfaces of dispersed particles can be investigated in situ[1].

In this presentation I will introduce nonlinear optical scattering, highlight new possibilities that are becoming available and show some of the latest developments. These include: the possibility of investigating molecular surface effects in colloidal phase transitions[2], how to extract molecular properties[3] and the possibility of observing embedded structures in (polymer) materials.

[1] - S. Roke, W. G. Roeterdink, J. E. G. J. Wijnhoven, A. V. Petukhov, A. W. Kleyn and M. Bonn, Phys. Rev. Lett., 91 (2003), 258302-1. [2] - S. Roke, J. Buitenhuis, M. Bonn and A. Van Blaaderen, J. Phys.: Condens. Matter., 17 (2005), S3469-S3475; S. Roke, J. Buitenhuis, A. van Blaaderen and M. Bonn, PNAS, 103 (2006), 13310-13314. [3] - A. G. F. de Beer and S. Roke, Phys. Rev. B, 75 (2007), 245438-1-8.

CPP 35.2 Fri 11:00 C 130

MD simulations of sheared brush-like systems — •Leonid Spirin[1], Torsten Kreer[2], and Kurt Binder[1] — [1]Johannes Gutenberg-Universitaet Mainz, Institut fuer Physik, Staudinger Weg 7, 55099 Mainz, Germany — [2]Institut Charles Sadron, 6 Rue Boussingault, 67083 Strasbourg, France

Friction forces between two solid surfaces bearing polymer brushes play a key role in many applications. However, systems with soft colloids between polymer brushes have not been investigated yet. Star polymers can be taken as a model of hairy micelles or soft colloids. We perform Molecular Dynamics simulations of such systems under shear. Statical and dynamical properties are investigated. In particular, we focus on the response to non-stationary external stimuli.

CPP 35.3 Fri 11:15 C 130

Reversible activation of a polyelectrolyte brush — V. Papaefthimiou[1], J.-U. Günther[2], C. A. Helm[2], S. Förster[3], G. H. Findenegg[1], and •R. Steitz[4] — [1]Technische Universität Berlin — [2]Ernst-Moritz-Arndt-Universität Greifswald — [3]Universität Hamburg — [4]Hahn-Meitner-Institut Berlin

Polyelectrolytes anchored on surfaces are important in various applications and are also a challenging topic for fundamental studies. In this work, a monolayer of the PEE114PSS83 [(poly(ethyl ethylene)114 poly(styrene sulfonic acid)83] diblock copolymer was transferred from the air/water interface to a deuterated polystyrene coated silicon (dPS/Si) surface, for evaluation as a tunable polyelectrolyte-brush containing system. The grafting density of the polymer film was controlled by changing the lateral pressure during the depositions. X-Ray Reflectivity and AFM measurements showed that a homogeneous layer of the block copolymer was formed, whose thickness (maximum 8 nm) increased with increasing grafting density. Neutron reflectivity studies against aqueous solutions revealed a hydrophobic PEE layer attached on the dPS/Si surface, and a carpet/brush polystyrene sulfonate (PSS) double layer in water. The effect of salt concentration on the brush nanostructure was investigated in aqueous solutions containing 0-1 M NaCl. It was found that the brush thickness decreases for salt concentrations above 0.1 M. In addition, reversible activation of the brush by changing the ionic strength of the subphase was demonstrated. These results confirm a potential use as a stimuli-responsive polymer for both fundamental studies and biological applications.

CPP 35.4 Fri 11:30 C 130

Polarisation modulation IR studies on silica surfaces functionalised with protein resistant coatings — •Stefan Zorn[1], Iain Dunlop[2], Alexander Gerlach[1], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen, Germany — [2]Max Planck Institut für Metallforschung, Stuttgart, Germany

We performed polarisation modulation infrared reflection absorption spectroscopy (PM-IRRAS) studies of organic silane coatings on silica surfaces and their protein resistance. PM-IRRAS measurements require conducting surfaces to get a signal and to benefit from the surface selection rules. In the case of silane chemistry an important tool to functionalise silicon and glass surfaces this is hardly possible. We developed a multilayer, consisting of a titanium layer and a sputtered silica layer on top which is easy to produce and enables us to perform PM-IRRAS measurements on silanised surfaces. We studied biotinylated PEG2000 layers, a widely used system for sensor surfaces, and their ability to resist unspecific protein binding and enables specifically streptavidin binding. We were able to demonstrate PEG adsorption on the substrates and the specific binding of streptavidin with characteristic absorption modes. We also discuss theoretical aspects of the signal on different layer systems with the help of simulations based on the Fresnel equations.

