

CHEMICAL AND POLYMER PHYSICS

CHEMISCHE PHYSIK UND POLYMERPHYSIK (CPP)

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OVERVIEW OF INVITED TALKS AND SESSIONS

(lecture rooms ZEU Lich, ZEU 160, ZEU 114, ZEU 118)

Invited Talks

CPP 1.1	Mon	09:30	(ZEU Lich)	Polymer Thin Films and Mixed Brushes: Some Applications to Nanoscience , Manfred Stamm
CPP 4.1	Mon	14:00	(ZEU Lich)	Optical tweezers - novel tools in nanophysics , Friedrich Kremer , Christof Gutsche, Kati Kegler, Mathias Salomo, Joerg Reinmuth, Wiktor Skokow
CPP 7.1	Tue	09:30	(ZEU 160)	Structure and interfacial rheology of aggregated two dimensional suspensions , Jan Vermant , Sven Reynaert, Madivala Basavaraj, Moldenaers Paula, Franssaer Jan
CPP 7.5	Tue	11:00	(ZEU 160)	Non-linear rheological properties of glassy colloidal dispersions , Matthias Fuchs , Oliver Henrich, Michael Cates, Matthias Ballauff, Jerome Crassous, Fathollah Varnik
CPP 9.1	Tue	14:00	(ZEU 160)	Rheology and Structure Kinetics of Filled Polymer Nanocomposites and Networks , Gert Heinrich
CPP 9.6	Tue	15:45	(ZEU 160)	Microstructure design for food applications , Bettina Wolf
CPP 19.1	Thu	09:30	(ZEU Lich)	Electronic structure of hybrid interfaces for polymer-based electronics , William R. Salaneck
CPP 19.5	Thu	11:00	(ZEU Lich)	Fast and stable integrated polymer circuits , Walter Fix
CPP 20.1	Thu	09:30	(ZEU 160)	Interplay of slip and viscoelasticity in dewetting of thin liquid films , Markus Rauscher , Andreas Münch, Barbara Wagner, Ralf Blossey
CPP 20.5	Thu	11:00	(ZEU 160)	Sorting in Structured Microfluidic Devices , Alexandra Ros , Jan Regtmeier, Thanh Tu Duong, Dario Anselmetti
CPP 21.1	Thu	14:00	(ZEU Lich)	Recent Advances in Charge Transport in Organic Field effect Transistors , Ananth Dodabalapur , Liang Wang, Lawrence Dunn, Debarshi Basu
CPP 22.1	Thu	14:00	(ZEU 160)	Confinement and manipulation of single molecules in micro- and nanochannels , Petra Schwille , Fedor Malik, Petra S. Dittrich, Madhavi Krishnan
CPP 22.6	Thu	15:45	(ZEU 160)	Unconventional Microfluidics , Ralf Seemann , Jean-Christophe Baret, K. Khare, Craig Priest, Stephan Herminghaus

Sessions

CPP 1	Thin Films and Surfaces I	Mon	09:30–12:15	ZEU Lich	CPP 1.1–1.9
CPP 2	Colloids and Nanoparticles	Mon	10:00–12:30	ZEU 160	CPP 2.1–2.9
CPP 3	Polymer Materials	Mon	10:00–12:30	ZEU 114	CPP 3.1–3.9
CPP 4	New Experimental Techniques	Mon	14:00–17:45	ZEU Lich	CPP 4.1–4.13
CPP 5	Polyelectrolytes	Mon	14:30–17:45	ZEU 160	CPP 5.1–5.12
CPP 6	Electronic Structure and Spectroscopy I	Mon	14:30–17:45	ZEU 114	CPP 6.1–6.12

CPP 7	SYMPOSIUM Disperse Polymer Systems I	Tue 09:30–12:15	ZEU 160	CPP 7.1–7.8
CPP 8	SYMPOSIUM Nonequilibrium Phenomena in Soft-Condensed Matter	Tue 14:00–16:45	ZEU Lich	CPP 8.1–8.10
CPP 9	SYMPOSIUM Disperse Polymer Systems II	Tue 14:00–17:00	ZEU 160	CPP 9.1–9.9
CPP 10	POSTER Nonequilibrium Phenomena in Soft Condensed Matter	Tue 17:00–19:00	P3	CPP 10.1–10.11
CPP 11	POSTER Disperse Polymer Systems	Tue 17:00–19:00	P3	CPP 11.1–11.48
CPP 12	POSTER Colloids, Nanoparticles and Self-Organizing Systems	Tue 17:00–19:00	P3	CPP 12.1–12.31
CPP 13	POSTER New Experimental Techniques	Tue 17:00–19:00	P3	CPP 13.1–13.14
CPP 14	Polymer Crystallization	Wed 14:00–15:30	ZEU Lich	CPP 14.1–14.5
CPP 15	Dynamics and Diffusion	Wed 14:00–15:00	ZEU 114	CPP 15.1–15.4
CPP 16	Electronic Structure and Spectroscopy II	Wed 14:00–17:30	ZEU 160	CPP 16.1–16.11
CPP 17	Thin Films and Surfaces II	Wed 15:45–17:30	ZEU Lich	CPP 17.1–17.7
CPP 18	Polymer Materials II	Wed 15:45–17:15	ZEU 114	CPP 18.1–18.6
CPP 19	SYMPOSIUM Functional Organic Thin Films I	Thu 09:30–12:30	ZEU Lich	CPP 19.1–19.9
CPP 20	SYMPOSIUM Microfluidics I: Boundary conditions, manipulation, and transport	Thu 09:30–12:30	ZEU 160	CPP 20.1–20.9
CPP 21	SYMPOSIUM Functional Organic Thin Films II	Thu 14:00–17:00	ZEU Lich	CPP 21.1–21.10
CPP 22	SYMPOSIUM Microfluidics II: Soft objects in flow, open geometries	Thu 14:00–17:00	ZEU 160	CPP 22.1–22.9
CPP 23	POSTER Functional Organic Thin Films	Thu 17:00–19:00	P2	CPP 23.1–23.54
CPP 24	POSTER Microfluidics	Thu 17:00–19:00	P2	CPP 24.1–24.17
CPP 25	POSTER Electronic Structure and Spectroscopy	Thu 17:00–19:00	P2	CPP 25.1–25.22
CPP 26	POSTER Dynamics and Diffusion	Thu 17:00–19:00	P2	CPP 26.1–26.14
CPP 27	POSTER Polymer Physics and Materials	Thu 17:00–19:00	P2	CPP 27.1–27.52
CPP 28	Biological Systems	Fri 10:30–12:30	ZEU Lich	CPP 28.1–28.8
CPP 29	Computational Techniques	Fri 10:30–11:45	ZEU 160	CPP 29.1–29.5

Annual General Meeting of the Section Chemical and Polymer Physics

Wed 18:30–19:30 ZEU Lich

Tagesordnung

1. Tagungsnachlese
2. Symposien 2007
3. Sonstiges

Für das leibliche Wohl ist gesorgt.

Sessions

– Invited, Contributed Talks and Posters –

CPP 1 Thin Films and Surfaces I

Time: Monday 09:30–12:15

Room: ZEU Lich

Invited Talk

CPP 1.1 Mon 09:30 ZEU Lich

Polymer Thin Films and Mixed Brushes: Some Applications to Nanoscience — ●MANFRED STAMM — Leibniz Institute of Polymer Research Dresden, Germany

Polymers exhibit interesting properties that are used in the bulk, but can similarly provide interesting aspects with thin films. Crosslinked polymer networks thus can be highly swollen in solvents, and with a thin polymer bilayer film this effect may be utilized to produce nanotubes by scrolling of the film /1/, when the lower layer is swollen by the solvent while the upper layer is inert. The film can be patterned at the surface and the structure transferred to the inner surface of the tube formed. A fairly robust way of surface functionalization is the attachment of polymer chains to the surface by covalent bonding. At high grafting density a brush-like layer will be formed, and surface properties can be changed significantly. Utilizing mixed polymer brushes the surface properties can be switched between different states due to local phase segregation /2/, and it is even possible to switch between ultra-hydrophobic and ultra-hydrophilic behavior by introduction of an additional surface roughness. Mixed polymer brushes may be used for the control of protein adsorption or the separation of liquids by the effect of controlled surface interaction.

/1/ V. Luchnikov, M. Stamm, O. Sydorenko, *Advanced Materials*, 17, 1177-1182 (2005) /2/ L. Ionov, B. Zdyrko, A. Sidorenko, S. Minko, V. Klep, I. Luzinov, M. Stamm, *Macromolecular Rapid Communications*, 25, 360-365 (2004)

CPP 1.2 Mon 10:00 ZEU Lich

Thin Film Rupture: From Elastic Fracture to Viscous Fingering — ●SYLVAIN GABRIELE¹, GÜNTER REITER², and PASCAL DAMMAN¹ — ¹Université de Mons Hainaut Laboratoire de PhysicoChimie des Polymères Place du Parc, 20 B-7000 Mons — ²Institut de Chimie des Surfaces Interfaces 15, rue Jean Starcky F-68057 Mulhouse

The stability of thin polymer films on top of a solid surface is of importance for numerous applications ranging from the lubrication to microlithographic resist films. When forced to cover a non-wettable substrate, thin liquid film could be unstable and dewet. We will focus on different geometries of dewetting (circular and planar) which exhibit a variety of artistic morphologies of instability. We report experimental observations that suggest that different viscoelastic instabilities are directly related to the dissipation mode: elastic or viscous. The first case of instability appears at the early stage of dewetting in the elastic regime and is related to stress dissipation by fracture propagation. The formation of cracks into the asymmetric rim can be interpreted as the instantaneous response of a circular dynamic elastic ring to an applied tangential stress. As a result, the fractures propagation forms a complex structure in a starry shape which provides a faster way to release the accumulated stress. After a characteristic time t_2 , rims show fluctuations in width and finally yield to an artistic finger-like pattern. The transversal instability of the rim is clearly reminiscent of the Rayleigh-Plateau instability. We argue that determining the onset of this rim instability represents a reliable way for measuring the disentanglement time of polymer which corresponds to the characteristic time t_2 .

CPP 1.3 Mon 10:15 ZEU Lich

Flow of a complex liquid near a solid interface: SPM studies — ●HENDRIK HÄHL, LUDOVIC MARQUANT, DANIEL PODZIMEK, RENATE FETZER, and KARIN JACOBS — FR 7.2 Experimentalphysik - Weiche Materie, Universität des Saarlandes, D-66123 Saarbrücken

Dewetting of structured liquids is a very complex process. We investigate thin block-copolymer films composed of polystyrene-block-polyethylen/propylen (PS/EP) retracting from silanized silicon wafers. The equilibrium layer structure of the block-copolymer film vanishes in the presence of shear flow, giving way to a more complex structure. By tapping mode SPM, we can detect PS cylinders in a matrix of PEP.

These cylinders are aligned parallel to the moving three-phase contact line. Additional to the free surface of the film, we are interested in the film behaviour near the solid substrate. We found a novel method to scan the microdomain structure of the block-copolymer film just at this interface with SPM resolution. The alignment of the cylinders we also found here gives evidence to a nonzero slippage velocity.

CPP 1.4 Mon 10:30 ZEU Lich

Pretransitional Wetting Structures at a Thermotropic Liquid Crystal/Water Interface — ●CHRISTIAN BAHR — Max Planck Institute for Dynamics and Self-Organization, Bunsenstr. 10, 37073 Göttingen

Recently, theoretical interest has emerged concerning colloidal interactions between spherical particles, which are suspended in the isotropic phase of nematic liquid crystals and are covered with a nematic wetting layer [1]. A corresponding experimental system could consist of an emulsion of water droplets in an isotropic liquid crystal. It is not known, however, if at isotropic liquid crystal/water interfaces nematic wetting layers exist or what properties they have. We present here an ellipsometric study of such an interface near the nematic – isotropic phase transition. Approaching the transition temperature T_{NI} from above, a nematic wetting layer appears at the interface if the water phase contains a surfactant inducing a homeotropic alignment of the nematic phase. On further approaching T_{NI} , the thickness of the nematic layer shows a pronounced increase and a possible logarithmic divergence at T_{NI} . The detailed behavior is significantly influenced by the concentration of the surfactant. The experimental results can be described by a mean-field model in which the surfactant concentration tunes the magnitude of an ordering interface potential.

[1] H. Stark, *Phys. Rev. E* **66**, 041705 (2002); J. Fukuda, H. Stark, H. Yokoyama, *Phys. Rev. E* **69**, 021714 (2004); M. Huber and H. Stark, *Europhys. Lett.* **69**, 135 (2005).

— 15 min. break —

CPP 1.5 Mon 11:00 ZEU Lich

Structural analysis of triblock / diblock copolymer blend films: A comparative GISAXS study of films obtained by spin-coating and solution casting — ●V. KÖRSTGENS¹, M.M. ABUL KASHEM¹, S. STÜBER¹, S.V. ROTH², and P. MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik-Department E13, James-Frank-Str. 1, D-85747 Garching, Germany — ²HASYLAB at DESY, Notkestr. 85, D-22603 Hamburg, Germany

Films of styrene-isoprene-styrene (SIS) triblock copolymer blended with styrene-isoprene (SI) diblock copolymer and a naphthenic oil are investigated with grazing incidence small angle X-ray scattering (GISAXS). Polymer films were prepared from toluene solution on glass slides by two different procedures: On the one hand spin-coating technique was applied and on the other hand films were solution casted and dried. Both types of films differ markedly in thickness and structure. Moreover surface and bulk structures can be distinguished. Surface sensitive probes such as atomic force microscopy and optical imaging complement the scattering experiment.

CPP 1.6 Mon 11:15 ZEU Lich

Regular Nano-dot Patterns by Dewetting of Thin Organic Films — ●STEPHAN RATH, MARK HEILIG, and HELMUT PORT — 3. Phys. Inst. Universität Stuttgart

The dewetting of thin organic films UHV-deposited on He-cooled substrate is analyzed by optical and AFM microscopies. By controlled annealing to room temperature such films can be transformed into patterns of isolated droplets. The description of the dewetting process takes advantage of the close similarity to pattern formation and dynamics in

thin polymer films (polystyrene). Typical dewetting stages are discerned: spinodal hole formation, inhomogeneous extension of the hole, transformation into droplets via fingering and Rayleigh instabilities followed by droplet coarsening.

Films of a fulgide derivative, deposited on quartz glass substrates in the thickness range between 2 and 22 nm, will be considered as example. On smooth substrate surfaces, however, only irregular pattern of droplets are formed. In order to achieve regular patterns which are of interest for applications in molecular electronics and photonics, structured substrates are used as templates. In this way regular patterns of nano-dots with variable sizes and lateral distances have been produced.

CPP 1.7 Mon 11:30 ZEU Lich

Deformation of polymer thin films on structured substrates — ●JULIEN LEOPOLDES and PASCAL DAMMAN — Laboratoire de Physico-Chimie des Polymères, 20 Place du Parc, B7000 Mons

Polymer surface patterning is a crucial issue for many technological applications such as the manufacture of memory storage devices, catalyse, biomimetics or microfluidics. Various techniques are available, mainly based on lithography. It is however unanimously acknowledged that new routes toward the self-assembling of chemical and/or topographical patterns are urgently needed, to reduce the cost and accelerate the progress of the development of the micro and nano structuring processes. A most promising approach is the decomposition of thin films under the destabilizing influence of long range Van der Waals forces, but the complex patterns obtained still render their technological value rather unclear. Moreover, the limited scales (100nm) on which Van der Waals forces can be accounted for is actually a great limitation to a broad range of applications. Here we reveal other perspectives to achieve the control of the destabilisation of thin films, and henceforth the resulting surface properties. The films are adsorbed on chemically patterned substrates and the alteration of the film surface is initiated up to thicknesses corresponding to several microns.

CPP 1.8 Mon 11:45 ZEU Lich

Low-temperature structures of dipolar films — ●SABINE H.L. KLAPP — Stranski-Lab for Physical and Theoretical Chemistry, Sekr. C7, Technical University Berlin, Strasse des 17. Juni 115, 10623 Berlin — Institute for Theoretical Physics, Sekr. PN 7-1, Technical University Berlin, Hardenbergstrasse 36, 10623 Berlin

Recent theoretical and experimental research has demonstrated that fluids with dominant dipole-dipole interactions can display new, unexpected behavior such as self-assembly of the particles into dipolar chains, and crystallization into novel structures (1). In the present contribution we focus on the behavior of dipolar systems confined to thin films and in two spatial dimensions, a situation which is particularly important for colloidal systems with (ferro-)magnetic interactions and for thin magnetic films. Using lattice summations and density functional theory we analyze possible lattice structures as well as the fluid side of the phase diagram. We also present Monte Carlo data for thin dipolar fluid films with a thicknesses between one and two monolayers.

1) S. H. L. Klapp, J. Phys.: Condens. Matter **17**, R525 (2005).

CPP 1.9 Mon 12:00 ZEU Lich

Micro-focus GISAXS Investigation of Polymer Brushes — ●JOCHEN S. GUTMANN^{1,2}, GINA-GABRIELA BUMBU¹, MARKUS WOLKENHAUER¹, YAJUN CHENG¹, and RÜDIGER BERGER¹ — ¹Max Planck Institute for Polymer Research, Ackermannweg 10, D-55128 Mainz, Germany — ²Institute for Physical Chemistry, Johannes Gutenberg University Mainz, Welderweg 11, D-55099 Mainz, Germany

Polymer brushes are selective coatings for micromechanical cantilever (MC) sensors, enabling the use of MC sensor technology in liquid environments. To prepare covalently grafted polymer layers on MC sensors, a poly(methyl methacrylate) (PMMA) brush layer was grown using a grafting-from ATRP synthesis [1]. The brush layer acts as a sensing layer when brought into contact with different solvents. In our experiments we have noticed that the deflection/stress of the PMMA covered MC after the first swelling systematically differs from the values before swelling. This behaviour may be assigned to a structural 'memory' of previous treatments, i.e. the solvent/non-solvent used and the drying procedure. We therefore focus on the influence of the solvent used for swelling on the morphology of the dried PMMA brushes. In order to investigate the lateral structure of the brush layer on the μm sized cantilevers, we used a micro-focus set-up for X-ray scattering under grazing incidence (μ -GISAXS), at the BW4 beam line.

[1] Bumbu G.-G., Kircher G., Wolkenhauer M., Berger R., Gutmann J.S., Macromol. Chem. Phys. 2004, 205 (13): 1713-1720

CPP 2 Colloids and Nanoparticles

Time: Monday 10:00–12:30

Room: ZEU 160

CPP 2.1 Mon 10:00 ZEU 160

Self organization of micelles at solid-liquid interfaces — ●MAX WOLFF^{1,2}, MARCO WALZ³, ANDREAS MAGERL³, and HARTMUT ZABEL¹ — ¹Lehrstuhl für Festkörperphysik, Ruhr-Universität Bochum, Bochum, Germany — ²Institut Laue-Langevin, Grenoble, France — ³Lehrstuhl für Kristallographie und Strukturphysik, Universität Erlangen-Nürnberg, Erlangen, Germany

Self organizing systems are known to open new possibilities in nanopatterning of materials. One interesting aspect is the influence of a solid substrate on ordering in liquids. To gather in-situ non-destructive information on the not directly accessible solid-liquid interfaces is difficult. We have demonstrated that by taking advantage of the high penetration power of neutrons and combining neutron reflectivity (NR), off-specular scattering and near-surface small angle scattering (NS-SANS) three dimensional structural information from the μm down to nm regime becomes accessible.