CPP 35.5 Fri 11:45 C 130

Unspecific adsorption of protein films: dynamics and morphology — •Yvonne Schmitt, Hendrik Hähl, Hubert Mantz, and Karin Jacobs — Saarland University - Department of experimental physics, 66123 Saarbrücken, Germany

Protein adsorption takes place whenever a surface is in contact with a protein solution and can for example lead to fouling. The control of adsorption therefore is of crucial importance for many boilogical and biomedical applications like dentistry and the design of implants. By performing in-situ AFM scans in a liquid environment it is possible to gain insight in the complex process of unsecific protein adsorption. The dynamics was monitored via a series of AFM images. The characterization of the spatial protein distribution is done by means of integral geometric methods (Minkowski-functionals) that allow to distinguish between random sequential adsorption and guided adsorption and gives an objective description of the morphology of the protein film. The experimental results will be compared with recent simulations in order to develop a comprehensive description of the the adsorption process which could possibly allow to predict the next adsorption sites for a given protein arrangement.

CPP 35.6 Fri 12:00 C 130

Activity and Conformation of Lysozyme Adsorbed on Surfaces of Nanodiamond/-silica — •Victor Wei-Keh Wu — Department of Chemical and Materials Engineering, National Kaohsiung University of Applied Sciences, 80782 Kaohsiung, Taiwan — Victor Basic Research Laboratory e. V. Gadderbaumer-Str. 22, 33602 Bielefeld, Germany, Email:victorbres3tw@yahoo.com.tw, Tel:+886-919-300-525.

Coverages and adsorption constants via fluorescence of free lysozyme before and after adsorption on the surfaces of nanodiamond/-silica of diameter 100 nm with their suspension solutions prepared with concentration of 25 mg in 10 mL PPBS of 7 mM at pH=11 have been obtained. 55 and 15 nm^2/g BET surfaces of nanodiamond/-silica after adsorptive-dose rate-static-volumetric method were obtained. 12 and 4 nm^2 as available surfaces for each lysozyme at saturation threshold 190 and 175 nM for lysozyme and nanodiamond/-silica, respectively, can be derived. Coverages 10∼65 % after adsorption on nanodiamond correspond 10∼75 % of the original lysozyme activity, if effects upon helicity for both at pH=5 and 11 were similar. Lysozyme can possibly keep its helicity well and show its optimal activity, even as surface on nanodiamond is covered nearly 100 % at 700 nM. On the contrary, it on surface of nanosilica can still keep its helicity well, only if its concentration is lower than 100 nM. It might be deformed or changed with its folding structure much in the region of 100-1000 nM. Nanosilica is rather incompetent in the sense of adsorption of lysozyme. **Ref**. 1. V. W.-K. Wu, CL. 35, 1380 (2006), 2. T.-T. Bao Nguyen, H.-C. Chang, and V. W.-K. Wu, Diamond and Related Materials, 16, 872 (2007).

CPP 35.7 Fri 12:15 C 130

Specific Ion Adsorption at Solid Surfaces — •Dominik Horinek, Douwe Bonthuis, and Roland R. Netz — Physik Department, Technische Universität München, 85748 Garching, Germany

Ion specific effects at solid surfaces are of fundamental importance in biology, physics, and chemistry. Contrary to electrostatic forces, which are well-described by analytical theories, there is no satisfying theory for all solvent-induced forces. We present molecular dynamics simulations for the calculation of potentials of mean force for ion adsorption at hydrophobic and hydrophilic surfaces. We discuss ion specific effects at infinite dilution as well as their implications for the surface tension and surface potential at finite salt concentrations based on an extended Poisson-Boltzmann modeling where we include the potentials of mean force from simulation. We obtain qualitative agreement with experiments.

CPP 36: Biopolymers and Biological Systems

Time: Friday 10:30–12:45 Location: C 264

CPP 36.1 Fri 10:30 C 264

Spin Label EPR on Biological Systems — •Malte Drescher — Emmy-Noether-Gruppe am FB Chemie, Universität Konstanz, Fach M639, 78457 Konstanz

In spite of significant progress, the challenging areas for structure determination in biological systems are still ample: Membrane proteins, protein-protein interactions and membrane association are important for biological function, but because of the amphipathic nature of the first and the intrinsic disorder of the latter systems, conventional methods of structure determination usually do not work. By advanced EPR methods the interaction between spin labels can be measured from 5 Å to 5 nm. Paramagnetic labels can be attached to proteins, nucleic acids and lipids, and as native paramagnetic centres are scarce, the method is background free. Examples of applications to proteins and membranes will be discussed.

CPP 36.2 Fri 10:45 C 264

Digital in-line soft X-ray holography as microscopy technique for biological samples — •Axel Rosenhahn[1], Ruth Barth[1], Florian Staier[1], Todd Simpson[2], Silvia Mittler[2], Stefan Eisebitt[3], and Michael Grunze[1] — [1]Angewandte Physikalische Chemie, Universität Heidelberg, Germany — [2]Department of Physics and Astronomy, The University of Western Ontario, Canada — [3]BESSY m.b.H., 12489 Berlin, Germany

Digital in-line soft X-ray holography (DIXH) is a lenseless approach towards microscopy at short wavelength. We present measurements which successfully prove that the original Gabor geometry can be applied to X-rays and a lateral resolution of 400 nm can be achieved. Objects of different thickness and materials were used to determine the imaging properties of holographic microscopy in the VUV and soft X-ray wavelength range. By tuning the x-ray energy, element specific contrast can be obtained e.g. at the carbon K edge. These results are promising with respect to the possibility to exploit intrinsic contrast mechanisms for biological samples. Using fibroblasts and other cells, the sensitivity of the technique to resolve small structures inside these extended objects will be discussed. Although the spatial resolution still needs to be improved, these experiments are a starting point for future, lenseless holospectroscopy.

CPP 36.3 Fri 11:00 C 264

Reptation of individual F-Actin Filaments in 3D Networks — •Masashi Degawa, Norbert Kirchgessner, Bernd Hoffmann, Rudolf Merkel, and Margret Giesen — Institut für Bio- und Nanosysteme 4, Forschungszentrum Jülich, 52425 Jülich Germany

The mechanical properties of the cell are determined by a 3D network of polymerized protein filaments, the cytoskeleton. For deeper understanding of cell biomechanics, it is crucial to understand the physical properties of such polymer network. In the past, we have concentrated on the study of individual F-actin filaments within the network. Dynamics of the filaments were studied in the time scale of μsec to a sec where the transverse fluctuation from the filament contour is dominant and results were well described by the Glassy Worm-like chain Model [1]. Here we present dynamic studies of the same system, however, in the time scale of min to an hr where the motion along the filament contour is now dominant. F-Actin are labeled with TRITC and visualized with line-scan confocal scanning microscope. We measure the filament contour as a function of time. Specifically we focus on the curvature of the filaments, which in recent work indicate glass like properties, where the ergodic theorem breaks down [2]. [1] J. Glaser, et al. submitted to Eur. Phys. J. (2007) [2] M. Romanowska, et al. submitted to Phys. Rev. Lett. (2007)

CPP 36.4 Fri 11:15 C 264

Time-dependent Chain Rupture of Single Double-stranded DNA — •Hua Liang, Nikolai Severin, Igor m. Sokolov, and Jürgen P. Rabe — Department of Physics, Humboldt University, D-12489 Berlin, Germany

The rupture of single covalent bonds is a fundamental scientific issue. Under applied force this is a statistical process with a characteristic time scale depending on the force loading rate. This has been predicted theoretically and proven experimentally for fast force loading rates (1). In the established experimental methods such as dynamic force spectroscopy and dragging molecules with dynamic flow (2), information on the rupture of a single covalent bond is obtained from the breakage of a single polymer chain. However, these methods do not allow to investigate breakage of a covalent bond upon application of a static force. On the other hand, theory predicts that covalent bond rupture under static force is qualitatively different from rupture under dynamic force. Here we report a newly developed method (3) which allows placing a single polymer chain, e.g. a single double-stranded DNA molecule under a static force for an hour or more. The first results elucidate the difference between bond breaking under static force and dynamic force application. The data also allow us insight into the energy landscape of a covalent bond.