We will demonstrate the importance of the properties of the solid-liquid interface, like the chemical termination, for the crystallization of three block polymer micelles. Additionally we will present data exploring the crystallization process for varying temperatures in great detail. We find a hysteresis not only in the size and formation of crystallites but also in the structure formed during crystallization and reorientation with increasing and decreasing temperatures. The presented findings from the neutron scattering experiments will be correlated to rheological studies.

CPP 2.2 Mon 10:15 ZEU 160

Energetics of Self-organization of 2D colloids in free-standing smectic-C films — ●CHRISTIAN BOHLEY and RALF STANNARIUS — Institut für Experimentelle Physik, Abteilung Nichtlineare Phänomene, Otto-von-Guericke-Universität Magdeburg, PF 4120, D-39016 Magdeburg

The formation of regular colloid patterns was shown experimentally for free smectic films at the transition from the smectic-C to the isotropic phase [1-3]. The self-organization of the isotropic droplets is caused by their mutual interaction, mediated by elastic distortions of the local liquid crystal (LC) director that are related to the anchoring conditions of the director at the droplet border. We describe analytically the energetics of a single droplet in the LC environment. A method of the complex analysis, the Conformal Mapping, is employed. Energetics of chain and grid patterns built from the isotropic colloids will be investigated numerically in order to explain the observed formations.

[1] C. Völtz, R. Stannarius, Phys. Rev. E **70**, 061702 (2004) [2] C. Völtz, R. Stannarius, Phys. Rev. E **72**, 011705 (2005) [3] R. Stannarius, C. Völtz, Phys. Rev. E **72**, 032701 (2005)

CPP 2.3 Mon 10:30 ZEU 160

Detailed structural analysis of wet-chemically synthesized II-VI semiconductor nanoparticles — ●FRANZISKA NIEDERDRAENK¹, PAWEŁ LUCZAK¹, ANDREAS STAHL¹, CHRISTIAN KUMPF¹, REINHARD NEDER², and EBERHARD UMBACH¹ — ¹Experimentelle Physik II, Univ. Würzburg — ²Inst. für Mineralogie und Kristallstrukturlehre, Univ. Würzburg

The determination of the detailed geometric structure of nanoparticles with diameters below 5 nm is of particular interest since these parti-

cles represent the transition regime between molecular and solid state physics. In principle, diffraction methods provide this information, but crystallographic analysis techniques, like the Rietveld refinement or a size determination with the Scherrer equation were developed for large particles (> 10 nm) and are not reliable any more below 5 nm.

To cope with this difficulty, we model the entire nanoparticle and use the Debye formula to calculate its powder diffraction pattern. This method allows us to directly determine intrinsic parameters which cannot be treated by most of the established crystallographic techniques, e.g. size-distributions, different shapes, stacking faults, strain, etc. The Debye formula has been embedded in an evolutionary algorithm, which enables an automatic refinement of the primary atomic model. Distributions of parameters are now considered, which are essential since they are likely to occur in wet-chemically synthesized particles. We present model calculations for ZnO, CdSe and CdSe/ZnS core-shell nanoparticles in the range of 2 - 10 nm and compare them with experimental data.

— 15 min. break —

CPP 2.4 Mon 11:00 ZEU 160

Janus particles at liquid/liquid interfaces — •NICOLE GLASER, ALEXANDER BÖKER, and GEORG KRAUSCH — Physikalische Chemie II, Universität Bayreuth, 95440 Bayreuth, Germany

Following recent theoretical predictions, we report on the first experiments on the interfacial assembly of so-called Janus nanoparticles, i.e. bifacial particles consisting of a gold and an iron oxide moiety, using pendant drop tensiometry. Our results show that the amphiphilicity derived from the Janus character of the particles leads to a significantly higher interfacial activity than observed for the respective homogeneous particles of the same size. This leads to a dramatic decrease in interfacial tension at the hexane-water interface during particle assembly. Furthermore, we demonstrate control over the interfacial activity by tuning the particle amphiphilicity via ligand exchange reactions.

CPP 2.5 Mon 11:15 ZEU 160

Mechanical properties of catanionic hollow faceted polyhedrons — •NICOLAS DELORME¹, MONIQUE DUBOIS², THOMAS ZEMB³, and ANDREAS FERY¹ — ¹Max Planck Institute for Colloid and Interface Research, Potsdam, Germany — ²SCM, CEA Saclay, Gif-sur-Yvette, France — ³LCF, CNRS/CEA URA 331, Gif-sur-Yvette, France

Mixtures of cationic and anionic surfactants dispersed in water show a rich polymorphism depending on the mixing ratio. For an excess of the anionic component, hollow faceted polyhedrons are formed which have been subject to detailed structural studies in the past. While our aim in this study is to understand the impact of electrostatic interactions on the mechanics of the catanionics, our results are also relevant for studies on viruses or faceted vesicles which are mechanically analogous. In this purpose, Atomic Force Microscopy (AFM) is used to measure elastic properties and other surface interaction forces. After the immobilization of the polyhedrons onto a flat surface using polyelectrolytes of tailored charge density, combining force measurements and imaging allowed demonstrating the strong dependence between the stiffness and the shape of the faceted polyhedrons. We have demonstrated that compared to a supported lipid bilayer in the gel-state, the catanionic membrane is very rigid, showing an effective bending modulus of up to 450 kT. In order to understand the origin of the rigidity of the catanionic membrane, the evolution of the mechanical properties were investigated as function of pH and salt concentration, which are known to change the electrostatic contribution to the bending stiffness.

CPP 2.6 Mon 11:30 ZEU 160

Raman scattering on double-wall carbon nanotubes under high pressure — •MATTHIAS MÜLLER¹, JANINA MAULTZSCH¹, FERENC SIMON², and CHRISTIAN THOMSEN¹ — ¹Inst. für Festkörperphysik, TU Berlin, 10623 Berlin — ²Inst. für Materialphysik, Universität Wien, A-1090 Wien

We report resonant Raman scattering on double-wall carbon nan-

otubes. The effects of applied pressure up to several GPa on the radial breathing modes and the high energy modes are studied. We investigated either structures with ¹²C or ¹³C isotopes used for the production of the inner tube. From the radial breathing modes we can assign the chiral index of the tubes[1]. Pressure shielding by the outer tubes was suggested by Arvanitidis et al.[2]. Using the ¹²C or ¹³C tube samples, we assign the Raman signal to inner and outer tube. We can therefore distinguish the possibly different effect of pressure on either inner or outer tube.

[1] Telg et al., Phys. Rev. Lett. 93, 177401 (2004). [2] Arvanitidis et al., Phys. Rev. B 71, 125404 (2005).

CPP 2.7 Mon 11:45 ZEU 160

Resonant Raman spectroscopy on isolated single-walled carbon nanotubes — •MARTIN FOUQUET, HAGEN TELG, JANINA MAULTZSCH, and CHRISTIAN THOMSEN — Institut für Festkörperphysik, Technische Universität Berlin, Germany

We performed resonant Raman measurements on isolated single-walled carbon nanotubes deposited on a silicon substrate. Varying the excitation energy, we collected intensity profiles of the radial breathing mode (RBM) and the high energy mode (HEM). From the RBM we assign the chiral index of each observed tube. We then analyze the dependence of the HEM on excitation energy of the assigned tube. In particular we compare the HEM lineshape of metallic and semiconducting nanotubes.

CPP 2.8 Mon 12:00 ZEU 160

Lattice dynamics of two-dimensional colloidal crystals — •PAVEL DYSHLOVENKO — Ulyanovsk State Technical University, 32 Severny Venets Street, Ulyanovsk 432027, Russia

Electrostatic interaction in two-dimensional colloidal crystals obeying the non-linear Poisson-Boltzmann equation is studied numerically. The force constants, which are the coefficients of the energy quadratic form of the crystal, are obtained for hexagonal and quadratic crystal lattices. The normal modes of oscillations and low frequency elastic properties of colloidal crystals are then calculated for a broad range of lattice constants and particles' parameters. Particular attention is given to many-particle effects in the crystals.

Significant discrepancy between the results of computer experiments and predictions of the harmonic crystal theory based on the idea of pair interaction was detected. The unified approach to quantitative estimation of many-particle effects and validity of the approximation of the nearest-neighbour interaction is proposed. It is shown that the contribution of many-particle interaction into the total electrostatic interaction in colloidal crystals is surprisingly significant for a broad range of crystal lattice constants and particles' sizes and charges.

CPP 2.9 Mon 12:15 ZEU 160

Fluctuation Forces between Colloids at Interfaces — •HARTWIG LEHLE^{1,2}, MARTIN OETTEL^{1,2}, and SIEGFRIED DIETRICH^{1,2} — ¹Max Planck Institut für Metallforschung, Heisenbergstraße 3, 70569 Stuttgart — ²ITAP, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart

We calculate the thermal Casimir force between nanoscopic rotationally symmetric colloids trapped at a fluid interface. Due to the constraints imposed by the presence of the colloids on the interface the spectrum of the interface fluctuations (capillary waves) is modified, leading to a free energy depending on the geometrical arrangement of the system. For the case of two colloids and a simple capillary wave Hamiltonian, we calculate the partition function of the system in a functional integral approach, where the boundary conditions imposed by the colloids on the interface are incorporated by the use of auxiliary fields. Analytical results for small and large colloid separations are compared to numerical results for the full range of separations. We discuss the physically distinct cases of a pinned (Dirichlet boundary condition) and a fluctuating contact line. For small separations, the leading part of the divergent fluctuation force is calculated with Dirichlet b. c. Since the fluctuation force is independent on the surface tension and the precise shape of the colloids, we predict a strong tendency to coagulation even in arrangements when the vdW force is close to zero.

CPP 3 Polymer Materials

Time: Monday 10:00–12:30

Room: ZEU 114

CPP 3.1 Mon 10:00 ZEU 114

Generalized Cauchy Relation For Reactive Polymers: Epoxies and Polyurethanes, a comparison — ●CHRISTELLE VERGNAT¹, MARTINE PHILIPP², RAVI BACTAVATCHALOU¹, JÖRG BALLER², WULF POSSART¹, ULRICH MÜLLER¹, PATRICK ALNOT³, ROLAND SANCTUARY², and JAN K. KRÜGER¹ — ¹Laboratoire Européen de Recherche Universitaire Saarland-Lorraine-Luxembourg Universität des Saarlandes D-66123 Saarbrücken — ²Université de Luxembourg, 162a, Avenue de la Faiencerie L-1511 Luxembourg — ³Université de Nancy, Bd des Aiguillettes F-54506 Vandoeuvre

The generalized Cauchy Relation $c_{11} = B c_{44} + A$ for isotropic materials is a linear transformation which strongly reduces the independence of the two remaining elastic constants c_{11} and c_{44} of the isotropic state. The pre-factor B usually reflects the global symmetry and has a value of three. The parameter A seems to be indicative to the difference between global and local symmetry of the material. At sufficient high probe frequencies the generalized relation even holds for the liquid state and doesn't change at the transition to the glassy state. As a matter of fact the generalized Cauchy relation is even maintained during the curing process of reactive polymers. Within this contribution we present Cauchy Relations for epoxies and polyurethanes. The results will be discussed in the context of local symmetry and local heterogeneity.

CPP 3.2 Mon 10:15 ZEU 114

The Chemical Glass Transition as seen by High Performance Brillouin spectroscopy: Epoxies and Polyurethanes, a comparison — ●MARTINE PHILIPP¹, CHRISTELLE VERGNAT², RAVI BACTAVATCHALOU², JÖRG BALLER¹, WULF POSSART², ULRICH MÜLLER², DIDIER ROUXEL³, ROLAND SANCTUARY¹, and JAN K. KRÜGER² — ¹Laboratoire Européen de Recherche Universitaire Saarland-Lorraine-Luxembourg Université de Luxembourg 162a, avenue de la Faiencerie L-1511 Luxembourg — ²Universität des Saarlandes D-66123 Saarbrücken — ³Université de Nancy I, Bd des Aiguillettes F-54506 Vandoeuvre

The nature of the glass transition and the nature of the glassy state are still a matter of debate. There are two contradictory hypothesis which do compete: The kinetic hypothesis and the transition hypothesis. According to the kinetic hypothesis the glass transition is due to a cross-over of the relevant intrinsic alpha-relaxation time with the time constant of the measurement probe in addition to the patience of the experimentalist. It is therefore of great interest to investigate a type of glass transition which by definition does not suffer from such a cross-over between the experimental time scale and the intrinsic relaxation times. For that purpose we present in this contribution investigations of the chemically induced glass transition. As model substances we have chosen the two reactive polymers: epoxy and polyurethane. As a sensitive probe for the detection of the chemical glass transition we use so-called mode-Grüneisen parameters. These parameters have been measured with high performance Brillouin spectroscopy. The results will be compared with other physical quantities as the specific heat and the refractive index.

CPP 3.3 Mon 10:30 ZEU 114

Strain dependent structural changes of spider dragline silk observed with single fiber x-ray diffraction — ●ANJA GLISOVIC¹, THORSTEN VEHOFF¹, RICHARD DAVIES², CHRISTIAN RIEKEL², and TIM SALDITT¹ — ¹Institut für Röntgenphysik, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — ²ESRF, 6 rue Jules Horowitz, BP220, 38043 GRENOBLE CEDEX, FRANCE

Spider silk is a biopolymer which has attracted more and more attention in recent years due to its unique combination of tensile strength and viscoelastic extensibility. In order to study the correlation between structure and mechanical properties we combined stress-strain measurements on single dragline fibers with x-ray diffraction. The experiments were carried out at ESRF's microfocus beamline ID 13 in Grenoble. With this method the structural changes of the fiber's crystalline parts could be studied. The changes of the crystallites are quite small and their contribution to the mechanical properties is discussed.

— 15 min. break —

CPP 3.4 Mon 11:00 ZEU 114

High-Performance Polypropylene pipes via biaxial processing — ●RALF KLEPPINGER¹, PATRICK VOETS², MARIA SOLIMAN², COLIN MORATH³, and IAN WARD³ — ¹DSM Research, Geleen, The Netherlands — ²SABIC EuroPetrochemicals, Geleen, The Netherlands — ³Department for Physics and Astronomy, Leeds University, Great Britain

Besides revealing a complex polymorphism that is affected by thermal history but also specific additives, recent studies have also revealed that polypropylene reveals a unique crystallization behavior when subjected to sufficiently strong shear fields. The interplay among both is of crucial importance with respect to the morphology and finally determines macroscopic properties of the material. Using polypropylene pipes as a practical example we demonstrate how processing-induced orientation in the material can either result in deterioration or enhancement of properties. Our results demonstrate that by using the die-drawing process a significant improvement of the properties of polypropylene pipes can be achieved.

CPP 3.5 Mon 11:15 ZEU 114

Scattering from polymer networks under elongational strain — ●CARSTEN SVANEBOG¹, RALF EVERAERS¹, and GARY S. GREY² — ¹Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Straße 38, 01187 Dresden — ²Sandia National Laboratories, Albuquerque, NM 87185, USA

Molecular dynamics simulations are used to sample the single-chain form factor of labelled sub-chains in model polymer networks under elongational strain. We observe very similar results for randomly cross-linked and for randomly end-linked networks with the same average strand length and see no indication of lozenge-like scattering patterns reported for some experimental systems. Our data analysis shows that a recent variant of the tube model quantitatively describes scattering in the Guinier regime as well as the macroscopic elastic properties. The observed failure of the theory outside the Guinier regime is shown to be due to non-Gaussian pair-distance distributions. Nevertheless, the results presented here [1] and in Ref. [2,3] open up the possibility to systematically link SANS studies of *microscopic* deformations to the *macroscopic* elastic properties of rubber-elastic systems.

[1] C. Svanebog, G. S. Grey, and R. Everaers. Euro. Phys. Lett. accepted.

[2] C. Svanebog, G. S. Grey, and R. Everaers. Phys. Rev. Lett., 93:257801, 2004.

[3] C. Svanebog, G. S. Grey, and R. Everaers. Polymer, 46:4283, 2005.

CPP 3.6 Mon 11:30 ZEU 114

The study of the relation between cavitation and microfibrillation in HDPE using time resolved synchrotron X-ray scattering during tensile deformation — ●KONRAD SCHNEIDER¹, SONDES TRABELSI², STAMM MANFRED¹, and RIEKEL CHRISTIAN³ — ¹Leibniz-Institut für Polymerforschung Dresden, Hohe Str. 6, 01069 Dresden — ²Forschungszentrum Karlsruhe GmbH, Institut für Synchrotronstrahlung, ANKA, Hermann-von-Helmholtz-Platz 1, 76344 Karlsruhe — ³European Synchrotron Radiation Facility (ESRF), BP 220, F38043 Grenoble, France

Real time synchrotron Small-Angle and Wide-Angle X-ray Scattering was performed during the tensile deformation of a high-density polyethylene copolymer. 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 stage composed of the phase of the lowering load in the force-displacement-curve and the strain hardening. Competitive phenomena like crystallite fragmentation and cavitations were found to occur simultaneously in the lowering phase of the load but at different length scale. We prove that the volume fraction of the voids increase during the fibrillation of the lamellae stacks. At increasing strain the changes of the radius of gyration of the cavities in stretching as well as in transversal direction were discussed. During strain hardening no further increase in the volume fraction of the voids was found. However, we make evidence for the establishment of a new long spacing order of the micro-block crystallites, which were stable despite the occurrence of the melting process.

CPP 3.7 Mon 11:45 ZEU 114

Investigation of Swollen Polymer/Gas-Systems: Atomistic Packing Models Based on Experimental Properties — ●MARTIN BÖHNING¹, MATTHIAS HEUCHEL², OLE HÖLCK¹, and MARTIN R. SIEGERT² — ¹Bundesanstalt für Materialforschung und -prüfung (BAM), Unter den Eichen 87, 12205 Berlin, Germany — ²GKSS Forschungszentrum, Institut für Polymerforschung, Kantstrasse 55, 14513 Teltow, Germany

Changes in glassy polymers induced by sorption of substantial amounts of small penetrant molecules can affect the amorphous packing structure as well as the molecular mobility of the polymer chains. These changes - manifested as swelling and plasticisation phenomena - can have radical influences on relevant properties, especially concerning the gas transport behaviour in membrane or barrier applications. Based on sorption and dilation measurements of CO₂ in different glassy polymers (e.g. polysulfone and a polyimide) detailed atomistic packing models have been created using MM/MD-simulation techniques. The analysis of representative models of swollen and unswollen states allows a detailed characterisation of these changes in terms of free volume distribution and molecular mobility. Solubilities and diffusivities of penetrants in these models were calculated using MD and GCMC methods. Results are evaluated in relation to phenomenological models and compared to experimental findings in order to prove the reliability and predictive abilities of this approach.

CPP 3.8 Mon 12:00 ZEU 114

Epoxy networks — ●MARIAN BRANDAU¹, MICHAEL SCHULZ², and STEFFEN TRIMPER¹ — ¹Fachbereich Physik, Martin-Luther-Universität, Friedemann-Bach-Platz, 06108 Halle — ²Abteilung Theoretische Physik, Universität Ulm, 89069 Ulm

We present the results of a Monte Carlo simulation for the kinetic of formation in epoxy networks. In particular, two time regimes are distinguished, namely a short time regime characterized by a radicalic polymerisation and a long time regime where slow formation processes are relevant. Whereas the first stage is reaction controlled, diffusion

processes determine the second one. On a more microscopic level two kinds of molecules with different functional groups are taken into account. While the so-called cross-linkers are characterized by three or four functional groups, the chain formers are bifunctional. The aim is to find out universal properties of the kinetic of formation such as the cluster size distribution function, and the behavior in the vicinity of the percolation threshold. Moreover, we consider the light-scattering function.