1. M. Grandbois et al, Science 283 (1999) 1727-1730;
2. D. Bensimon et al, Physical Review Letters 74 (1995) 4754-4757;
3. N. Severin et al, Nano Letters 6 (2006) 2561-2566.

CPP 36.5 Fri 11:30 C 264

Cyclization of short DNA fragments: the effects of electrostatic interactions — •A. G. Cherstvy[1] and R. Everaers[2] — [1]Theorie-II, IFF, FZ Juelich, D-52425 Juelich, Germany — [2]Ecole Normale Superieure de Lyon, 46 Allee d'Italie, 69364 Lyon Cedex 07, France

Cyclization of short DNA fragments is known to be a reliable method for measuring the elastic response of DNA molecules to twisting and bending [1]. Although the DNA is one of the most highly charged biopolymers known in nature, the standard theories developed for calculation of the ring formation probabilities by semiflexible polymers [2] neglect completely the electrostatic interactions along DNA chain. We show how the Shimada-Yamakawa theory for DNA cyclization factors [2] is modified due to the presence of charges on DNA. We also study [3] to which extent the phenomenon of Manning's conterion condensation on a straight highly charged cylinder [4] will differ for a DNA ring. We are interested also how the Odijk-Skolnick-Fixman theory of electrostatic persistence of weakly bent rod-like polyelectrolytes [5] will be modified for small circles of DNA.

[1] K. Rippe, et al., Trends Biochem. Sci., 20, 500 (1995). [2] J. Shimada and H. Yamakawa, Macromol., 17 689 (1984). [3] A. G. Cherstvy and R. Everaers, work in preparation. [4] G. S. Manning, J. Phys. Chem. B, 111 8554 (2007). [5] T. Odijk, J. Pol. Sci., 15 477 (1977).

CPP 36.6 Fri 11:45 C 264

Reversible photothermal dehybridization of DNA attached to gold nanoparticles — •Maximilian Reismann[1], Jan Bretschneider[2], Ulrich Simon[2], and Gero von Plessen[1] — [1]I. Inst. of Physics (IA), RWTH Aachen University, Germany — [2]Inst. for Inorganic Chemistry, RWTH Aachen University, Germany

Heat released from laser-irradiated metal nanoparticles can be applied to control biomolecules attached to the nanoparticles. Several studies have investigated destructive processes caused by nanoparticle-assisted photothermal heating, such as hyperthermia of malignant cells. In contrast, the photothermal control of non-destructive, *i.e.* reversible, biomolecular reaction processes has rarely been studied. Here we investigate the reversible photothermal control of the DNA dehybridization process. For this purpose, gold nanoparticle networks are synthesized using complementary single-stranded DNA as linker molecules. The well-known color change of such nanoparticle networks that occurs upon disassembly or assembly is applied to continuously monitor the state of the networks using optical spectroscopy. The DNA-nanoparticle network suspensions are heated by irradiation with focused c.w. laser light. This heating causes a disassembly of the networks, indicating the dehybridization ('melting') of the DNA double strands. After laser irradiation, the networks reassemble, thus indicating the reversibility of the dehybridization process. It is shown that the DNA melting occurs predominantly within the 100 μm wide laser focus, where the intensity is highest, thus enabling a highly local control of the reaction.

CPP 36.7 Fri 12:00 C 264

Structural Changes of Casein Micelles in a Calcium and an Enzym (Rennet) Gradient Film — •Ronald Gebhardt[1], Manfred Burghammer[1], Christian Riekel[1], Stephan Volkher Roth[2], and Peter Müller-Buschbaum[3] — [1]European Synchrotron Radiation Facility, BP 220, F-38043 Grenoble Cedex 09, France — [2]HASYLAB at DESY, Notkestr. 85, 22603 Hamburg, Germany — [3]TU München, Physik-Department, LS E13, James-Franck-Str.1, 85747 Garching, Germany

Caseins are phosphoproteins consisting of blocks with high amounts of hydrophobic and hydrophilic amino acids. Due to their amphiphilic nature they are able to built up casein micelles which are broadly distributed in size. The stability of the casein micelles is ensured by an outer kappa-casein layer. Concentration gradients of calcium and rennet were choosen to destabilize the association structures in casein films. While rennet cuts off the hairs of the layer, calcium leads to a compactation of the micelles and a decrease of the layer thickness by satturating the negative charged caseins. This first step of milc conversion, followed normally by aggregation and flocculation and finaly gel formation, can be well investigated in casein gradient films using grazing incident small angle scattering with a micrometer sized beam (microGISAXS). Differnt structural conformations along the reaction pathway are frozen inside the film and can be detected with high statistical relevance in a nondestructive way.