CPP 3.9 Mon 12:15 ZEU 114

A non-cubic network phase in ABC copolymers via e^- -tomography — ●GERD E SCHROEDER¹, STEPHEN T HYDE¹, HERMIS IATROU², NIKOS HADJICHRISTIDIS², SATOSHI AKASAKA³, and HIROKAZU HASEGAWA³ — ¹Applied Maths, Research School of Physical Sciences, Australian National University, 0200 Canberra, Australia — ²Chemistry Department, University of Athens, Panepistimiopolis, Zografou 15771, Athens, Greece — ³Department of Polymer Chemistry, Graduate School of Engineering, Kyoto University, Katsura, Nishikyo-ku, Kyoto 615-8510 Japan

We report the discovery of a novel bicontinuous tetragonal phase in the linear ABC triblock terpolymer system polystyrene, polyisoprene and polydimethylsiloxane. The data is consistent with spacegroup Fddd and is distinctly non-cubic. The channel topology of the mesophase is distinct from the cubic Gyroid and Diamond mesophases. It consists in 2 identical intertwined labyrinths with 3- and 4-connected nodes. Our mesophase differs from an earlier report of a copolymer phase (also in a linear terpolymer system) with the same spacegroup by Bates *et al.* who deduced a single channel morphology, based on TEM and SAXS data [1]. Our proposal is based on 3D e^- -tomography data. The channel geometry is identified via a *medial surface* (MS) algorithm. The MS is a generalised channel graph consisting in surface patches rather than line segments and is, in contrast to line graphs, a complete descriptor of both topology and geometry.

[1] T. Epps, E. Cochran, T. Bailey, R. Waletzko, C. Hardy, and F. Bates, *Macromolecules* **37**, 8325–8341 (2004)

CPP 4 New Experimental Techniques

Time: Monday 14:00–17:45

Room: ZEU Lich

Invited Talk

CPP 4.1 Mon 14:00 ZEU Lich

Optical tweezers - novel tools in nanophysics — ●FRIEDRICH KREMER, CHRISTOF GUTSCHE, KATI KEGLER, MATHIAS SALOMO, JOERG REINMUTH, and WIKTOR SKOKOW — University of Leipzig, Institute of Experimental Physics I

Optical tweezers are microscopic tools with extraordinary resolution. (resolution in space: ± 1 nm, resolution in force: ± 50 fN) In the talk three different experiments will be discussed: 1.) Measurement of the force-extension dependence of single chains of double stranded DNA having a length between 1000 base pairs (bp) to 6000 bp. It is shown that the wormlike chain model fits the data. 2.) Measurement of forces of interaction between single blank and DNA-grafted colloids. The forces are measured in two directions, parallel and perpendicular to the axis between the two colloids under study. Bringing the DNA-grafted colloids in close contact (< 100 nm for 4000 bp DNA) enables one to measure directly the forces necessary to interdigitate the DNA-brushes. Under these conditions frictional stick-slip phenomena take place, when the colloids are moved perpendicularly to its central axis. 3.) Measurement of the flow resistance of single colloids grafted with DNA of lengths between 1000 bp to 6000 bp. The experiments can be described by Stokes law with an effective hydrodynamic radius being dependent on the flow velocity, the length, the grafting-density and the ionic strength of the surrounding medium.

CPP 4.2 Mon 14:30 ZEU Lich

Gold Nanorods as Novel Nonbleaching Plasmon-Based Sensors for Molecular Orientations and Local Refractive Index Changes — ●JAN BECKER and CARSTEN SÖNNICHSEN — Nanobiotechnology group, Institute for Physical Chemistry, University of Mainz, Germany (www.nano-bio-tech.de)

Gold nanorods of typical dimensions of 25nm x 60nm can be observed in a darkfield microscope because of their strong light scattering at the plasmon resonance. The scattered light of these gold rods is strongly polarized along their long axis making them an ideal orientation probe.

We study the rotations of single gold nanorods weakly bound to a glass surface by observing the intensity fluctuations in polarized light. We observe some fast rotating rods (10ms time scale) and some very slow rotating rods likely trapped in shallow surface potentials.

Furthermore, the wavelength of the plasmon depends on the volume and aspect ratio of the gold nanorod, but also on the refractive index of the local environment. We study this plasmon shift for different particle shapes to find the optimal local refractive index sensor using a novel automated acquisition setup. Nanorods are found to be more sensitive than spherical particles, triangles, cubes and hollow spheres.

CPP 4.3 Mon 14:45 ZEU Lich

FTIR-Goniometry — ●PATRICK KOELSCH, MICHAEL TAMMER, and FRIEDRICH KREMER — University of Leipzig, Faculty of Physics and Earth Science, Linnestrasse 5, 04103 Leipzig

Fourier Transform Infrared (FTIR)-Goniometry is a novel spectroscopic tool in which the principle of goniometry (as known from x-ray scattering) is combined with (polarized) IR spectroscopy. In practice a thin (μm thick) sample is intentionally inclined in adjustable spatial directions with respect to the optical axis of the spectrometer. An algorithm will be presented to deduce the mean orientation and the distribution of the different molecular moieties in the sample from the measured transmission. Thereby advantage is taken from the specificity of the IR spectral region as a “fingerprint” regime.

This offers a manifold of novel perspectives for molecular physics and materials science. Examples will be discussed.

CPP 4.4 Mon 15:00 ZEU Lich

Transitions in Nanometer thin films - Investigations by AC-Chip calorimetry — ●HEIKO HUTH, ALEXANDER MINAKOV, and CHRISTOPH SCHICK — University of Rostock, Institute of Physics, Universitätsplatz 3, 18051 Rostock, Germany

Calorimetry is known as a very powerful tool for the characterization of a wide variety of materials and their transitions. The combination of sili-

con technology and calorimetry opens up new possibilities in this research area as demonstrated recently (1). Based on a differential AC-calorimeter we show an improved experimental setup combining the advantages of the different methods. The measurements are done at slow scanning or at constant bath temperature. The frequency chosen provides a well defined time scale of the experiment. In several cases, e.g. at glass transition, a direct comparison with results from other dynamic methods like dielectric spectroscopy is possible. Due to the differential setup we achieve a sensitive in the pico Joule per Kelvin range allowing to measure samples below one nanogram and consequently films down to 1 nm thickness (2, 3). Because of the small total heat capacity (addenda + sample) not only a high sensitivity is achieved but AC measurements at relative high frequencies are possible too. The capabilities are demonstrated by different nanometer thin polymeric films.

[1] D. W. Denlinger; E. N. Abarra; K. Allen; P. W. Rooney; M. T. Messer; S. K. Watson; F. Hellman, Rev. Sci. Instrum. 65 (1994) 946

[2] H. Huth, A. Minakov, C. Schick, Netsu Sokutei 32 (2005) 69

[3] Lupascu V., Huth H., Schick C. and Wubbendorff M. Thermochim. Acta 432 (2005) 222

CPP 4.5 Mon 15:15 ZEU Lich

Visualizing the metal centers in metallocomplexes by scanning tunneling spectroscopy — ●M.S. ALAM¹, V. DREMOV¹, P. MÜLLER¹, R. ALSASSER², U. KORTZ³, M. RUBEN⁴, L.K. THOMPSON⁵, and J.M. LEHN⁶ — ¹Physikalisches Institut III, Universität Erlangen — ²Institut für anorganische Chemie, Universität Freiburg — ³School of Engineering and Sciences, International University Bremen — ⁴Institut für Nanotechnologie, FZ Karlsruhe — ⁵Dept. of Chemistry, Memorial University, St. John's, NL, Canada — ⁶ISIS, Université Louis Pasteur, Strasbourg, France

As the contrast in STM images mixes both topographic and electronic effects in a complicated way, mapping of complex molecules is not straightforward. However, scanning tunneling spectroscopy (STS) measurements reveal direct information about the energy levels close to the molecule's Fermi level. Using our home built STM working under ambient conditions, we succeeded to combine high resolution topography mapping with simultaneous current-voltage characteristics measurements on single molecules deposited on HOPG surfaces. We present our recent results on Co [2X2], Mn [3X3] grid-type molecules, Cu₂₀ wheel-shaped polyoxoanions, as well as on Cu coordination polymers. In our STS measurements we found a rather large signal at the expected positions of the metal centers in our molecules, i.e. the location of the individual metal ions in their organic matrix is directly addressable by STS even if these ions are covered by the organic ligands.

— 15 min. break —

CPP 4.6 Mon 15:45 ZEU Lich

Energy Dispersive Small Angle X-Ray Scattering — ●TUSHAR SANT¹, WOLFRAM LEITENBERGER², TOBIAS PANZNER¹, and ULLRICH PIETSCH¹ — ¹Institute for Physics, University of Siegen, Walter Flex Strasse 3, D-57068 Siegen, Germany. — ²Institute for Physics, University of Potsdam, Am Neuen Palais 10, D-14469 Potsdam, Germany.

Small Angle X-ray Scattering is well known technique for characterizing polymers, colloids and biological samples. We performed energy dispersive small angle X-ray scattering (EDSAXS) experiments using white synchrotron radiation at Energy Dispersive Reflectivity (EDR) beamline at BESSY II. We measured EDSAXS spectra for Gold nanoparticles with diameter of about 12 nm and 40 nm solvated in water. The extracted colloidal radius taken from EDSAXS spectra agree well with these obtained by monochromatic SAXS measurements at an in-house set-up. The main advantage of EDSAXS technique is the most reduced time consumption which required 3 minutes at EDR but 3 hrs for monochromatic measurement. This is useful for the systematic investigation of large series of samples or study of slow dynamical processes. The specific experimental conditions at BESSY II limit the accessible q range of investigation. This in turn puts the limit for the measurable size of the particles.

CPP 4.7 Mon 16:00 ZEU Lich

High resolution setups at BW4 - from microfocus to USAXS — ●STEPHAN V. ROTH, RALPH DÖHRMANN, MARTIN DOMMACH, CHRISTIAN SCHROER, MARION KUHLMANN, and RAINER GEHRKE — HASYLAB at DESY, Notkestr. 85, D-22603 Hamburg

The wiggler beamline BW4 at HASYLAB is dedicated to ultra-small-angle x-ray scattering (USAXS) in material science. After ten years of

successful operation major upgrading and refurbishment has been performed, starting in 2003. We describe the recent upgrade of the USAXS-camera, the available SAXS setups and the present status of BW4 on the basis of standard samples and recent experiments. In brief, the key improvements at BW4 are as follows: 1) The maximum USAXS resolution - defined by the size of the beam stop - is $d_{max} > 1\mu\text{m}$ at a sample-to-detector distance $L_{SD} = 13\text{m}$. 2) In grazing incidence USAXS (GIUSAXS) the resolution has been pushed well beyond $d_{max} > 3\mu\text{m}$. 3) A new SAXS setup using a newly designed piezo-driven portable slit is available. This allows to optimize intensity and resolution for $L_{SD} \leq 4\text{m}$. 4) A new microfocus option has been established using Beryllium compound refractive lenses. Currently a moderate microfocus of $30 \times 17\mu\text{m}^2$ can be achieved. This new option allows for scanning applications like μSAXS and μGISAXS with the sample size reduced by two orders of magnitude.

CPP 4.8 Mon 16:15 ZEU Lich

Periodic NMR excitation in very thin slices: Interplay of diffusion and relaxation — ●ACHIM GÄDKE and NIKOLAUS NESTLE — TU Darmstadt, Institute of condensed matter physics, Hochschulstr. 6, D-64289 Darmstadt, Germany

NMR experiments involving thin excited slices are of interest both for conventional micro-MRI and for mechanically detected magnetic resonance. Especially in the latter case, the thickness of the excited slices may be well below $1\mu\text{m}$. In samples containing fast-diffusing liquid components such as water, the diffusive exchange of spin magnetization between the excited slice and its surroundings on the time scale of the NMR experiments plays a major role. Some time ago, we have studied the influence of the diffusion balance on the apparent longitudinal relaxation behaviour measured in a saturation-recovery experiment. This study suggests that in a $1\mu\text{m}$ slice with a Gaussian profile, the apparent longitudinal relaxation time of water may be below 1 ms. In this experiment, full spin relaxation was possible between two excitation cycles. In micro-MRI or in mechanically detected NMR, by contrast, the excitation is periodic. In this case, the diffusive magnetization balance between the excited slice and its surroundings needs considering excited magnetization from previous excitation cycles, too. This diffusion balance will also depend on the presence of diffusion barriers and relaxation sinks outside the excited slice. Results from both simulation studies and experiments concerning these two effects are presented, and their implications micro-MRI and mechanically detected NMR are discussed.

CPP 4.9 Mon 16:30 ZEU Lich

Visualization of liquid water in PEM Fuel Cells with Neutron Radiography — ●INGO MANKE^{1,2}, NIKOLAY KARDJILOV², CHRISTOPH HARTNIG³, ANDRÉ HILGER^{2,4}, MARKUS STROBL⁴, MANFRED GRÜNERBEL³, WOLFGANG TREIMER⁴, WERNER LEHNERT³, and JOHN BANHART^{1,2} — ¹Technische Universität Berlin, Fakultät 3 — ²Hahn-Meitner-Institut Berlin, SF 3 — ³Centre for Solar Energy and Hydrogen Research (ZSW) — ⁴University of Applied Science (TFH), FB 2

A key issue in the development of Polymer Electrolyte Membrane Fuel Cells (PEMFC) is the optimization of the mass transport, i.e. the transport of liquid water, in the gas diffusion layers and the gas channels of the flow field. The water is produced by conversion of hydrogen fuel and oxygen into electrical energy. However, the production of too much water can disturb the gas flows and causes a breakdown in the output power. Neutron Radiography (NR) is a unique experimental technique to study the two-phase flow inside operating PEMFCs. Neutrons penetrate quite thick metal components and at the same time they are highly sensitive to hydrogen containing materials. The accumulation of water was investigated under different operating conditions. Beginning from *dry* and going to *wet* conditions, time and location of the water accumulation were recorded, analyzed and quantified by NR. First liquid water droplets develop in the gas diffusion layers. After some time water drops appear at the side of the gas channels in the flow field. The drop sizes are increasing until the whole channel is filled and the gas flow inside the whole channel is filled and the gas flow inside the corresponding channels is blocked.

CPP 4.10 Mon 16:45 ZEU Lich

3-d Cylindrical Pulsed X-Band ESR-Imaging — ●MICHAEL GLIED^{1,2}, MALTE DRESCHER², and ELMAR DORMANN² — ¹now at 1. Physikalisches Institut, Universität Stuttgart, D-70550 Stuttgart, Germany — ²Physikalisches Institut, Universität Karlsruhe (TH), D-76128 Karlsruhe, Germany

ESR-Imaging is a technique using similar principles to the established NMR-imaging; however, the fast electron spin relaxation time constants are an experimental challenge. Spin echo backprojection reconstruction imaging in the X-band using a static magnetic field gradient is the favourable application for material science where temperature variation in metal cryostat is necessary. Nevertheless, studying quasi-one dimensional organic conductors only a pulsed phase encoding gradient can be tolerated in the conduction direction in order to avoid imaging artefacts caused by electron spin diffusion.

We present an appropriate three dimensional imaging scheme, combining static gradient backprojection reconstruction and pulsed gradient fourier imaging to scan the reciprocal space in cylindrical coordinates and obtain three dimensional images of various physical parameters like spin density, relaxation time or defect concentration.

Conduction electron density images with a volume element size of $13 \times 13 \times 17 \mu\text{m}^3$ as well as images of the spin lattice relaxation time, obtained by inversion recovery, with a volume element size of $13 \times 13 \times 68 \mu\text{m}^3$ are presented for fluoranthene radical cation salt single crystals of typical sizes of $0.4 \times 0.4 \times 1 \text{mm}^3$.

CPP 4.11 Mon 17:00 ZEU Lich

Confocal micro-Raman spectroscopy: A tool to discriminate calcified biominerals in land living crustaceans — ●SABINE HILD and ANDREAS ZIEGLER — Central Facility for Electron Microscopy; University of Ulm, Albert-Einstein-Allee 11, 89081 Ulm

Land living crustaceans, like Porcellio scaber (Isopoda), have the ability to elaborate various types of calcified biominerals e.g. calcium phosphate, calcite, and amorphous calcium carbonate (ACC). Crystalline minerals are located mainly in the mineralized exoskeleton (cuticle) of the animals. Amorphous minerals, like ACC, which is thought to be a precursor for crystalline CaCO_3 , occur primarily in transient reservoirs for calcium. To get information about the morphology of the inorganic phase and their spatial distribution imaging techniques like REM and SFM are suitable. However, the various modifications of the biominerals cannot be discriminated by these techniques. Scanning confocal *Raman spectroscopy (SCRS) enables to investigate the chemical composition of materials with a high resolution. In this study Raman spectral imaging in combination with SFM have been used to characterize and localize amorphous and crystalline minerals in a calcified tissue of P. scaber. First SCRS experiments reveal both crystalline and amorphous CaCO_3 within the cuticle. Our model organism develops also transient reservoirs, which are fully X-ray amorphous. The reservoirs contain only ACC embedded in an organic matrix, which is proposed to stabilize the ACC. Additionally detected phosphate derivatives suggests that they may also influence the stabilization of amorphous calcium carbonate.

CPP 4.12 Mon 17:15 ZEU Lich

Nanometer-sized temperature-sensors using the upconversion signal in single colloids of Lanthanide-doped NaYF_4

— ●STEFAN SCHIETINGER¹, BJÖRN LAURITZEN¹, STEPHAN HEER², HANS-ULRICH GÜDEL², and OLIVER BENSON¹ — ¹AG Nano-Optik, Institut für Physik, Humboldt-Universität zu Berlin, Hausvogteiplatz 5-7, 10117 Berlin (Germany) — ²Department of Chemistry and Biochemistry, University of Bern, Freiestrasse 3, CH-3000 Bern 9 (Switzerland)

Because of low absorption of biological tissue in the near-infrared (NIR), luminescent biolabels based on two-photon absorption processes in this spectral region are of great interest. NaYF_4 colloids doped with $\text{Yb}^{3+}/\text{Er}^{3+}$ with a size of 10-30 nm can be excited by photon upconversion. The excitation is based on sequential absorption of one photon by the Yb^{3+} ions followed by the absorption of a second photon and the energy transfer to Er^{3+} ions emitting the upconversion signal. Due to the contribution of a real metastable level in the Yb^{3+} , excitation rates are much higher than in two-photon absorption processes using a "virtual" quantum mechanical state¹.

Two states emitting around 540 nm are coupled thermally and therefore their intensity ratio is $\propto \exp(-\Delta E/k_B T)$. We were able to measure the temperature dependence in the biological interesting region around 300 K of a single nanocrystal. We therefore suggest not only the use of these colloids as stable and high efficient biomarkers, but also their employment as local temperature-sensors on a nanometer scale.

1 W. Krämer *et al.*, Chem. Mater. 16, 1244, (2004)

CPP 4.13 Mon 17:30 ZEU Lich

Blowing DNA bubbles — ●NIKOLAI SEVERIN¹, WEI ZHUANG¹, CHRISTOF ECKER¹, ALEXEI A. KALACHEV², IGOR M. SOKOLOV¹, and JÜRGEN P. RABE¹ — ¹Department of Physics, Humboldt University Berlin, Newtonstr. 15, D-12489 Berlin, Germany — ²Plasmachem GmbH, Rudower Chaussee 29, D-12489 Berlin, Germany

Liquids at the interface with a solid differ from their bulk state since they order in molecular layers parallel to the substrate surface. With a surface forces apparatus, the layers can be squeezed out one by one at increasing normal forces, indicating solid-like behavior in the direction normal to the substrate. Similar layered behavior is observed for free liquid thin films on a surface. Computer simulations, measurements of shear forces and tracer dye diffusion, however, indicate liquid-like behavior parallel to the substrate. Therefore, we regard an ultra-thin layer of a liquid on a solid substrate as a quasi 2D-liquid. Here we demonstrate that such a layer may be used to transmit forces isotropically across a surface. A scanning force microscope (SFM) tip was employed to generate a 2D-pressure, which then exerts a force on a single macromolecule embedded in the 2D-liquid. In particular, supercoiled ds-DNA has been unraveled, moved, stretched, overstretched to 2.0 times its B-form length and then torn apart at (1.1 ± 0.2) nN.

CPP 5 Polyelectrolytes

Time: Monday 14:30–17:45

Room: ZEU 160

CPP 5.1 Mon 14:30 ZEU 160

Fluctuation and correlation effects in charged macromolecular systems studied by molecular dynamics simulations — ●ARBEN JUSUPI and MATTHIAS BALLAUFF — Physikalisches Chemie I, Universität Bayreuth, 95440 Bayreuth, Germany

We have performed MD simulations of a charged macroion surrounded by counterions. Various scattering contributions result from correlations between counterions, macroion, and between both of them. Experimentally, these scattering contributions can be measured by anomalous small-angle X-ray scattering (ASAXS) experiments. As a result the cross-correlation between the rigid macroion and counterions yields always a meanfield expression for the counterion density distribution even if the counterions exhibit correlated fluctuations. In contrast, in star-like polyelectrolytes, representing a fluctuating macroion, meanfield approximations are valid only if the functionality is sufficiently high. A systematic

investigation of the strength of correlated fluctuations and their effect in scattering intensities is demonstrated for these systems.

CPP 5.2 Mon 14:45 ZEU 160

Engineering Heterogeneously Charged Surfaces by Dendrimer Adsorption: Mechanisms and Interaction Forces — ●GEORG PAPASTAVROU, RAMON PERICET-CAMARA, SAMUEL RENTSCH, and MICHAL BORKOVEC — University of Geneva, Laboratory of Colloid and Surface Chemistry, Science II CHIAM, Quai Ernest Ansermet 30, 1211 Geneva, Switzerland

The adsorption of poly(amidoamine) (PAMAM) dendrimers of generations G8 and G10 to a mica surface has been studied by AFM as function of ionic strength and pH. The observed trends of the surface coverage can be described within the effective hard sphere model for Random Sequential Adsorption (RSA). Surfaces with a well-defined den-

sity of dendrimers with different surface coverages ranging from 0.05 up to 0.4 can be prepared by selecting an appropriate dendrimer generation, ionic strength of the background electrolyte, and pH-value. These surfaces, although of random nature, exhibit characteristic length scales in the nanometer range for the distances between neighboring adsorbed dendrimer molecules and the approach can be applied as well to colloidal particles. We present measurements on the interaction forces between such heterogeneously charged surfaces by the colloidal probe technique and examine especially the conditions under which the Derjaguin approximation can be applied in the sphere-sphere geometry.

CPP 5.3 Mon 15:00 ZEU 160

Polyelectrolytes and polyelectrolyte complexes in solution — ●ULRICH SCHELER and UTE BÖHME — Leibniz Institute of Polymer Research Dresden, Hohe Strasse 6, D-01069 Dresden, Germany

Electrostatic interaction determines the properties of polyelectrolytes in solution. Due to the electrostatic repulsion they adopt a more extended conformation than uncharged polymers in a good solvent. When the ionic strength of the solution is increased, polyelectrolytes adopt a more compact conformation which is reflected in an enhanced diffusion coefficient measured by PFG NMR. This effect becomes more prominent for counterions with higher valence. This effect has been studied on the example of poly(styrenesulfonate) of 77 kg/mol with a monovalent salt (NaCl) and a poly(diallyldimethylammonium chloride) PDADMAC of 5 kg/mol. Upon the addition of PDADMAC acting as a multivalent counterion, the diffusion coefficient is increased more drastically and a primary polyelectrolyte complex is formed. The effective charge of the complexes, measured by electrophoresis NMR, changes according to the composition of the complexes.

CPP 5.4 Mon 15:15 ZEU 160

Thermosensitive surfaces by self-assembly of PNIPAM microgels on polyelectrolyte layers — ●THOMAS HELLWEG¹, STEPHAN SCHMIDT², and REGINE VON KLITZING³ — ¹TU Berlin, Stranski-Lab. (ER 1), Strasse des 17. Juni 112, 10623 Berlin — ²MPI-KGF, 14424 Potsdam — ³Institut für Physikalische Chemie, Christian-Albrechts-Universität Kiel, Ludewig-Meyn-Str. 8, 24118 Kiel

The present contribution describes the behaviour and ordering of thermosensitive PNIPAM and PNIPAM-co-P(AAC) microgels when deposited on layers of the polyelectrolyte PEI. The obtained surface structures change as a function of deposition method (spin-coating or dip-coating) and also as a function of the interaction between microgel and PEI. The electrostatic part of the interaction can be controlled by pH or ionic strength.

Ordered monolayers of microgel particles were obtained and characterized by in-situ ellipsometry measurements. The films are still responsive and change thickness with increasing temperature making them possible candidates for sensoric surfaces.

— 15 min. break —

CPP 5.5 Mon 15:45 ZEU 160

Structuring of polyelectrolytes in thin aqueous nanofilms — ●DAN QU¹, KATARZYNA CIUNEL², JAN SKOV PEDERSEN³, TOMMY NYLANDER⁴, and REGINE V. KLITZING⁵ — ¹MPI für Kolloid- und Grenzflächenforschung, D-14224 Potsdam — ²Stranski-Laboratorium, TU Berlin, Str. d, 17. Juni 112, D-10623 Berlin — ³Department of Chemistry, University of Aarhus, Langelandsgade 140, DK-8000 Aarhus C — ⁴Department of Chemistry I, Lund University, Box 124 SE-221 00 Lund — ⁵Institut für Physikalische Chemie, CAU Kiel, Ludewig-Meyn-Strasse 8, D-24118 Kiel

Confinement effects on the structuring of polyelectrolyte chain in aqueous media are studied within nanofilms. The effect of interfaces is studied by choosing films with different surfaces, which are foam films (air/liquid/air), wetting films and films between two solid interfaces. The measurements are carried out in a Thin Film Pressure Balance (TFPB), a Colloidal Probe Atomic Force Microscope (CP-AFM) and a Surface Force Apparatus (SFA). In the semi-dilute regime the confined polyelectrolyte solutions show a force oscillation in a TFPB and in a CP-AFM. While in CP-AFM the whole oscillation is detectable, the TFPB measures only the repulsive parts which leads to steps in the isotherm. The step width corresponds to the period of the oscillation which leads to the conclusion that the properties of the interfaces do not affect the structuring of the polyelectrolytes. In addition the comparison between CP-AFM and SAXS studies shows that there is no confinement effect on the

characteristic lengths of the polyelectrolyte system and the counterion distribution.

CPP 5.6 Mon 16:00 ZEU 160

Ion Profile in Polyelectrolyte Multilayers Studied by Standing Wave X-ray Fluorescence — ●HAUKE SCHOLLMAYER^{1,2}, REGINE VON KLITZING³, PATRICK GUENOUN¹, and JEAN DAILLANT¹ — ¹LIONS bât. 125, CEA Saclay, F-91191 Gif Cedex, France — ²Institute for X-Ray Physics, Georg-August-University, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — ³Institut für Physikalische Chemie, CAU Kiel, Ludewig-Meyn-Str. 8, D-24118 Kiel, Germany

The alternating electrostatic adsorption of cationic and anionic polyelectrolytes has attracted some attention over the last years. These multilayer complex films are a good model system to study permeability of ions. They are prepared using layer-by-layer adsorption of oppositely charged polyelectrolytes. Only little work was done on the study of permeabilities of protons and ions through these layers. In most cases fluorescence dyes were used to measure the ion distribution in the films. The influence of these dyes on the ion diffusion through the polymeric film is not known. In particular for thin films these dyes disturb the system. Furthermore this technique is limited to specific molecules respective to the dye. A comprehensive study of the ion distribution and ion diffusion in these layers, in particular without grafting a disturbing molecule, is missing. For this we used standing waves x-ray fluorescence to measure the ion distribution of polyelectrolyte multilayers. With that technique it is possible to measure the permeabilities of polyelectrolyte multilayers with respect to small ions of different size and charge.

CPP 5.7 Mon 16:15 ZEU 160

Micelle formation of amphiphilic poly(2-alkyl-2-oxazoline) block copolymers — ●C.M. PAPADAKIS¹, T. BONNÉ¹, R. IVANOVA¹, P. ŠTĚPÁNEK², K. LÜDTKE³, and R. JORDAN³ — ¹Physikdepartment E13, Technische Universität München, James-Frank-Str. 1, D-85747 Garching — ²Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Prague — ³Lehrstuhl für Makromolekulare Stoffe, Chemiedepartment, Technische Universität München, 85 747 Garching

Amphiphilic copolymers find numerous applications, e.g. for drug delivery or as nanoreactors. Poly(2-oxazoline) block copolymers constitute a very versatile system: The amphiphilicity can be controlled by the choice of side groups, and in aqueous solution, unimers, micelles or micellar hydrogels are formed, depending on the block copolymer architecture.

Fluorescence correlation spectroscopy (FCS) experiments on aqueous solutions of poly[(2-nonyl-2-oxazoline)_n-b-(2-methyl-2-oxazoline)_m], P[(MOx)_m(NOx)_n], diblock copolymers with a small fraction of identical, fluorescence-labeled polymers as tracers allowed us to study the micelle formation at very low concentrations [1]. In contrast, low molar mass fluorescence tracers lead to an overestimation of the micellar diffusion coefficients, because of the exchange dynamics of the tracer. Micelles formed by P[(MOx)_m(NOx)_n(MOx)_m] triblock copolymers are smaller than the ones from the corresponding diblock copolymers, as expected from the additional constraints for the hydrophobic blocks.

[1] T.B. Bonné, K. Lüdtkke, R. Jordan, P. Štěpánek, C.M. Papadakis, Coll. Polym. Sci. **282**, 833 (2004)

CPP 5.8 Mon 16:30 ZEU 160

Imaging of rodlike polyelectrolyte micelles — ●INGO LIEBERWIRTH, ANJA KRÖGER, JÖRG BELACK, and GERHARD WEGNER — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz

Mimicking the intricate structures and complex function of biological macromolecules with synthetic polymers is an attractive challenge. Research in this area will provide fundamental insights into the behavior and function of biopolymers and produce new materials as well for advanced applications in areas ranging from materials science to medicine. Biogenic polymers can frequently be considered as wormlike polyelectrolytes that have the tendency to self-aggregate into well-defined superstructures.

Serving as a model system, the self-assembly of rod-like polyelectrolytes consisting of a poly(p-phenylene) backbone with sulfonic acid and dodecyl side groups was investigated by transmission electron microscopy (TEM). In consistency with the DLS and SAXS measurements, the observed morphologies yield cylindrical micelles with morphologies ranging from individual strands and loops to gel-like networks.

A feature which is clearly established is the formation of closed loops and lasso-like structures starting from the individual micelles. Based on the reasonable assumption that the packing of the constituent PPPSH

chains within the individual micelles is of nematic and thus fluid character, a mechanism for the formation of closed loops has been suggested.

CPP 5.9 Mon 16:45 ZEU 160

Polypyrrole Nanowires Grown From Single Adsorbed Polyelectrolyte Molecules — ●ANTON KIRIY¹, VERA BOCHAROVA¹, MANFRED STAMM¹, HARTMUT VINZELBERG², and INGOLF MÖNCH² — ¹Leibniz Institute of Polymer Research Dresden, D-01069 Dresden — ²Leibniz Institute for Solid State and Materials Research, D-01069 Dresden

One-dimensional nanostructures of conductive polymers have attracted a great interest as building blocks for future miniaturized nanoelectronic devices and highly sensitive chemical or biological sensors. We have developed a simple chemical route to conductive polypyrrole nanowires by the grafting of polypyrrole from isolated synthetic polyelectrolyte molecules. The location and length of the synthesized Ppy nanowires are defined by the location and length of adsorbed single-molecule templates. Diameter of the nanowires varies from few nanometers to hundreds of nanometers and can be adjusted by polycondensation time and concentration of reagents. The dc conductivity of individual polypyrrole nanowires approaches the conductivity of polypyrrole in the bulk. A possibility to use the nanowires as active elements of sensors on acids and bases was evaluated. These results open broad opportunities for fabrication of electronic devices and sensors at molecular level (Bocharova, V.; Kiriya, A.; Vinzelberg, H.; Mönch, I.; Stamm, M. *Angew. Chem. Int. Ed.* 2005, 44, 6391).

CPP 5.10 Mon 17:00 ZEU 160

Structure and Dynamics of Bottle-brush Polymers — ●S. RATHGEBER¹, T. PAKULA¹, A. WILK¹, K. MATYJASZEWSKI², K.L. BEERS², and P. PANINE³ — ¹Max Planck Institute for Polymer Research, Mainz, Germany. — ²Carnegie Mellon University, Pittsburgh, USA. — ³ESRF, Grenoble, France.

The talk will address the structure and dynamics of bottle-brush polymers (BB) in solution. Due to high branching densities the hybrid character of BB between a flexible polymer and compact colloid is reflected their structure and dynamics. We investigated the dilute solution properties with static scattering methods, Monte Carlo simulations and measured the internal dynamics with neutron-spin echo spectroscopy. Collective breathing modes of the side chains in the brush lead to a slowing down of the dynamics on length scales of the brush diameter D . Attachment of longer, more space demanding side chains does not induce higher persistence to the overall brush. The persistence length λ is independent of the side chain length N_s . Thus, the ratio λ/D is decreasing with increasing N_s and lyotropic behavior becomes unlikely. We also looked at the lyotropic behavior and the rheological response of highly concentrated BB solutions. Structural changes occurring in a disordered and in a, perpendicular to the shear field pre-aligned sample, in response to the external shear field were measured by time-resolved x-ray scattering. Above a threshold torque the BB start to align in flow direction inducing a shear thinning process lasting two hours accompanied by a reduction in viscosity by two orders of magnitude. Above a higher threshold torque the alignment of the BB spontaneously flips into the flow direction.

CPP 6 Electronic Structure and Spectroscopy I

Time: Monday 14:30–17:45

Room: ZEU 114

CPP 6.1 Mon 14:30 ZEU 114

Energy-transfer of the organic donor-acceptor system triphenyldiamine-perylenebisimide studied by time-resolved spectroscopy — ●CHRISTIANE SCHARF¹, KATJA PETER², PETER BAUER², CHRISTOPH JUNG¹, MUKUNDAN THELAKKAT², and JÜRGEN KÖHLER¹ — ¹Department of Experimental Physics IV and BIMF, University of Bayreuth, D-95440, Germany — ²Department of Macromolecular Chemistry I and BIMF, University of Bayreuth, D-95440, Germany

We investigated energy transfer processes in the organic donor-acceptor system triphenyldiamine-perylenebisimide employing time-resolved spectroscopy. In order to do so, the fluorescence lifetimes of the isolated components have been determined as a function of the concentration of the chromophores and as a function of the polarity of the solvent. Subsequently, energy-transfer experiments were conducted in a solution of

CPP 5.11 Mon 17:15 ZEU 160

Melting of Polyelectrolyte Multilayer Capsules Investigated with AFM Force Spectroscopy — ●RENATE MUELLER and ANDREAS FERY — Max Planck Institute of Colloids and Interfaces, 14424 Potsdam

Microcapsules formed from polymer networks play an important role in both applications like encapsulation (drugs, cosmetics) and in microbiology where these structures are abundant (cell walls, virus capsids). We use Polyelectrolyte multilayer capsules as model systems to study the physico-chemical background of polymeric microcapsule mechanics.

The combination of the colloidal probe AFM technique and an optical microscope allows us to investigate the compliance of individual shells and derive elastic constants of the shell's wall material [1]. Here we explore how temperature affects the mechanical properties of our system. We find a strong softening for capsules formed from Poly(styrene sulfonate)/Poly(diallyldimethylammonium chloride), which we explain as transition from a glassy/rubbery to a viscoelastic state [2]. Shape changes occur in the viscoelastic state like shrinking for spherical shells [3] or more complex phenomena for non-spherical objects; we discuss them as surface tension effects. The shape can be frozen upon returning to $T = 25^\circ\text{C}$, thus the shape can be controlled on the nanoscale. Additional calorimetric experiments on the system will clarify the nature of the softening transition.

[1] F. Dubeuil et al., *Eur. Phys. J. E*, **2003**, 12, 215-221.

[2] R. Mueller et al., *Macromolecules*, **2005**, 38, 9766-9771.

[3] K. Köhler et al., *Macromolecules*, **2005**, 109, 18250-18259.

CPP 5.12 Mon 17:30 ZEU 160

Strong and weak adsorption of polyelectrolyte chains onto the oppositely charged sphere — ●ANDREY CHERSTVY^{1,2} and ROLAND WINKLER¹ — ¹Institut für Festkörperforschung, Theorie-II, Forschungszentrum Jülich, D-52425 Jülich, Germany — ²Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzerstrasse 38, 01187 Dresden, Germany

We investigate the complexation of long thin polyelectrolyte (PE) chain with an oppositely charged sphere. In the limit of strong adsorption, when PE chain adapts a definite wrapped conformation on the sphere, we analytically solve the linear Poisson-Boltzmann equation and calculate the electrostatic potential and the energy of the PE complex. We discuss possible attractive interactions between two such non-homogeneously charged complexes and its application to nucleosome core particles. In the limit of weak adsorption, when chain fluctuations are important and PE is crowded around the sphere, we solve the Edwards equation for PE conformations in the Hulthen potential, used as an approximation for the Debye-Hückel potential of the sphere. We predict the shape of the monomer profile away from the sphere and the critical conditions for PE adsorption. We find that the critical sphere charge density depends in a different manner on the Debye screening length than for PE adsorption onto flat surfaces. Our critical adsorption condition is consistent with experiments on complexation of PE with oppositely charged surfactant micelles. We also present results of numerical solutions of the self-consistent field equations for PE adsorption in assemblies of PEs with the oppositely charged spheres.

free donors and free acceptors. The results of these experiments are in reasonable agreement with predictions based on Förster theory. Finally, experiments were performed on donor-acceptor systems covalently bound by a $\text{C}_{12}\text{H}_{24}$ -linker.

CPP 6.2 Mon 14:45 ZEU 114

Femtosecond spectroscopic study of carminic acid-DNA interactions — ●RADU COMANICI¹, BIANCA GABEL¹, THOMAS GUSTAVSSON², RUSU CATALIN¹, and KRYSCHI CAROLA¹ — ¹Institute of Physical Chemistry I, FAU, D-91058 Erlangen — ²CEA/Saclay, DSM/DRECAM/SCM, F-91191 Gif-sur-Yvette

Photo-excited carminic acid and carminic acid-DNA associates have been examined using a variety of spectroscopy techniques, e.g. the femtosecond resolved fluorescence up-conversion and transient absorption spectroscopy. The observation of dual fluorescence emission, one peaks at 470 and the other 570 nm, shows that carminic acid undergoes an

excited-state (S1) intramolecular proton transfer (ESIPT). Transient absorption spectroscopy measurements of carminic acid in BPES yielded four lifetimes of the excited state (S1): 8 ps, 15 ps, 33 ps and 46 ps. On the other hand, only two lifetimes, 34 ps and 47 ps, were observed by fluorescence up-conversion. The four S1 lifetimes were ascribed to the coexistence of respectively two tautomer (normal and tautomer) forms of carminic acid, in the undissociated state (CAH) and in the deprotonated state (CA⁻). Fluorescence up-conversion measurements of carminic acid-DNA associates showed that the coupling to DNA is associated with the prolongation of the fluorescence lifetimes. This effect is taken as evidence for the formation of intercalation complexes between the carminic acid and the DNA. The intercalative binding of the carminic acid to DNA is confirmed by the fluorescence titration experiments.