R. Gebhardt , M. Burghammer , C. Riekel, S. V. Roth , and P. Müller-Buschbaum (2007) Macromol. Biosci. accepted

CPP 36.8 Fri 12:15 C 264

Protein dynamics-induced modulation of excitation energy transfer — •Marc Brecht, Volker Radics, Jana Berit Nieder, Hauke Studier, and Robert Bittl — Fachbereich Physik, Freie Universität Berlin, Arnimalle 14, 14195 Berlin, Germany

Electron and energy transfer in proteins are key processes in bioenergetics. Their understanding on a molecular level can serve as important guideline for the design of nanoscale assemblies. Energy transfer between pigment molecules requires a match between their transition energies for energy emission and absorption. The tuning of these pigment energies in proteins is achieved by pigment-protein interactions. In general, these interactions are regarded as static properties determined by the three-dimensional structure of pigment-protein complexes. Employing single-molecule fluorescence spectroscopy on photosystem I [1] we demonstrate that protein dynamics, even at cryogenic temperatures, significantly influences the transition energy of pigments and, as a consequence, modulates energy transfer pathways. Our finding shows that the energy transfer pathway in photosystem I is not uniquely defined by the three-dimensional structure of the complex. This variability of energy transfer pathways introduced by protein dynamics might be important for the extreme robustness of photosystems [2].

[1] Brecht, M., Studier, H., Elli, A. F., Jelezko, F., and Bittl, R. (2007) Biochemistry, 46(3):799-806. [2] Brecht M., Radics V., Nieder J. B., Studier H., Jelezko F., Bittl R. submitted

CPP 36.9 Fri 12:30 C 264

Thermodynamics of proteins: pressure and temperature denaturation curves — •Johannes Wiedersich[1,2], Simone Köhler[1], Josef Friedrich[1], and Arne Skerra[3] — [1]Lehrstuhl für Physik Weihenstephan, TU München — [2]Physikdepartment E13, TU München — [3]Lehrstuhl für Biologische Chemie, TU München

The folding and unfolding of proteins shows a complex scenario, the details of which are not yet fully understood. One important aspect concerns the stability of proteins. By means of fluorescence spectroscopy we obtain the equillibrium constant for the denaturation of the engineered fluorescein-binding protein FluA as a function of both pressure and temperature. From the full thermodynamic analysis of the transition curves all of the involved global thermodynamic parameters of protein folding are determined, in particular the changes in entropy and volume, compressibility, thermal expansion and specific heat.

We demonstrate that the phase diagram of protein folding is closed and assumes an elliptic shape. The thermodynamic condition for such an elliptic phase diagram is related to the degree of correlation between fluctuations of the changes in volume and enthalpy at the phase boundary. This correlation is moderately low, on the order of 0.05 in our case. Our study suggests that the elliptic phase diagram is a consequence of the inherent conformational disorder of proteins and that it may be viewed as the thermodynamic manifestation of the high degeneracy of conformational energies that is characteristic for this class of macromolecules.

CPP 37: Molecular Dynamics

Time: Friday 10:30–12:30 Location: C 230

CPP 37.1 Fri 10:30 C 230

Investigation of polymer dynamics in acrylnitrile butadiene rubber — •Juliane Fritzsche and Manfred Klüppel — Deutsches Institut für Kautschuktechnologie e.V., Eupener Straße 33, D-30519 Hannover, Germany

The field of application of elastomers is determined by their frequency dependent dielectric and dynamic-mechanical properties. The dynamic spectrum of such materials becomes very important for understanding the correlation between parameters of the molecular and supramolecular structure on one hand and macroscopic properties on the other.

The frequency dependent mechanical behaviour is obtained by dynamic-mechanical analysis (DMA) and dielectric spectroscopy. Dielectric broadband relaxation spectroscopy covers a frequency range between 10-1 and 109 Hz. In this range molecular and collective dipolar fluctuations, charge transport and polarization effects at inner and outer boundaries take place and determine the dielectric properties of the material. However, molecular and collective dipolar fluctuations are related to characteristic parts of a molecule (functional group) or the molecule as a whole and give raise to characteristic relaxation processes. The investigation of these processes is one of the most important applications of this method as information about the polymer dynamics can be obtained.