CPP 6.3 Mon 15:00 ZEU 114

Time-Resolved Measurements of Intramolecular Energy Transfer in Single Donor/Acceptor Dyads — ●GERALD HINZE¹, FABIAN NOLDE², KLAUS MÜLLEN², and THOMAS BASCHÉ¹ — ¹Institut für Physikalische Chemie, Universität Mainz, Jakob-Welder-Weg 11, 55099 Mainz, Germany — ²Max-Planck-Institut für Polymerforschung, Ackermannweg 10, 55128 Mainz, Germany

Electronic excitation energy transfer has been measured in single donor/acceptor dyads. The specific design of donor/acceptor and the spacer in between force a rigid geometry of the overall molecular structure. Distance and orientation of the two chromophores were chosen such that both, donor as well as acceptor emission is observed. The significantly smaller photostability of the donor allows for time-resolved measurements of the acceptor emission with and without energy transfer from the donor. By analyzing the differences of the rise/decay profiles of the acceptor emission for both pathways, we could determine time constants of energy transfer with high accuracy. At the same time, emission spectra could be obtained for each dyad. Due to inhomogeneous broadening of the electronic transitions, spectral features and therefore energy transfer efficiencies vary from molecule to molecule.

We find a correlation between the spectral overlap and the energy transfer rates which seems to be in accordance with standard Förster theory. However, on average the energy transfer proceeds faster ($f \approx 1.8$) than what would have been expected.

CPP 6.4 Mon 15:15 ZEU 114

Charge Transfer Processes as the Source of Emission Intermittency of Semiconductor Quantum Dots — ●ABEY ISSAC¹, F. CICHOS², and C. VON BORCZYKOWSKI¹ — ¹Optical Spectroscopy and Molecular Physics — ²Photonics and Optical Materials, Institute of Physics, Chemnitz University of Technology, D-09107 Chemnitz, Germany

The emission intermittency of quantum dots (QDs) is one of the striking phenomena of single quantum objects. Its occurrence is unwanted and wanted at the same time since it interrupts the observation of the QDs but resembles to be one of the simplest switching events possible in a nano-object. Based on extensive measurements on the emission intermittency of single CdSe quantum dots in different dielectric environments, we show that this intermittency is controlled by the dielectric properties of the local environment [1]. Both, the duration of the emitting periods as well as of the dark periods respond to the dielectric function of the matrix material. This is a direct sign for a photo-induced charge transfer process as the source of the intermittency. Referring to recent theoretical models [2], we demonstrate that features of a diffusion controlled charge transfer process can be identified in the experimental statistics of single quantum dot intermittency. The combination of experiment and theory allows exploring the involved energy states, energy barriers and dielectric reorganization energies. [1] J. Tang et al. J. Chem. Phys. 123, 054704 (2005) [2] A. Issac et al. Phys. Rev. B. 71, 161302(R) (2005)

— 15 min. break —

CPP 6.5 Mon 15:45 ZEU 114

The Relation of Photoblinking and Photobleaching for Single Dye Molecules — ●JÖRG SCHUSTER, JÖRG BRABANDT, and CHRISTIAN VON BORCZYKOWSKI — Institute of Physics, TU Chemnitz, D-09107 Chemnitz

An inherent fingerprint of single molecule detection is the observation of photoblinking on different time scales. In recent papers [1] we could show, that for several dye molecules a blinking mechanism exists,

which is characterized by power law statistics of on- and off-times. The so called "power law blinking" is connected to an increasing duration of off-times during the observation of a single emitter. Thus, the discrimination between long dark periods and irreversible photodestruction of the molecules becomes impossible. In ensemble experiments the presence of dark periods manifests as reversible photobleaching [2].

In our contribution we present, how both types of photobleaching can be analyzed by single molecule observations. The suggested analysis is further supported by computer simulations which include power law blinking and irreversible photobleaching. Data are also discussed within the framework of a recent theory on the intermittency of semiconductor nanocrystals by Marcus et al. [3] which describes also several aspects of dye molecule blinking.

[1] Schuster et al., APL 87 (2005), 051915 and herein

[2] Orrit et al., J. Phys. Chem. A 107 (2003), 6770

[3] Marcus et al., PRL 95 (2005), 107401

CPP 6.6 Mon 16:00 ZEU 114

Interferometric Pump-Probe Spectroscopy of Single Gold Nanoparticles — ●MARKUS LIPPITZ^{1,2}, MEINDERT A. VAN DIJK¹, and MICHEL ORRIT¹ — ¹MoNOS, Huygens Laboratory, Leiden University, Niels Bohrweg 2, 2333 CA Leiden, The Netherlands — ²present address: Institut für physikalische Chemie, Universität Mainz, Jakob-Welder-Weg 11, 55099 Mainz, Germany

We report the first time-resolved absorption measurements of single gold nanoparticles, with a sensitive common-path interferometer [1,2]. The variation of the plasmon resonance after absorption of a near-infrared pump pulse is probed in the visible wavelength range. It can be separated in two parts: The prompt part of the signal arises from an increased plasmon resonance width due to hot electrons, and provides high-contrast images of particles as small as 10 nm. On a longer timescale, an oscillating transient (period about 16 ps for 50 nm diameter) reveals mechanical vibrations of the particle by periodic shifts of the plasmon frequency.

The selection of individual particles reveals the full heterogeneity of the ensemble, and the intrinsic damping of the vibrations, which is hidden in bulk measurements. Besides the fundamental breathing mode already seen in ensembles, we find a new mode at lower frequency involving shear deformation. Ultra-fast laser spectroscopy of single gold particles opens new insight into the mechanical properties of nanometer-sized objects.

[1] M.A. van Dijk et al., Acc. Chem. Res., 2005, 38, 594

[2] M.A. van Dijk et al., Phys. Rev. Lett., accepted, preprint cond-mat/0506401

CPP 6.7 Mon 16:15 ZEU 114

Orientation of Absorption Dipoles in Rigid Bichromophoric Systems as determined by Single Molecule Techniques — ●BURKHARD FÜCKEL¹, GERALD HINZE¹, FABIAN NOLDE², KLAUS MÜLLEN², and THOMAS BASCHÉ¹ — ¹Institut für Physikalische Chemie, Universität Mainz, Jakob-Welder-Weg 11, 55099 Mainz, Germany — ²Max-Planck-Institut für Polymerforschung, Ackermannweg 10, 55128 Mainz, Germany

The orientation of the absorption transition dipoles has been investigated in several rigid bichromophoric systems using polarization resolved single molecule spectroscopy. Depending on whether both chromophores within the bichromophores were the same or not, two different experimental techniques have been applied. In case of chemically identical chromophores fluorescence transients with polarization modulated excitation have been acquired prior and after bleaching of one of the components. Bichromophoric systems with different chromophores (donor/acceptor type) on the other hand allow for wavelength selective addressing of the chromophores. By analyzing the polarization dependence, we occasionally find significant deviations of the orientations of the transition dipoles from the values predicted by the molecular structure. This surprising observation is attributed to a symmetry breaking induced by the heterogeneous environment.

CPP 6.8 Mon 16:30 ZEU 114

Nanometer scale properties of self-assembled semiconductor quantum dot/dye hetero-arrays — ●MOHAMED ABDEL-MOTALEB¹, EDVARD ZENKEVICH², JÖRG SCHUSTER¹, ABHEY ISSAC¹, FRANK CICHOS³, and CHRISTIAN VON BORCZYKOWSKI¹ — ¹Optical Spectroscopy and Molecular Physics, Institute of Physics, TU Chemnitz, D-09107 Chemnitz — ²Institute of Molecular and Atomic Physics, National Academy of Sciences of Belarus, Minsk, Belarus — ³Photonics and Optical Materials, Institute of Physics, TU Chemnitz, D-09107 Chemnitz

One of the outstanding but inherent features of single quantum objects (molecules, quantum dots - QD) is the observation of luminescence intermittency. In recent experiments we have shown [1] [2] [3] that besides intramolecular properties (triplet states), photo-ejected charges cause intermittency dynamics on times scales over several orders of magnitude ranging from ms to h. These dynamics are related to QD photoluminescence intensities both of single particles and ensembles and are among others controlled by dielectric properties of the QD/dye arrays and/or the environment. This offers the possibility to investigate on a nanometer scale dielectric properties of functionalized organic molecules [4] self-assembled on semiconductor surfaces. Possible applications such as nanoscopic sensors will be discussed.

[1] Cichos et al. Phys. Rev. B, 70, 1153141 (2004)

[2] Issac et al. Phys. Rev. B 71, 161302(R) (2005)

[3] Schuster et al. Appl. Phys. Lett., 87, 051915 (2005)

[4] Zenkevich et al. J. Phys. Chem. B 109, 8679 (2005)

CPP 6.9 Mon 16:45 ZEU 114

Delayed luminescence in conjugated polymers — ●DIRK HERTEL and KLAUS MEERHOLZ — Institute of Physical Chemistry, University of Cologne, Luxemburger Str. 116, 50939 Cologne, Germany

Luminescent conjugated polymers are increasingly used as active components in optoelectronic devices such as light emitting diodes (LEDs). One obstacle for high volume OLED applications is the limited luminescence efficiency of conjugated polymers. According to spin statistics the formation of excited states from uncorrelated charge carriers yields 25% singlet and 75% triplet states, the latter do usually not contribute to electroluminescence. There is abundant indirect evidence for the existence of triplet states in conjugated polymers, but little is known about their generation and kinetics. The application of time gated luminescence spectroscopy enabled us to observe delayed fluorescence (DF) and phosphorescence (Ph) in conjugated polymers of the spiro-polyfluorene type. These materials are used for state of the art polymer LEDs. From combined experimental investigations of the time and intensity dependence of DF and Ph as well as the temperature dependence of DF we are able to show that DF in a spiro-polyfluorene homopolymer is dominated by triplet-triplet annihilation (TTA). Recently we have extended our investigation to spiro- copolymers to study the influence of electron transport and hole transport units on the DF and Ph. To clarify the role of charge recombination on DF the dependence of DF and Ph on applied electric fields is discussed. Time gated luminescence spectroscopy is as well a powerful tool to check the purity of conjugated materials.

CPP 6.10 Mon 17:00 ZEU 114

Anisotropy of the transport mechanisms in organic quasi 1D conductors — ●DAVID SAEZ DE JAUREGUI and ELMAR DORMANN — Physikalisches Institut, Universität Karlsruhe (TH), D-76128 Karlsruhe

Arene radical cation salts (rcs) are synthetic metals consisting of polycyclic aromatic hydrocarbons (i.e. naphthalene, fluoranthene, pyrene or perylene) and inorganic complex anions (i.e. PF₆, AsF₆ or SbF₆). Due to a π -orbital overlap of the arene molecules and a not completely filled conduction band the rcs are quasi-one dimensional conductors. They perform a Peierls transition between a metallic high temperature phase

with a pseudo-gap caused by fluctuations and charge density ground.

These rcs provide excellent model systems for investigations of the transport dynamics, because both the electronic charge as well as the electron spin motion can be detected. Using microwave conductivity measurements and X-band-pulse-ESR techniques with applied static field gradients the electron charge motion and the electron spin diffusion were examined for different orientations and a broad temperature regime below and above the semiconductor-metal phase transition. This was done for rcs with different paramagnetic defect concentrations. The influence of defects is a decrease of the anisotropic behavior of the organic conductors. The real "intrinsic" anisotropy of the electrical conductivity and the spin diffusion coefficient must be derived by extrapolation to vanishing defect concentration.

CPP 6.11 Mon 17:15 ZEU 114

Thermodynamic theory of light-induced material transport in amorphous azobenzene polymer films — ●MARINA SAPHIANNIKOVA¹ and DIETER NEHER² — ¹Leibniz Institute of Polymer Research, Hohe Str. 6, 01069 Dresden, Germany — ²Institute of Physics, University of Potsdam, Am Neuen Palais 10, 14469 Potsdam, Germany

It was discovered 10 years ago that the exposure of an initially flat layer of an azobenzene containing polymer to an inhomogeneous light pattern leads to the formation of surface relief structures, accompanied by a mass transport over several micrometers. However, the driving force of this process is still unclear.

We propose a new thermodynamic approach that explains a number of experimental findings including the light-induced deformation of free standing films and the formation of surface relief gratings for the main inscription geometries. Our basic assumption is that under homogeneous illumination an initially isotropic sample should stretch itself along the polarization direction to compensate the entropy decrease produced by the photoinduced reorientation of azobenzene chromophores. The magnitude of the elastic stress, estimated by taking the derivative of the free energy over the sample deformation, is shown to be sufficient to induce plastic deformation of the polymer film. Orientational distributions of chromophores predicted by our model are compared with those deduced from Raman intensity measurements.

CPP 6.12 Mon 17:30 ZEU 114

Photo-induced deformations in azobenzene-containing side-chain polymers: molecular dynamics study — ●JAROSLAV ILNYTSKIY¹, MARINA SAPHIANNIKOVA², and DIETER NEHER¹ — ¹Institute for Physics, University of Potsdam, Am Neuen Palais 10, 14469 Potsdam, Germany — ²Leibniz Institute of Polymer Research, Hohe Str. 6, 01069 Dresden, Germany

The photo-induced deformations in azobenzene containing side-chain polymers and elastomers are studied by means of molecular dynamics (MD) simulations on semi-atomistic models. The phase diagrams for both polymers are built and initial configurations in nematic and smectic phases are prepared in a number of ways. By driving the elastomer system through the orientational phase transition, the reversible contraction of the sample have been reproduced. The photo-mechanical response of both polymers involved the modelling of the photoisomerization of the azobenzenes. That was done in a simplified way, by considering solely the effect of reorientation of the *trans* isomers perpendicularly to the light polarization. We found the effect strongly dependent on the optical field strength. In weak fields the photo-chemical phase transition takes place and for the case of nematic elastomer the reversible shrinking along the optical field is observed. In the case of side-chain polymer in stronger fields, the rapid initial shrinking of the sample (similar to the case of elastomer) is followed by slow self-organisation of new smectic layers with the chromophores perpendicular to the light polarization (the light induced order).

CPP 7 SYMPOSIUM Disperse Polymer Systems I

Time: Tuesday 09:30–12:15

Room: ZEU 160

Invited Talk

CPP 7.1 Tue 09:30 ZEU 160

Structure and interfacial rheology of aggregated two dimensional suspensions — ●JAN VERMANT¹, SVEN REYNAERT¹, MADIVALA BASAVARAJ¹, MOLDENAERS PAULA¹, and FRANSSAER JAN² — ¹Department of Chemical Engineering, K.U. Leuven, Belgium — ²Department of Metallurgy and Materials Science, K.U. Leuven, Belgium

Tailoring the structure and rheological properties of particle-laden interfaces is of importance in a number of practical applications such as the stabilization of emulsions, polymer blends and foams. In the present work, different methods are compared to generate weakly aggregated two-dimensional suspensions with controlled interactions. Adequate combinations of electrolyte and surfactant destabilized particulate monolayers, both at the water-oil and water-air interface. The structural and kinetic aspects of the induced structures are compared to the underlying changes in the interparticle interactions, and the conditions under which reproducible results could be induced are reported and discussed. Also effects of particle shape are explored. Secondly, a magnetic needle interfacial rheometer is used to characterize the rheological behaviour of the particle monolayer. Preliminary results show the presence of a two-dimensional yield stress and control over the surface rheology much like for the three dimensional weakly aggregated suspensions.

CPP 7.2 Tue 10:00 ZEU 160

The Influence of Triblock Copolymers and Low Molecular Weight Homopolymers on the Structure of Microemulsions — ●TINKA SPEHR and BERND STÜHN — Institute of Condensed Matter Physics, Technical University Darmstadt, D-64289 Darmstadt

We use small angle X-ray scattering (SAXS) to study a microemulsion consisting of water droplets coated by the anionic surfactant AOT dispersed in decane. At a constant water-to-AOT ratio the dependence of droplet radius, polydispersity and structure factor of the pure microemulsion on droplet density and temperature were investigated. Unexpectedly the radius of the water core decreases with increasing droplet volume fraction. At a volume fraction of droplets of ten percent we added different amounts of the amphiphilic triblock copolymer PEO-PI-PEO, which has hydrophilic headgroups and a hydrophobic middle part (PEO: polyethyleneoxide, PI: polyisoprene). There is clear evidence for an increasing crosslinking of the droplets with increasing polymer concentration. Already a low number of polymer molecules per droplet causes network formation as opposed to the complementary system (o/w-microemulsion with nonionic surfactant) for which the interconnection of the droplets via an amphiphilic triblock copolymer has previously been shown [1]. Structure factors were extracted from the SAXS profiles. Furthermore the effect on droplet structure caused by the incorporation of low molecular weight PEO homopolymers will be discussed. [1] M. Schwab and B. Stühn; J. Chem. Phys. 14, 6461 (2000)

CPP 7.3 Tue 10:15 ZEU 160

Correlation between morphology, rheology and foamability of immiscible PPE/SAN blends — ●HOLGER RUCKDAESCHEL¹, ANDREAS GOELDEL¹, SAMPATH BANGARU¹, JAN K.W. SANDLER¹, VOLKER ALTSTAEDT¹, HOLGER SCHMALZ², and AXEL H.E. MUELLER² — ¹Polymer Engineering, University of Bayreuth, Universitaetsstrasse 30, 95447 Bayreuth, Germany — ²Macromolecular Chemistry II, University of Bayreuth, Universitaetsstrasse 30, 95447 Bayreuth, Germany

The morphology as well as the interfacial properties of immiscible polymer blends are of key importance for the processing behaviour and the materials performance. In this particular study, both phenomena were analysed in detail for blends of poly(2,6-dimethyl-1,4-phenylene ether) (PPE) and poly(styrene-co-acrylonitrile) (SAN). Melt-processing and batch-foaming were used as processing techniques. The morphology development following melt-processing revealed a strong dependence on the blend composition as well as on the viscosity ratio between the constituents. Subsequent batch-foaming of the two-phase blend highlighted further special features which could be correlated both to the melt-elongational behaviour and to the blend morphology. Furthermore, the addition of further components was identified to be one efficient route to adjust the rheological as well as the interfacial properties of the blend. In particular, the effect of triblock terpolymers as compatibilising agents

as well as the effect of a selectively miscible third blend component were demonstrated. This final approach ensures to control both the morphology development and the foamability of PPE/SAN blends.

CPP 7.4 Tue 10:30 ZEU 160

Linear viscoelastic shear oscillation investigations of melt mixed blends of polycarbonate with multiwalled carbon nanotubes and polyethylene — ●PETRA PÖTSCHKE and MAHMOUD ABDEL-GOAD — Leibniz Institute of Polymer Research Dresden, Hohe Strasse 6, 01069 Dresden, Germany

The concept of double percolation was adapted to melt mixed blends of a conductive polycarbonate composite containing 2 wt% multiwalled carbon nanotubes (PC-2NT) and polyethylene (PE). The blends were melt mixed using a small scale twin-screw compounder over the whole composition range. This study presents linear viscoelastic shear oscillation tests on these blends performed at 280°C. We investigated the question, if melt rheological measurements are able to detect the co-continuous composition range in such systems unequivocally. The percolation of the nanotubes in PC is clearly detected by an increase in complex viscosity by lowering oscillation frequency and the formation of a plateau of G' at low frequencies. Viscosity and moduli of the selected high density PE are higher than those of PC-2NT which gives favourable conditions for the formation of a continuous PC-2NT phase at low concentrations. Whereas all blends show values of G'' between those of the parent materials, some of the composites in the middle concentration range exceed the parent values of G' and complex viscosity, especially at low frequencies. It was found from morphological studies and selective extraction experiments that the co-continuous structure formation starts at 20 vol% PC-2NT. At this composition, we also find maximum values of G' , G'' and complex viscosity over the whole frequency range.

— 15 min. break —

Invited Talk

CPP 7.5 Tue 11:00 ZEU 160

Non-linear rheological properties of glassy colloidal dispersions — ●MATTHIAS FUCHS¹, OLIVER HENRICH¹, MICHAEL CATES², MATTHIAS BALLAUFF³, JEROME CRASSOUS³, and FATHOLLAH VARNIK⁴ — ¹Fachbereich Physik, Universitaet Konstanz — ²School of Physics, The University of Edinburgh — ³Physikalische Chemie I, Universitaet Bayreuth — ⁴MPI fuer Eisenforschung, Duesseldorf

Soft materials, such as particle dispersions, quite universally exhibit a strongly decreasing viscosity as function of shear rate ('shear thinning'). We study theoretically an universal mechanism explaining the reduction of the viscosity or stress in such disordered colloidal systems.

Our first-principles approach [1] to the non-linear rheology of dense colloidal suspensions predicts an universal transition between the yielding of amorphous solids and non-Newtonian (shear-thinning) fluid flow. The approach builds upon a microscopic description of structural relaxations in quiescent suspensions provided by the mode coupling theory. The advection of density fluctuations is the dominant mechanism captured, while hydrodynamic interactions, non-linear flow profiles and ordering phenomena are neglected. Comparisons with experiments in model colloidal dispersions support the approach [2], as do computer simulations of Newtonian supercooled liquids, which find a finite dynamic yield stress at low temperatures [3].

[1] M. Fuchs and M. E. Cates, Phys. Rev. Lett. 89, 248304 (2002); Faraday Discuss. 123, 267 (2003); J. Phys.: Condens. Matter 17, 1681 (2005)

[2] M. Fuchs and M. Ballauff, J. Chem. Phys. 122, 094707 (2005)

[3] F. Varnik and O. Henrich, submitted (2005)

CPP 7.6 Tue 11:30 ZEU 160

2-Fluid Description of Disperse Polymer Systems — ●HARALD PLEINER¹ and JAMES L. HARDEN² — ¹Max Planck Institute for Polymer Research, Mainz — ²Johns Hopkins University, Baltimore

We combine the recently developed nonlinear hydrodynamic description of viscoelastic fluids [1] with a general 2-fluid hydrodynamics of 2-component and 2-momentum systems [2] to give a generalized-hydrodynamics model for disperse polymers. The former covers the usual non-Newtonian effects, like shear thinning, strain hardening,

stress overshoot, normal stress differences and non-exponential stress relaxation, while the latter deals with the relative velocity and its relaxation, the stress division between the two subsystems, the convective velocity problem and the anomalous concentration dynamics.

[1] H. Pleiner, M. Liu and H.R. Brand, *Rheologica Acta*, **39**, 560 (2000) and **43**, 502 (2004). [2] H. Pleiner and J.L. Harden, in *Nonlinear Problems of Continuum Mechanics*, Special issue of Notices of Universities. South of Russia. Natural sciences, p.46 (2003) and cond-mat/0404134.

CPP 7.7 Tue 11:45 ZEU 160

Flow behavior of two-phase polymer blends — •BERNHARD A. WOLF, VERENA E. ZIEGLER, and MATTHIAS SCHNELL — Institut für Physikalische Chemie der Johannes Gutenberg-Universität Mainz, Germany

The processing of polymer mixtures (for instance in extruders at high temperatures) is usually taking place in the heterogeneous state. Under these conditions two liquid phases (the melts of normally almost immiscible polymers) coexist and the viscosities of these mixtures are not only determined by the properties of the components, but modified considerably by the morphology of the system.

The lecture demonstrates for two binary polymer blends of different degrees of incompatibility [poly(ethylene oxide)/poly(dimethylsiloxane) and poly(dimethylsiloxane)/poly(dimethylsiloxane-*ran*-methylphenylsiloxane)], how the spatial arrangement of the coexisting phases (as observed with an optical microscope during shear) influences the viscosities and the storage plus loss moduli of the mixture. Furthermore it deals with the changes resulting from the addition of compatibilizers. The measurements demonstrate that the viscosities as well as the storage moduli are normally markedly larger than predicted under the assumption of additivity of the properties of the pure

components. The variations of these quantities with blend composition and with shear rate indicate under which conditions droplet/matrix structures or co-continuous morphologies are stable.

CPP 7.8 Tue 12:00 ZEU 160

Shear and melt elongation of polycarbonate/multiwalled carbon nanotubes composites — •U.A. HANDGE¹ and P. PÖTSCHKE² — ¹Institute of Polymers, Dept. of Materials, ETH Zürich, 8093 Zürich, Switzerland — ²Leibniz Institute of Polymer Research Dresden, Dept. of Polymer Reactions and Blends, Hohe Strasse 6, 01069 Dresden, Germany

The discovery of carbon nanotubes initiated intensive research activities which also led to applications of these remarkable molecules. For example, composites that consist of commercial polymers and carbon nanotubes can serve as possible antistatic or conductive materials. Processing of polymers is intimately associated with their rheological properties. In this work, we studied the rheological properties of pure polycarbonate and a polycarbonate/multiwalled carbon nanotubes (PC/MWCNT) composite in the melt. The weight fraction of the multiwalled carbon nanotubes for the composite was 2 wt.% and the test temperature was $T = 190^\circ\text{C}$. We performed linear viscoelastic shear oscillations and elongational tests that were followed by recovery experiments using the uniaxial elongational rheometer RME. The analysis of the linear viscoelastic shear oscillations of the composite revealed that at low and large frequencies elastic forces dominated. In melt elongation, the transient viscosity of the PC/MWCNT composite did not differ much from the elongational viscosity of pure polycarbonate. However, the recovered stretch of the composite was significantly smaller than the corresponding values for pure polycarbonate. We discuss these results by taking into account the extension of the macromolecules in elongational flows and the yield stress of the composite.

CPP 8 SYMPOSIUM Nonequilibrium Phenomena in Soft-Condensed Matter

Time: Tuesday 14:00–16:45

Room: ZEU Lich

CPP 8.1 Tue 14:00 ZEU Lich

Optimal control of self-organized dynamics in cellular signaling — •DIRK LEBIEDZ — IWR, Im Neuenheimer Feld 368, 69120 Heidelberg

Recently, increasing experimental evidence has become available supporting the significance of self-organization and pattern formation for information processing in cellular signal transduction. The underlying complex mechanisms can only be understood by help of detailed mathematical modeling and simulation. In that context, model based control studies of self-organized dynamics are promising for two major reasons. First, to study potential dynamic regulatory mechanisms, and second, to explore possibilities for specific manipulation of biochemical system dynamics by external stimuli and targeted modifications realized for example by tailored drug application. Optimal control allows the general formulation of inverse problems with time-varying input parameters as well as specific control aims in the form of objective functionals to be minimized. We present applications of advanced numerical optimization to ordinary and partial differential equation models for cellular signal transduction systems and demonstrate how optimal control can be exploited for studying both inherent regulatory mechanisms and specific external manipulations. [1] D. Lebiecz, U. Brandt-Pollmann, Manipulation of self aggregation patterns and waves in a reaction-diffusion-system by optimal boundary control strategies, *Phys. Rev. Lett.* **91**, 208301 (2003) [2] D. Lebiecz, S. Sager, H.G. Bock, P. Lebiecz. Annihilation of limit-cycle oscillations by identification of critical perturbing stimuli via mixed-integer optimal control, *Phys. Rev. Lett.*, **95**, 108303 (2005)

CPP 8.2 Tue 14:15 ZEU Lich

Numerical study of electrostatic colloidal interaction at interface — •PAVEL DYSHOVENKO¹ and PIOTR WARSZYŃSKI² — ¹Ulyanovsk State Technical University, 32 Severny Venets Street, Ulyanovsk 432027, Russia — ²Institute of Catalysis and Surface Chemistry, ul. Niezapominajek 8, 30-239 Kraków, Poland

Electrostatic interaction of a pair of colloidal particles immersed in electrolyte in the vicinity of a charged plane is studied numerically within the framework of the non-linear Poisson-Boltzmann equation in two dimensions. Particular attention is given to the many-particle effects and non-linearity. The question under consideration is related to the important practical problem of colloidal adsorption/deposition. The relevant details of numerical procedure are briefly discussed. The results of the

numerical experiments indicate that the inter-particle interaction near a charged plane differs appreciably from the interaction of free particles. For the problem considered, the repulsion of two like-charged particles weakens for large values of plane's charge, both positive and negative. In contrast, the repulsion exceeds the one of free particles when the wall is charged moderately.

CPP 8.3 Tue 14:30 ZEU Lich

Capillary Rise of Liquids in Mesoporous Silica — •PATRICK HUBER¹, KLAUS KNORR¹, and ANDRIY KITYK² — ¹Technische Physik, Universität des Saarlandes, D-66041 Saarbrücken — ²Institute for Computer Science, Technical University of Czestochowa, PL-42200 Czestochowa

In order to study liquid flow in restricted geometries we have investigated the capillary rise (spontaneous imbibition) of water and n-alkanes in mesoporous Vycor glass (mean pore diameter 10 nanometer). An analysis of the mass uptake of the porous monoliths versus time, $m(t)$, allows us to determine a characteristic speed of the imbibition process, v_{imb} , which gives access to the ratio of surface tension σ and viscosity η of the confined liquids: $v_{imb} \sim \sigma/\eta$. For imbibing water as well as for the n-alkanes investigated (C_8H_{18} - $\text{C}_{30}\text{H}_{62}$) we find a \sqrt{t} -Lucas-Washburn type behavior for both the mass uptake and the position of the advancing liquid front. The relative imbibition speeds of the different *nanoconfined* liquids scale as expected from the ratio of the *bulk* fluid parameters. The width of the advancing two-phase boundary as a function of time is extracted from light scattering data sets recorded during imbibition. It is discussed with regard to state-of-the art theories of kinetic roughening of such boundaries in disordered media.

[1] M. Alava, M. Dubee, M. Rost, *Imbibition in disordered media*, *Adv. Phys.* **53**, 83 (2004).

CPP 8.4 Tue 14:45 ZEU Lich

Phase-field description for the budding of two-component vesicles — •ROGER FOLCH and UWE THIELE — Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, D-01187 Dresden, Germany

We present a diffuse-interface or phase-field model[1] for the *dynamics* of the budding process of a vesicle induced by phase separation on its membrane. Possible two-dimensional budding mechanisms are explored

in addition to known three-dimensional scenarios [2]. The model extends previous developments to simulate two-fluid flow[3] and the dynamics of a vesicle under flow[4] to include the internal dynamics of the membrane (phase-separation) and thus account for its non-static mechanical properties.

[1] R. González-Cinca, R. Folch, R. Benítez, L. Ramírez-Piscina, J. Casademunt and A. Hernández-Machado (cond-mat/0305058), in *Advances in Condensed Matter and Statistical Mechanics*, pp. 203–236, ed. by E. Korutcheva and R. Cuerno, Nova Science Publishers (New York, 2004).

[2] R. Lipowsky and R. Dimova, *J. Phys. Condens. Matt.* **15**, 31 (2003).

[3] R. Folch, J. Casademunt, A. Hernández-Machado and L. Ramírez-Piscina, *Phys. Rev. E* **60**, 1724; *ibid.* 1734 (1999).

[4] J. Beacourt, F. Rioual, T. Séon, T. Biben and C. Misbah, *Phys. Rev. E* **69**, 011906 (2004).

CPP 8.5 Tue 15:00 ZEU Lich

Suppression of demixing in a small gap between parallel plates: From Cahn-Hilliard to model H — ●SANTIAGO MADRUGA and UWE THIELE — Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, D-01187 Dresden, Germany

We analyse the spinodal decomposition of a mixture in the gap between parallel plates [1]. Linear results obtained with the full transport equations for (a) solely diffusive transport described by the Cahn-Hilliard equation and (b) diffusive and convective transport described by model H consisting of coupled Navier-Stokes and Cahn-Hilliard equations [2] are compared to an effective thin film description.

Detailed results are given for the dependence of the critical gap width (below which decomposition is suppressed) on the physico-chemical properties of the bounding plates. Criteria for the validity of the thin film description are given.

[1] R. Kenzler *et al.*, *Comp. Phys. Comm.* **133**, 139–157 (2001).

[2] D. M. Anderson, G. B. McFadden, and A. A. Wheeler, *Ann. Rev. Fluid Mech.* **30**, 139–165 (1998).

CPP 8.6 Tue 15:15 ZEU Lich

The depinning transition of a driven droplet on a heterogeneous substrate — ●UWE THIELE¹ and EDGAR KNOBLOCH² — ¹Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, D-01187 Dresden, Germany — ²Department of Physics, University of California, Berkeley CA 94720, USA

On non-ideal real substrates used in experiments the onset of droplet motion under driving along the substrate is strongly influenced by chemical or physical defects. A finite driving force is necessary to overcome the pinning influence of the heterogeneities occurring on a micro- or mesoscale. This is thought to be responsible, for instance, for the observed hysteresis between advancing and receding contact angles.

In the present paper we aim at understanding not only the processes that lead to pinning, but also the bifurcation that leads to depinning and the subsequent behavior of a moving droplet. We study driven droplets on a heterogeneous inclined plate using a long-wave evolution equation for the film thickness profile in two cases: (a) a periodic sinusoidal modulation of the disjoining pressure, and (b) strongly localized hydrophilic or hydrophobic 'defects'. As a result the drop may be pinned at the rear by an enhanced wetting region, or at its front by a region of reduced wettability. The results are obtained by a combination of branch following methods, linear stability theory and direct numerical simulation of the model equation.

— 15 min. break —

CPP 8.7 Tue 15:45 ZEU Lich

Transport coefficients of polymer solutions and blends near a glass and a liquid-liquid phase transition — ●WERNER KÖHLER, ALBERT VOIT, JÜRGEN RAUCH, and ALEXEI KREKHOV — Physikalisches Institut, Universität Bayreuth

Transport coefficients in polymer solutions and blends can usually be written in terms of a thermodynamic (osmotic modulus) and a kinetic (friction) factor. We discuss self diffusion, collective diffusion, and thermal diffusion of dilute to concentrated polymer solutions and polymer blends in the vicinity of a glass and a liquid-liquid phase transition. The dramatic increase of local friction near T_g is accompanied by a slowing down of mass diffusion, whereas the Soret coefficient, which is a measure for the susceptibility to external temperature fields, remains unaffected by the glass transition. In sharp contrast is its divergence near a critical point which is caused by the critical slowing down of collective diffusion and an almost constant thermal diffusion coefficient. We show how this diverging susceptibility can be utilized for patterning of critical polymer blends both in the one and in the two phase regime.

[1] A. Voit, A. Krekhov, W. Enge, L. Kramer, W. Köhler. *Phys. Rev. Lett.* **92** (2005) 214501

[2] J. Rauch, W. Köhler. *J. Chem. Phys.* **119** (2003) 119777

CPP 8.8 Tue 16:00 ZEU Lich

Nonequilibrium subdiffusion of a Brownian particle in a quasicrystalline potential — ●MICHAEL SCHMIEDEBERG and HOLGER STARK — Universität Konstanz, Fachbereich Physik, D-78457 Konstanz

We study the motion of a single colloidal particle in an optical lattice with two-dimensional quasicrystalline symmetry. From Brownian-dynamics simulations we find that initially the particle exhibits subdiffusional motion over several decades in time until it crosses over to pure diffusion in the long-time limit. We demonstrate that the subdiffusion is due to a temporally extended relaxation process towards thermal equilibrium where the particle then enters the diffusive regime. The duration of the transient subdiffusion increases for decreasing temperature. We observe a similar behavior for the motion of particles in random potentials which demonstrates that quasicrystalline systems are useful for studying aspects of disordered systems.

CPP 8.9 Tue 16:15 ZEU Lich

Unfolding of a globular polymer in shear flow — ●ALFREDO ALEXANDER-KATZ and ROLAND R. NETZ — Physik Department, Tech. Univ. Muenchen, James-Frank Str., D-85748, Garching, Deutschland

In the process of clotting in small vessels, platelets form a plug in an injured zone only in the presence of a protein known as the von Willebrand Factor (vWF). The absence or malfunction of the vWF leads to a bleeding disorder, the so-called von Willebrand disease. It is believed that the protein is globular when released into the blood flow. In this talk, we present a study of a simple model of vWF in shear flow. Using hydrodynamic simulations, we show that a globular polymer undergoes globule-stretch transitions above a critical shear rate. Finally, we discuss the scaling of the critical shear rate with the length of the polymer, and compare it to the physiological values attainable in the body.

CPP 8.10 Tue 16:30 ZEU Lich

A Fluctuation Theorem for Wet Granular Matter — ●AXEL FINGERLE and STEPHAN HERMINGHAUS — MPI for Dynamics and Self-Organization, Bunsenstr. 10, 37073 Göttingen, Germany

Although there are various formulations of fluctuation theorems extending the second law of thermodynamics, the time inversion symmetry of the equations of motion is the key principle in every derivation. Wet granular matter has been described successfully by the Minimal Capillary Model [S. Herminghaus, *Adv. Phys.*, **54**, 221 (2005)]. This dynamical system has a non-trivial time inversion map due to the hysteretic interaction by liquid bridges between grains. We present numerical results and give simple analytic arguments to determine why the exponential suppression of 'violations' of the second law remains valid even for a time inversion map that is non-local in time.

CPP 9 SYMPOSIUM Disperse Polymer Systems II

Time: Tuesday 14:00–17:00

Room: ZEU 160

Invited Talk

CPP 9.1 Tue 14:00 ZEU 160

Rheology and Structure Kinetics of Filled Polymer Nanocomposites and Networks — ●GERT HEINRICH — Leibniz Institute of Polymer Research Dresden, Hohe Strasse 6, D-01069 Dresden, Germany

Dynamic-mechanical and rheological studies provide an excellent access to the morphology and dynamics of complex filled polymers and to tests of corresponding models. Based on several dynamic-mechanical and shear flow experiments we discuss common features of structural filler reorganization in diverse filled elastomers and in polymer nanocomposites consisting of a thermoplastic melt (LDPE) and nanofillers (Mg/Al based Layered Double Hydroxide). In the elastomer case the discussion is possible when studying the kinetics of the modulus recovery with experimental set-ups where the stiffness response on repeated amplitude steps is measured. In the stress growth experiment the nanocomposites exhibit a pronounced non-linear behaviour observed as a shear overshoot. The time, at which the overshoot appears, decreases as the LDH loading increases. This effect can be described using the Wagner model, in which the non-linearity parameter increases with the particle loading and the relaxation time of the system decreases with the increase in shear rate. Additionally, in the high loaded nanocomposites, we observe shear oscillations presumably caused by the presence of a LC texture formed by the anisotropic filler particles. We propose that LDH particles in the PE melt are organised in domains (perhaps, orientational) which size is drastically diminished upon shear application.