In this presentation we will show the investigation of a acrylnitrile butadiene rubber unfilled and filled with different loadings of silica and carbon black. We obtained the dynamic-mechanical behaviour and the dielectric properties in a wide frequency range.

CPP 37.2 Fri 10:45 C 230

Molecular dynamics simulations of polymer brushes — •Gui-Li He[1], Holger Merlitz[1,2], Jens-Uwe Sommer[2], and Chen-Xu Wu[1] — [1]Xiamen University, Department of Physics, 361005 Xiamen, China — [2]Leibniz-Institut für Polymerforschung Dresden, 01069 Dresden, Deutschland

We have carried out molecular (Langevin) dynamics simulations of polymer brushes up to very high grafting densities. We report on the fluctuation properties, the excess free energy and the brush-crystallization at extreme grafting densities. The importance of finite extensibility in order to understand chain properties at high substrate coverage is demonstrated. Recent simulation results of mixed binary brushes are shown.

References: 1. Gui-Li He, Holger Merlitz, Jens-Uwe Sommer and Chen-Xu Wu, Static and dynamic properties of polymer brushes at moderate and high grafting densities: A molecular dynamics study, Macromolecules 40, p. 6721 (2007)

2. Gui-Li He, Holger Merlitz, Jens-Uwe Sommer and Chen-Xu Wu, Polymer brushes near the crystallization density, Eur. Phys. J. E (in press)

CPP 37.3 Fri 11:00 C 230

Interfacial dynamics of polymers in contact with solid substrates — •Anatoli Serghei and Friedrich Kremer — University of Leipzig, Linnestr. 5, Leipzig, 04103, Germany

Polymers exhibit alterations of their microscopic (and hence macroscopic) properties in the vicinity of solid interfaces. In the present contribution a novel experimental approach is demonstrated which enables one to investigate molecular fluctuations of polymer segments in the immediate (nanometric) vicinity of solid substrates. This development, employing nanostructures as spacers, renders to Broadband Dielectric Spectroscopy - traditionally a volume specific technique - the ability to measure the interfacial dynamics of organic materials in contact with solid substrates. The method readily allows to adjust the interfacial interactions by a controlled deposition of various (metallic but as well organic) layers onto the surface of the supporting electrodes. Experimental results on the interfacial dynamics of several polymers will be discussed, in systematic dependence on the interfacial interactions.

CPP 37.4 Fri 11:15 C 230

Surface diffusion of single polymer chains - a molecular dynamics study — •Christian Vree and S. G. Mayr — I. Physikalisches Institut, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

Bulk diffusion and transport of polymers in melts and solutions have attracted large scientific interest during the past decades in particular with respect to the influence of solvants, chain length, conformation and temperature. Contrary, surface kinetics of polymers are still poorly understood, although there is increasing interest in this field. Surface diffusion is of great importance in thin film physics, i.e. in physical vapor deposition methods. Therefore it is essential to understand the microscopic mechanisms of surface diffusion in more detail.

Here we present molecular dynamics studies of a polymer chain on a surface of a thin film of the same type of polymer. A cubic box with periodic boundary conditions in x- and y-direction and free surfaces in z-direction with typical dimensions of $42\sigma \times 42\sigma \times 30\sigma$, where σ is the bond length in Lennard-Jones units, acts as the substrate, where a single chain is placed on. Non-bonded particles interact via a truncated Lennard-Jones potential, while bonded particles interact via the FENE-potential suggested by Kremer and Grest (J. Chem. Phys. **92**, 5057, 1990). We find that the mobility on the surface is increased compared to the bulk value by about a factor of 2, while the time scaling does not change significantly.

This work is financially supported by the DFG SFB 602 (TP B3), as well as the GIF No. 1428-303.1/2004.