CPP 9.2 Tue 14:30 ZEU 160

A microscopic look at the reinforcement of silica filled rubber — ●EKKEHARD STRAUBE¹, ALBERTO BOTTI², WIM PYCKHOUT-HINTZEN³, and DIETER RICHTER³ — ¹Uni Halle-Saale — ²Uni Roma TRE, Italy — ³Forschungszentrum Jülich

The deformed state of filled rubbers under uniaxial strain has been investigated by a combination of SAXS and SANS. Using an extraction procedure the single chain scattering behavior as well as filler properties could be obtained. For the first time the deformation of the rubbery matrix on the length scale of a network chain is determined and no overstrain is observed. Likewise, the determination of filler deformation and filler destruction enables a first microscopic observation of possible mechanisms of the stress-softening Mullins-effect.

CPP 9.3 Tue 14:45 ZEU 160

Structure Property Relationships of Different Polymer Based Nanocomposites — ●ANDREAS SCHÖNHALS, NING HAO, MARTIN BÖHNING, and HARALD GOERING — Bundesanstalt für Materialforschung und prüfung, Unter den Eichen 87, D 12205 Berlin

Polymer based nanocomposites continue to receive tremendous attention for different applications. They show remarkable property improvements (increased tensile properties, decreased gas permeability, decreased solvent uptake, increased thermal stability and flame retardance) when compared to conventionally * scaled composite materials. Different polymer based nanocomposites are prepared where polypropylene, polycarbonate and polystyrene are used as polymer matrices. Montmorillonite clay, silicium carbide, multiwalled carbon nanotubes and polyhedral oligomeric silsesquioxanes (POSS) are used as nanoparticles. The property structure relationships of these nanocomposites are investigated by dielectric spectroscopy and gas transport measurements (permeation, sorption). The results are discussed with regard to the nanofiller dispersion and the phase structure of the nanocomposites. Special attention is paid to characterize the interfacial region between the polymeric matrix and the different nanofillers. This regards also to estimate the length scale of interaction between the nanoparticles and the matrix.

CPP 9.4 Tue 15:00 ZEU 160

Preparation and Viscoelastic Properties of Fibre Networks — ●CHRISTIAN FRIEDRICH, BENJAMIN GRIMMINGER, and CIPRIAN IACOB — Freiburg Materials Research Center (FMF), Albert-Ludwigs-Universität, Stefan-Meier-Str. 21, 79104 Freiburg

The dispersion of carbon nanotubes (CNTs) is of crucial importance for the understanding of their mechanical properties as well as for the enhancement of their application potential. Therefore, we dealt with methods enabling the molecular dispersion of CNTs in appropriate matrices. We found that CNTs are best dispersed in ionic liquids such as 1-butyl-3-

methyl imidazolium tetrafluoroborate (BMIBF₄) together with cosolvents and surfactants. The obtained dispersions were characterized morphologically and rheologically. For the highest concentrations, the rheological response of these compounds resembles that of fibre networks. Using models developed for semiflexible biopolymer networks we can understand the obtained results quantitatively. In contrast to actin-networks, the CNT-networks display rather energetic elasticity than entropic. We discuss the reasons for this peculiarity.

CPP 9.5 Tue 15:15 ZEU 160

Structure creation in pressure sensitive adhesives — ●E. MAURER¹, S. LOI¹, D. WULFF², N. WILLENBACHER², M. RUCKPAUL², and P. MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik-Department E13, James-Frank-Str. 1, D-85747 Garching, Germany — ²BASF Aktiengesellschaft, Carl-Bosch-Str.38, D-67056 Ludwigshafen, Germany

Pressure sensitive adhesives (PSA) play an important role as materials in the glue industry as well as in everyday life. The adhesion properties are depending decisive on the bonding history, which means parameters like contact pressure and time, temperature and debonding rate. Previous experiments were restricted to optical investigations addressing the macroscopic fibril structure. With ultra small angle x-ray scattering (USAXS) the microscopic length scales of the polymeric material have been investigated in the presented work. For this purpose an apparatus, combining both, a reproducible mechanical experiment of adhesive bonding and debonding and the requirements of in-situ scattering experiments, was built. Due to the weak scattering synchrotron radiation was required. The observed scattering signals show pronounced features originating from a highly ordered substructure of the adhesive material [1]. Several types of PSAs, homopolymers as well as statistical copolymers have been investigated.

[1] E.Maurer, S.Loi, D.Wulff, N.Willenbacher, P.Müller-Buschbaum; Physica B 357, 144 (2005)

— 15 min. break —

Invited Talk

CPP 9.6 Tue 15:45 ZEU 160

Microstructure design for food applications — ●BETTINA WOLF — Corporate Research Colworth, Unilever Colworth Park, Sharnbrook, Bedford MK44 1LQ, UK

In the food industry it is of great importance to control the stability and texture of structured products. Traditionally, biopolymers and more often mixtures thereof are used. One of the factors controlling the behaviour of such materials is the morphology of the biopolymer phases, being able to control and manipulate this is thus advantageous for product texture / property control. Of particular interest to us has been for some time to establish routes for influencing the morphology of particulate biopolymer gel phases, and to study the influence of particle shape and particle material properties on the rheological behaviour. Routes developed are based on permanently arresting morphologies developed in shear flow allowing for formation of gelled particles of arbitrary shape as well as ellipsoidal and cylindrical gelled particles. Other research interests in the field of microstructure and rheology concern the understanding of individual microstructure components on the rheological behaviour of full product formulations, development of appropriate instrumental techniques for the product itself as well as understanding its in-use behaviour.

CPP 9.7 Tue 16:15 ZEU 160

What is the link between gelation and partial solubility in the galactomannan polysaccharides? — ●MICHAEL POLLARD and PETER FISCHER — Laboratory for Food Process Engineering, Swiss Federal Institute of Technology, Zürich CH-8006

We are interested in the structure-property relations of the galactomannan storage polysaccharides found in the endosperm of Legumes. These nonionic, linear polysaccharides are used as thickeners/stabilizers, co-gellants, and fat replacers in ice creams, sauces, and other food products. The primary biosynthetic product is a poly((1-4)-beta-D-mannose) having degree of polymerization ~1000, with a statistical distribution of single-unit (1-6)-alpha-D-galactose side groups. These side-groups confer aqueous solubility via H-bonding at degrees of substitution greater than 20%; linear mannans are otherwise water-insoluble "cellulosic" polymers.

Locust Bean (*Ceratonia siliqua*) galactomannans display temperature-dependent aqueous solubility and a tendency to form weak gels without co-gellants present. Both properties are exploited to provide triggered viscosity increases and enhanced gel properties in ready-mix and frozen products, but the physical basis is poorly understood. The low galactose content and apparent statistical-blocky character of their distribution both probably play a role in the dissolution and gelation properties, but quantitative links have been very difficult to establish. We argue here that dissolving LB galactomannans effectively fractionates by chemical composition and possibly chain length, implying that the gels observed upon cooling may be a manifestation of very slow L-L demixing.

CPP 9.8 Tue 16:30 ZEU 160

Structure and dynamics of asymmetric block copolymers in thin films — ●LARISSA TSARKOVA, ANDRIANA HORVAT, and GEORG KRAUSCH — Physikalische Chemie II, Universität Bayreuth, 95444 Bayreuth

With tapping mode scanning force microscopy (SFM) we study the development of non bulk morphologies in a layer of polystyrene-*block*-polybutadiene cylindrical domains (C) supported by two chemically different substrates. The mechanism of the thickness induced phase transition shows clear dependence on the substrate induced surface field. On a neutral surface (carbon coating) ordered clusters of the perforated lamella (PL) phase coexist with grains of the C phase. A fraction of the non bulk PL morphology reflects the thickness gradient within a single layer of structures. A strong surface field largely suppresses the mobility of the majority polybutadiene component on the silicon substrate resulting in a C to lamella phase transition. The important contribution of the

chains lateral mobility on the structural development is demonstrated by in-situ SFM measurements of the microdomain dynamics. Computer simulations based on dynamic density functional theory (MesoDyn) are in a good agreement with the experimental observations.

CPP 9.9 Tue 16:45 ZEU 160

In-line monitoring of dispersion of nanofillers in polymer melts by optical spectroscopy — ●BERND STEINHOFF and INGO ALIG — Deutsches Kunststoff-Institut Darmstadt, Schlossgartenstr. 6, D-64289 Darmstadt, Germany

For polymers a pronounced enhancement of material properties such as toughness, thermal stability or permeability can be obtained by adding small amounts of nanosized fillers. For the improvement of such properties a nanoscale dispersion within the polymer matrix is crucial. For effective processing reliable and rapid process control is therefore essential. Optical spectra of dispersions exhibit in addition to the absorption bands a contribution from light scattering. Since light scattering is sensitive to optical heterogeneities, morphological information can be obtained from that scattering background. Based on this consideration optical spectroscopy has been tested for in-line control of the degree of dispersion of nanofillers in polymer melts during extrusion. The melt were extruded through a slit die equipped with UV/VIS and NIR transmission probes. The degree of dispersion was varied by changing the mixing conditions (e.g. direct melt mixing or dilution of a masterbatch) and the amount of a compatibilizer. Due to electron microscopy and x-ray analysis it has turned out that from the scattering background the average size of the dispersed particles can be extracted.

CPP 10 POSTER Nonequilibrium Phenomena in Soft Condensed Matter

Time: Tuesday 17:00–19:00

Room: P3

CPP 10.1 Tue 17:00 P3

Free Cooling of the One-dimensional Wet Granular Gas — ●VASILY ZABURDAEV, MARTIN BRINKMANN, and STEPHAN HERMINGHAUS — MPI for Dynamics and Self-Organization, Bunsenstr.10, 37073 Göttingen, Germany

In the present work we consider a one-dimensional gas of hard balls covered with a thin liquid film. A liquid bridge, formed at each collision, is responsible for the hysteretic and dissipative interaction. Each rupture of a liquid bridge requires a fixed amount of energy, and thus determines a threshold of relative velocities below which the two colliding particles form a bounded state losing their relative kinetic energy. We aim to study the cluster formation process in the free cooling system. Macroscopic laws of energy dissipation and cluster growth are studied in this model on the basis of numerical simulations supported by a scaling-like system of equations. We show that the sticky gas regime is an attracting asymptotic limit of the wet granular gas and does not depend on the liquid bridges strength. The next neighbor velocities correlations play the key role in the establishing of this regime.

CPP 10.2 Tue 17:00 P3

Global homogeneity of non-cubic bicontinuous space partitions — ●GERD E SCHROEDER¹, ANDREW FOGDEN², and STEPHEN T HYDE¹ — ¹Applied Maths, Research School of Physical Sciences, Australian National University, 0200 Canberra, Australia — ²Institute for Surface Chemistry, P.O. Box 5607, SE-11486 Stockholm, Sweden

Infinite periodic minimal surfaces (IPMS) form the structural basis of cubic phases in copolymer, lipid or surfactant self-assemblies. Although few non-cubic equilibrium phases have been reported to date, there are compelling reasons to study non-cubic IPMS: first, they offer possible transition structures between bicontinuous cubic phases. Second, the reason why soft systems (that favour homogeneity but not explicitly symmetry) exhibit phases of cubic symmetry is still uncertain.

We use the concept of *medial surfaces* to quantify *packing homogeneity*, i.e. variations of the channel radius within the structure [1]. This analysis is carried out on IPMS families that are degradations of the cubic P, D and G surfaces (the rPD, rG, tG, tD tP, and H).

We show that the cubic G and D are locally maximally homogeneous, whereas the cubic P has at least one relative that is more homogeneous. We discuss the implications for molecular self-assembly (chain stretching), and compare this result to analyses of curvature fluctuations [2].

[1] A. Fogden, S.T. Hyde, Eur. Phys. J. B **7**, 91–104 (1999)

[2] G.E. Schröder, S.J. Ramsden, A.G. Christy, S.T. Hyde, Eur. Phys. J. B **35**, 551–564 (2003)

CPP 10.3 Tue 17:00 P3

Nonlinear dynamics of elastic nano-filaments — ●HIROFUMI WADA and ROLAND NETZ — Physik Department, Technical University Munich, 85748 Garching, Germany

Dynamics of flexible filaments in viscous fluids, which is dominated by hydrodynamic dissipation and elasticity, is characterized by an intriguing interplay between geometry and physics. Examples are the motion of vortex lines in superconductors, the buckling and super-coiling of rubber tubes or long DNA molecules, and the swimming of bacteria flagella. We developed a dynamic simulation model of elastic filaments in low Reynolds number fluids, in which full couplings between stretch, bend and twist are properly taken into account and the hydrodynamic interaction is also incorporated within the Stokesian technique. We study non-linear dynamics of filaments subjected to various external forces and boundary conditions. In particular, we describe the stretching instability of a flexible helical spring and the super-coiling behavior of an over-twisted straight filament, and provide some insights into the kinetics of those non-equilibrium phenomena.

CPP 10.4 Tue 17:00 P3

Hydrodynamic simulations of polymers at surfaces — ●CHRISTIAN SENDNER and ROLAND NETZ — Physik Department, TU Muenchen, James Franck Strasse, 85748 Garching

We investigate the dynamics of a semiflexible polymer at a surface in the low-Reynolds-number limit. We include full hydrodynamic interactions between polymer segments and the boundary. The response of the polymer to external electric fields as well as to shear flow at finite temperatures is considered, using simulations and scaling arguments. Hydrodynamic interactions influence the conformation of the polymer leading to orientation effects and an effective repulsion from the surface. This might be useful for controlled desorption of short DNA strands in DNA-chip applications.

CPP 10.5 Tue 17:00 P3

Mediated Forces in out of Equilibrium Systems — ●ALI NAJAFI — Max-Planck Institut for Physics of Complex Systeme, Nothnitzer str. 38, 01187 Dresden, Germany

We study the fluctuation-induced forces in systems with non-

equilibrium nature. We show that in a system with nonuniform temperature profile a net force is exerted on a single flat plate that restricts the scale-free fluctuations of a scalar medium. This force resembles the thermophoresis or the Soret effect. Another class of non-equilibrium systems corresponds to the case where a topological defect moves in a phononic background. We show that inertial coupling between a single defect and ambient phonons leads to variety of interesting phenomena. Similar to the problem of dynamical Casimir effect the energy dissipation and mass renormalization of a moving defects are the results of this mediated interactions. Phonon-mediated coupling between many defects also investigated. We show that a regular lattice of such interacting defects will have anisotropic and anomalous mass and elastic constants.

CPP 10.6 Tue 17:00 P3

Structure formation in thin block-copolymer films — •LUDOVIC MARQUANT, HENDRIK HÄHL, DANIEL PODZIMEK, RENATE FETZER, MARTIN MEIER, and KARIN JACOBS — FR 7.2 Experimentalphysik - Weiche Materie, Universität des Saarlandes, D-66123 Saarbrücken

We are investigating rearrangement phenomena within structured liquids. Our system consists of a thin block-copolymer film of polystyrene-block-polyethylen/propylen (PS/EP) deposited on a non-wetting substrate. Due to a preannealing procedure the microdomains of the polymer melt equilibrate and form an ordered layered structure. Upon shear stress which is induced by the dewetting of the film this structure undergoes a rearrangement in the vicinity of the three-phase-contactline (air-substrate-film) and forms PS cylinders parallel to the edge of the film, embedded in a PEP-matrix. By tapping mode scanning probe microscopy we investigate this phenomenon at the solid/liquid interface. Here, the alignment of these cylinders gives evidence to a nonzero velocity at the interface, indicating slippage.

CPP 10.7 Tue 17:00 P3

Friction of macromolecules in solution: Effects of high-order correlations. — •ALEXANDER UVAROV and STEPHAN FRITZSCHE — Universität Kassel, D-34132 Kassel, Germany

Apart from the rotational and translational motion of macromolecules, the concept of friction have been found helpful to understand their shape as well as the formation and deformation of such macromolecules. During the past decade, therefore, a large number of experiments and molecular dynamic (MD) simulations have been carried out to understand the friction properties of macromolecules. An alternative treatment of such molecules is based on statistical methods, if they are described in terms of their molecular subsystems, (*beads*), and if the influence of the solvent particles on the dynamics of the macromolecule is incorporated into the friction tensors of the macromolecule [1].

In this contribution we derived and explain the explicit expression for the friction tensors which can be applied in order to calculate the diffusion coefficient as function of the mass ratio of the molecules, relative to the mass of the solvent particles. In addition, we also discuss the effects of the transition between slip and stick boundary conditions by calculating the boundary condition coefficient of the macromolecule for different mass ratios as well as different bead-solvent potentials. The results from this semi-phenomenological theory are found to compare very well with MD simulations over a wide range of mass ratios [2].

[1] A. Uvarov and S. Fritzsche, Phys. Rev. E, accepted (2005);

[2] J. R. Schmidt, J. L. Skinner, J. Phys. Chem. B. **108**, 6767 2004.

CPP 10.8 Tue 17:00 P3

Monitoring Defect Dynamics by Local Minkowski Measures — •SABINE SCHERDEL¹, CHRISTIAN FRANKE¹, MARTIN KREIS², and ROBERT MAGERLE¹ — ¹Chemische Physik, TU Chemnitz, D-09107 — ²Physikalische Chemie II, Universität Bayreuth, D-95440

To structure large surface areas block copolymer films are often used as templates. However, the dynamic and structure formation in thin block copolymer films is still under research. In particular surfaces and interfaces or different experimental conditions have a strong effect on the obtained structures. We investigate these mechanisms experimentally with in-situ scanning probe microscopy. The resulting movies are large and complex data sets. We have used local Minkowski measures to characterize defects appearing in thin films. This allows us to examine

systematically the structure of defects and their neighbourhood. Furthermore, we can describe the behaviour of individual defects with a few parameters and examine the influence of the geometry in the vicinity of defects.

CPP 10.9 Tue 17:00 P3

Defect Dynamics in Thin Films of Block Copolymers — •MARCUS BÖHME¹, MARTIN KREIS², SABINE SCHERDEL¹, NICOLAUS REHSE¹, and ROBERT MAGERLE¹ — ¹Chemische Physik, TU Chemnitz, D-09107 Chemnitz — ²Physikalische Chemie II, Universität Bayreuth, D-95440 Bayreuth

We investigate the dynamic processes in thin films of a cylinder forming polystyrene-*block*-polybutadiene block copolymer swollen in chloroform vapour. With tapping mode atomic force microscopy we study in situ the dynamics of defect structure during annealing of the liquid film. Our experiments show correlations between the dynamics of neighbouring defects, annealing of defects via formation of transient phases, shape fluctuations of cylinders and lamellae, as well as the dynamics of individual perforations in a hexagonally perforated lamellae.