CPP 37.5 Fri 11:30 C 230

Disentanglement in thin polymer films — •Hendrik Meyer — Institut Charles Sadron, CNRS UPR22, Strasbourg, France

Molecular dynamics simulations of thin polymer films confined between structureless walls show accelerated in-plane dynamics with decreasing film thickness. Using the primitive path analysis (PPA) introduced by Everaers et al [Science 303 (2004) 823] for chain length up to N=1024, we can show that the entanglement density decreases with decreasing film thickness. However, the effect becomes pronounced only for films thinner than the bulk radius of gyration where also the structure of the chains becomes modified by the confinement [1]. The PPA algorithm can be modified to estimate the contribution of self-entanglements: The latter become more important for thinner films, however, they do not counterbalance the global decrease of entanglements.

[1] H. Meyer et al Eur. Phys. J. Sp.Top. 141 (2007) 167.

CPP 37.6 Fri 11:45 C 230

Binding and Diffusion of individual dye molecules in ultrathin liquid films — •Daniela Täuber, Jörg Schuster, and Christian von Borczyskowski — Research G.: From local constraints to macroscopic transport, TU-Chemnitz, Institut für Physik, 09107 Chemnitz

The structure and dynamics of liquids close to solid interfaces is of central interest for numerous practical applications involving microfluidic structures. By tracking of single dye molecules we have been able to reveal details of the molecular structure of ultrathin liquid films on interfaces in previous work [1].

Molecular motion in thin liquid film is not purely diffusive but includes also temporary sticking or binding of probes to the solid surface. Based on a series of recent experiments we demonstrate that sticking probabilities as well as the diffusion constants of various dyes in ultrathin TEHOS films are slowly changing on a time scale of days. Although the two phenomena are strongly interconnected, we can show that they are caused by two independent processes, namely i) the thinning of the film due to evaporation, and ii) a change of the chemical composition of the surface which will lead to a decrease of the sticking probability a few days after sample preparation. A simple surface chemistry model is presented to explain those observations. In addition we show that thinning of the films is accompanied by a slow down of diffusional motion, which supports further our findings of a strongly anisotropic diffusion due to the layering structure of the films [1].

[1] J. Schuster, F. Cichos, Ch. von Borczyskowski: Euro. Phys. J. E. 12 (2003), 75-80

CPP 37.7 Fri 12:00 C 230

Chain motion in poly(ethylene oxide) crystallites as studied by NMR — Anja Achilles, Albrecht Petzold, Thomas Thurn-Albrecht, and •Kay Saalwachter — Institut für Physik, Martin-Luther-Universität Halle Wittenberg, 06099 Halle (Saale)

Many stereoregular polymers exhibit pronounced large-scale dynamics in the crystalline phase. “Helical-jump” processes mediate chain transport over large distances through the crystallites, and they are often related to the mechanically active $\alpha_{(c)}$ relaxation and macroscopic properties such as yield processes and ultradrawability. While the timescale of such processes has been studied for many different polymers [1], their dependence on morphological parameters, such as crystalline and amorphous layer thickness, has received less attention.

In this contribution, we report on NMR investigations of helical jumps in PEO crystallites, using advanced high-resolution ^{13}C exchange spectroscopy as well as simple analyses of the ^{1}H time-domain signal. These results are correlated with SAXS-determined changes in the morphology and crystallinity as a function of molecular weight and the crystallization conditions.

[1] W.-G. Hu, K. Schmidt-Rohr, *Acta Polym.* **50**, 271 (1999)

CPP 37.8 Fri 12:15 C 230

Morphological Differences in Semi-crystalline Polymers: Its Implications on Local Dynamics and Chain Diffusion — •Robert Graf[1], Yefeng Yao[1], Sanjay Rastogi[2], and Hans Wolfgang Spiess[1] — [1]Max-Planck-Institut für Polymerforschung, 55128 Mainz, Deutschland — [2]Eindhoven University of Technology, 5600MB Eindhoven, The Netherlands

Morphological differences in semi-crystalline polymers due to different crystallization conditions have strong implications on the chain motion. Using a broad variety of solid state NMR techniques probing the molecular dynamics on different time and length scales, the local dynamics in the non-crystalline regions of solution crystallized linear polyethylene was found to be is lower than in a melt crystallized sample under the same conditions, but the opposite is observed for chain diffusion between non-crystalline and crystalline regions. The activation enthalpy for chain diffusion, however, is the same, indicating that entropic differences in the non-crystalline regions strongly influence the chain diffusion of the same polymer in different morphologies.

Reference:

Y-F. Yao, R. Graf, H.W. Spiess,D.R. Lippits, S. Rastogi, Phys. Rev. E, in press.