CPP 10.10 Tue 17:00 P3

The General Physics Theory for 21 Century — •TOFIG GASSYM — Gehri Strasse 7, 6010 Kriens, Switzerland

By solving the coupled system of kinetic equations for interacting system of electrons positrons and photons at high external electric, arbitrary magnetic and at the propagation of strong electromagnetic waves non-equilibrium and non-stationary distribution function (DF) of photons and charge carriers by taking into account of arbitrary heating and mutual drag of carriers and photons was found. Author was sure that received him DF function of photons must lay on the basis of Theoretical Physics of 21 Century, as the equilibrium Planck's DF of black-body radiation lied on the basis of Quantum Physics of 20 Century. Authors many years mental work confirmed the rightness of searched him way and leads to the conclusion that Kinetic Theory is more general and fundamental theory of nature, which unified Non-stationary Dynamics (the left-hand side) with Non-stationary Statistical Mechanics (the right-hand side) of Kinetic Equation. Other sections of Theoretical Physics such as Newtonian, Hamiltonian and Relativistic Classical Mechanics, Quantum Physics may be received from Kinetic Theory under the special conditions and are the special parts of this theory. The problems irreversibility and instability, the paradox of time, quantum paradox and others are solved. This new General Theory explains all the problems and troubles of foundations and interpretation of quantum mechanics and relativity. It is shown the possibility of superluminal motion of light pulses and wavepackets through the medium and photonic barriers.

CPP 10.11 Tue 17:00 P3

Superluminal motion in interacting system of electrons, positrons and photons. — •TOFIG GASSYM — Gehri Strasse 7, 6010 Kriens, Switzerland

By solving the coupled system of kinetic equations for interacting system of electrons, positrons and photons in high electric E, arbitrary magnetic H and at the propagation of strong electromagnetic waves non-stationary and non-equilibrium distribution function (DF) of photons and charge carriers with arbitrary heating and the mutual drag of carriers and photons is found. It is shown that DF has the stationary limit at $uq/(\hbar\omega_q) < 1$ and grows by time exponentially for $uq/(\hbar\omega_q) > 1$. At the point $uq = \hbar\omega_q$ (i.e. $u = c$) state is ground with $N(q) = N(q, T_i) = \text{const.}$ have not singularity. At this point $u = V_H = c$, $E = H$ and EHV_H and electromagnetic field becomes transversal and free and emitted. From this point at $u > c$ begins the transition of carriers "dressed" by photons to the following energetic levels. It is the mechanism of inverse population of Lasers. Separating stationary DF $N(q) = N(q, T_i) (1 - uq/(\hbar\omega_q))^2$ to the isotropic and anisotropic parts at uq as in theory of relativity we have: $N_s(q) = N(q, T_{co}) (1 - u/c)^2$; $N_a(q) = (uq/(\hbar\omega_q)) N_s(q) = (u/c) N_s(q)$. Relativistic factor enters to expressions as $(1 - u/c)^2$, instead $(1 - u/c)^{-1/2}$ in Einsteins theory, which considers the case of absence of external fields. Thus we liquidate the main problems of superluminality and show the possibility of superluminal motion of light through the medium, at $u > c$ in accordance with a lot of experiments.

CPP 11 POSTER Disperse Polymer Systems

Time: Tuesday 17:00–19:00

Room: P3

CPP 11.1 Tue 17:00 P3

Raman characterization of polypropylene-clay nanocomposites — ●GOLNARA NIKOLAEVA¹, KIRILL PROKHOROV¹, PAVEL PASHININ¹, VIKTOR GERASIN², and EVGENI ANTIPOV² — ¹A.M. Prokhorov General Physics Institute, Russian Academy of Sciences, 38 Vavilov St., 119991 Moscow, Russia — ²A.V. Topchiev Institute of Petrochemical Synthesis, Russian Academy of Sciences, 29 Leninsky Pr., 119991 Moscow, Russia

We studied nanocomposites made of isotactic polypropylene (PP) and natural montmorillonite modified with a quaternary ammonium salt. The mass content of the clay in the composites varied from 1.5 to 20 percents. The production technology was melt-blending at 200°C and subsequent quenching in water. X-ray analysis of the composites revealed intercalation of polymer macromolecules in the clay interlayer space. The modulus of elasticity of the composites was higher than that of the neat PP and reached its maximum value at 1.5 percents of the clay content.

Raman spectra of the composites were measured with laser excitation at 472.7 nm. At this excitation wavelength, we observed a strong band of luminescence, the intensity of which increased with the increase in the clay content. However, the 2600–3100 cm⁻¹ frequency range of the Raman spectra contained intense lines that can be used for detailed characterization of the composite structure. In particular, when studying the behavior of the intensity of the A-symmetry line at 2963 cm⁻¹, we concluded that the orientation ability of the macromolecules during uniaxial drawing of the samples decreases with the increase of the clay content.

CPP 11.2 Tue 17:00 P3

Clay Dispersions — ●HENRICH FRIELINGHAUS¹, HELEN HERMES², WIM PYCKHOUT-HINTZEN¹, and DIETER RICHTER¹ — ¹Forschungszentrum Jülich GmbH, Institut für Festkörperforschung, 52425 Jülich, Germany — ²Physik der weichen Materie, IPkM, Heinrich-Heine-Universität Düsseldorf, 40225 Düsseldorf, Germany

Dispersions of montmorillonite clay particles in water are investigated by small angle neutron scattering. This method measures structures in the range of several 10 Å up to several 1000 Å. Complementary x-ray scattering experiments at intermediate angles complete the structural studies at shorter distances. Many dispersions showed a small fraction of tactoids, i.e. stacks of single platelets. A new developed model for small angle neutron scattering successfully describes the disc-like behaviour of the single platelets coexisting with a small fraction of tactoids. This model is about to be applied also for polymer-clay nanocomposites, since the distribution function of the stacking can be varied.

CPP 11.3 Tue 17:00 P3

Confined Polymers in Microemulsions — ●SIMONA MACCARONE, HENRICH FRIELINGHAUS, JÜRGEN ALLGAIER, and DIETER RICHTER — Forschungszentrum Jülich GmbH, Institut für Festkörperforschung, 52425 Jülich, Germany

It has been established that amphiphilic diblock copolymers increase the efficiency of surfactants in microemulsions (polymer boosting effect). These studies always considered large oil and water domains of size d compared to the typical polymer size R_g . Thus the confinement parameter R_g/d was small in these first studies. The ongoing studies of this paper consider medium and higher confinement, where small angle neutron scattering measurements reveal a new behaviour, which can be compared to computer simulations by T. Auth. The theory predicts an enhanced sensitivity of the polymer at medium confinement and a reversed behaviour at larger confinement. The higher sensitivity at medium confinement is only slightly visible experimentally, whereas the reversed behaviour (anti-boosting) is clearly present. These results are interesting for applications and interpretations of biological membranes.

CPP 11.4 Tue 17:00 P3

New Sticker Polymers as Efficiency Boosters in Microemulsions — ●MARTIN BRODECK, GAETANO MANGIAPIA, HENRICH FRIELINGHAUS, CHRISTIAN FRANK, JÜRGEN ALLGAIER, and DIETER RICHTER — Forschungszentrum Jülich GmbH, Institut für Festkörperforschung, 52425 Jülich, Germany

Amphiphilic diblock copolymers have been established to enhance the efficiency of surfactants dramatically (polymer boosting effect). The focus of the present paper focuses on sticker polymers with just a small

oil-soluble block. Even though the amphiphilicity of these polymers is rather low, they act as efficiency boosters as effectively as diblock copolymers. The microscopic structure of the domains is measured in small angle neutron scattering studies and compared with the macroscopic phase behaviour. Latest measurements involve sticker polymers with a higher functionality (larger arm number) and are compared to the simple sticker polymers. A theory by T. Auth and G. Gompper predicts a stronger sensitivity of the polymer effect with higher functionality. Ongoing work is aimed at four-functional sticker polymers.

CPP 11.5 Tue 17:00 P3

Assembly of SiO₂ nanoparticles into the interstitial sites of ordered polymethylmethacrylate beads — ●SIMONE HERTH — Rensselaer Nanotechnology Center, Rensselaer Polytechnic Institute, Troy, NY, USA

For nanocomposite materials, their optical, magnetic, and electrical properties could be improved by placing the nanoparticles equidistant to one another or by decreasing the width of the interparticle distance distribution. One attempt to achieve this special arrangement is the assembly of nanoparticles into the interstitial sites of an ordered lattice of uniform polymer beads, such as polymethylmethacrylate (PMMA), by centrifugation. Due to the different densities of PMMA and SiO₂, the PMMA would normally always settle down on top of the SiO₂ nanoparticles during the centrifugation process. For that reason, the SiO₂ nanoparticles were linked with the PMMA beads by a silane linker prior to centrifugation. Scanning electron micrographs of the dried pellets revealed a short range order of the PMMA beads, a good dispersion of SiO₂ nanoparticles, and a good adhesion of the SiO₂ nanoparticles to the PMMA beads.

CPP 11.6 Tue 17:00 P3

Magnetic particles in supported polymer nano-structures — ●M.M. ABUL KASHEM¹, S.V. ROTH², and P. MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik-Department E13, James-Frank-Str. 1, D-85747 Garching, Germany — ²HASYLAB at DESY, Notkestr. 85, D-22603 Hamburg, Germany

Polymer nano-structures with incorporated magnetic particles mark a new class of composite materials. Composite structures are formed from a P(S-b-I) matrix and a magnetic filler (metal oxide). The great potential of these composites derives from the substantial modification of the thermal, mechanical and electrical characteristics of polymers which results when the polymer is combined with a filler. The polymer nano-structures, acting as a template, enable a completely new arrangement of the particles which is inaccessible with common magnetic materials. The controlled incorporation of the particles results from the presence of a hairy polymer layer covering the magnetic particles. On top of solid supports the polymer layers including particles are prepared by spin-coating. The nano-structures are created by additional preparation steps by an interplay of dewetting and micro-phase separation. Within this self-assembly process the polymer matrix as well as the magnetic particles are ordered. The resulting structures are presented.

CPP 11.7 Tue 17:00 P3

Microbeam-GISAXS investigation of flow induced structures — ●E. BAUER¹, S.V. ROTH², and P. MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik-Department E13, James-Frank-Str. 1, D-85747 Garching, Germany — ²HASYLAB at DESY, Notkestr. 85, D-22603 Hamburg, Germany

Flow in nanoscale geometries is of importance in many areas as for example in chip production, printing techniques and bio-medical sensing devices. While on a local scale the surface structure is nicely pictured by AFM, scattering is usually applied to obtain a mean statistical information. With grazing incidence small-angle x-ray scattering (GISAXS) a length regime comparable to AFM is addressed. A local scattering information becomes accessible by combining GISAXS with a micron sized x-ray beam and scanning of the sample relative to the beam. We demonstrate the actual possibilities of this technique by locally probing the influence of selected boundary conditions on the movement of liquid fronts to reach a deeper understanding of the influence of the selected boundaries on flow at different lengths scales. In the presented example a blend solution (PS:PBr(0.34)S = 1:9) in toluene was deposited as a drop on top of a polyimide-coated substrate.

CPP 11.8 Tue 17:00 P3

Aggregation of block copolymers and surfactants studied by fluorescence correlation spectroscopy. — ●H. ZETTL¹, M. RUPPEL², M. BURKHARDT², A.H.E. MÜLLER², and G. KRAUSCH¹ —¹Physikalische Chemie II, Universität Bayreuth, 95440 Bayreuth — ²Makromolekulare Chemie II, Universität Bayreuth, 95440 Bayreuth

In recent years new block copolymers with very low critical aggregation concentrations (*cac*) have been synthesized. With classical techniques like light scattering and conductivity the exact determination of these *cac*'s becomes increasingly difficult. Fluorescence correlation spectroscopy (FCS) allows to analyse the diffusion behaviour of single dye molecules to study the aggregation processes of polymers and low molecular weight surfactants. We show aggregation studies starting from well investigated surfactant systems up to complex block copolymers in aqueous solutions and organic solvents.

CPP 11.9 Tue 17:00 P3

Dynamics of the miscible blend PEO / PMMA — ●KATARZYNA NIEDZWIEDZ, ANDREAS WISCHNEWSKI, MICHAEL MONKENBUSCH, LUTZ WILLNER, and DIETER RICHTER — Institute for Solid State Research, Research Center Juelich, Germany

In spite of intensive studies on binary polymer systems it is still impossible to predict the properties of a blend system on basis of what is known about the behaviour of each component of the mixture. Although it is well known that the dynamics of each component is affected by blending, the dynamic miscibility and in particular the question whether or not there exists a corresponding length scale is still matter of strong controversy. Of particular interest are blends where the dynamics of the pure components is well separated in time, i.e. with a very different glass transition temperature T_g of the pure components. We present a series of neutron spin echo and neutron backscattering data of the miscible polymer blend poly(ethylene oxide) (PEO, $T_g = 200$ K) / polymethylmethacrylat (PMMA, $T_g = 400$ K). At temperatures below the T_g of PMMA, the PEO component is still mobile but shows a strong difference in the segmental pair- and self-correlation functions, i.e. in the collective and self motion, respectively. An explanation for these surprising results will be presented.

CPP 11.10 Tue 17:00 P3

Nanostructure of copolymers of ethylene and 5-ethylidene-2-norbornene and aluminum/polyethylene composites study by very cold neutrons scattering — ●SERGEY KUZNETSOV¹, YURI LAPUSHKIN¹, ANDREY UDOVENKO¹, IRINA MESHKOVA², VITALII GRINEV², LEV RASPOPOV², ALEKSANDR SHCHEGOLIKHIN², ELENA KISELEVA², OLGA KUDINOVA², LIUDMILA NOVOKSHONOVA², and ANATOLII SHELAGIN³ — ¹Lebedev Physics Institute, Moscow, Russian Federation — ²Semenov Chemical Physics Institute, Moscow, Russian Federation — ³Moscow Physics Technical Institute, Moscow, Russian Federation

Very cold neutron (VCN) scattering was used to control the nanostructure of copolymers of ethylene and 5-ethylidene-2-norbornene (E/EN) and polymer nanocomposites. The technology of E/EN copolymerization was developed to obtain the heat-resistant materials with high glass transition temperature and increased transparency. Supermolecular structure (SMS) of the E/EN copolymers with different EN concentrations was investigated. It was shown that EN concentration growth lead to decrease the co-polymer crystallinity. We didn't see the VCN scattering on the E/EN copolymer nanostructure at EN concentration in copolymer >30 molar %. VCN scattering was also used to control the agglomeration of Al particles in Al/PE nanocomposites obtained by polymerization filling method. The dimensions of Al particles were determined. The macro-properties of Al/PE composites with various dimensions and concentrations of Al particles were compared.

CPP 11.11 Tue 17:00 P3

Conformational properties of dendritic block copolymer of first generation — ●MARIOS KOSMAS — Chemistry Department, University of Ioannina, Greece

Our previous works on linear and star polymers are extended to dendritic block copolymer chains of an extra generation and two different species. On the ends of a star of f_a branches of molecular weight N_a each, which constitute the inner region of the dendrimer the new generation is built. This outer generation consists of f_a new stars each one of f_b branches having totally $f_a f_b$ branches eachone having a molecular weight N_b . Working at the critical dimensionality $d=4$ above which

polymer chains behave ideally we determine the radius of gyration of the dendritic block copolymer and average angles between the branches, in an effort to see the effects of the two different molecular weights, the two different number of branches and the rest characteristics of the chain and the solvent, on the conformational behavior of the macromolecule. Two macroscopic properties are analysed. The positions of the end groups which determine the activity of the macromolecule and the empty spaces inside the chain which make the macromolecule a good carrier of smaller species.

CPP 11.12 Tue 17:00 P3

Polyethylene-terephthalate ferroelectrets: Foam preparation and piezoelectric properties — ●MICHAEL WEGENER, WERNER WIRGES, AXEL MELLINGER, OLENA VORONINA, and REIMUND GERHARD-MULTHAUPT — University of Potsdam, Department of Physics, Am Neuen Palais 10, D-14469 Potsdam, Germany

Novel cellular polyethylene-terephthalate (PETP) films have been prepared and investigated as alternative ferroelectrets. Ferroelectrets are polymer-air composites with a cellular structure and with electrically charged void surfaces where charges of opposite polarity form large macroscopic dipoles [1]. The change of void (and thus dipole) sizes during application of mechanical stress generates a piezoelectric activity of several hundred pC/N as demonstrated on polypropylene foams [1] and as recently reported for PETP foams [2], a second ferroelectret material.

Here, we describe several methods for foam preparation, such as voiding during treatment in supercritical carbon dioxide or during stretching of filler-loaded polymer sheets as well as procedures for foam-structure optimisation, such as stretching and inflation. Furthermore, we describe charging procedures for charging of void surfaces. Finally, we discuss the piezoelectric and elastic properties of the new ferroelectret materials.

[1] M. Wegener and S. Bauer, Microstorms in cellular polymers: A route to soft piezoelectric transducer materials with engineered macroscopic-dipoles, *ChemPhysChem* 6, 1014-1025 (2005).

[2] M. Wegener, W. Wirges, and R. Gerhard-Multhaupt, Piezoelectric polyethylene terephthalate (PETP) foams - Specifically designed and prepared ferroelectret films, *Adv. Eng. Mat.*, accepted for publication.

CPP 11.13 Tue 17:00 P3

Interface fluctuations, membrane elasticity and renormalization effects in microemulsions — ●OLAF HOLDERER, HENRICH FRIELINGHAUS, DMYTRO BYELOV, MICHAEL MONKENBUSCH, JÜRGEN ALLGAIER, and DIETER RICHTER — Institut für Festkörperforschung, Forschungszentrum Jülich GmbH, D-52425 Jülich

Neutron spin echo (NSE) spectroscopy is a well-suited method for studying the dynamic properties of microemulsions, consisting of oil, water and a surfactant. Here, the focus is set to bicontinuous microemulsions, having equal amounts of water and oil and varying surfactant concentration. The dynamic properties of the surfactant membrane are tuned by the addition of diblock copolymers or homopolymers. Structural parameters as the characteristic distance or correlation length in bicontinuous microemulsions are obtained by small angle neutron scattering (SANS). The renormalized bending modulus is obtained from the SANS experiments by matching the Gaussian random fields theory with a Ginzburg-Landau approach. NSE experiments are evaluated by numerically integrating $S(q,t)$ from the Zilman-Granek theory, where the bending modulus is the only free fitting parameter. It is shown that the analysis of the dynamics gives a direct access to the "bare" membrane bending modulus κ , which is compared to the renormalized one as obtained from SANS. The difference between the two ways of determining κ is the renormalization factor, as predicted by theory.

CPP 11.14 Tue 17:00 P3

Rigid Amorphous Fraction of Semicrystalline Polymers and Polymer Nanocomposites — ●ANDREAS WURM, ALBERT SARGSYAN, and CHRISTOPH SCHICK — University of Rostock, Institute of Physics, Universitätsplatz 3, 18051 Rostock, Germany

For semicrystalline polymers the observed relaxation strength at glass transition is often significantly smaller than expected from the non-crystalline fraction. This observation leads to the introduction of a rigid amorphous fraction (RAF) which does not contribute to the heat of fusion or X-ray crystallinity nor to the relaxation strength at glass transition. The RAF is non-crystalline and in a glassy state above the common glass transition temperature.

From heat capacity the temperature and time dependence of the RAF can be obtained. For PC, PHB and sPP it is possible to study the creation

and disappearance of the RAF in situ during isothermal crystallization and on stepwise melting.

A RAF can be detected for polymer nano-composites too. The amount and the thermal stability of the RAF in such systems will also be discussed.

CPP 11.15 Tue 17:00 P3

Multicompartment micellar gels of amphiphilic poly(2-oxazoline) triblock copolymers — ●C.M. PAPANAKIS¹, R. IVANOVA¹, T. BONNÉ¹, K. PRANZAS², K. MORTENSEN³, K. LÜDTKE⁴, T. KOMENDA⁴, and R. JORDAN⁴ — ¹Physikdepartment E13, Technische Universität München, James-Frank-Str. 1, D-85747 Garching — ²Institut für Werkstofforschung, GKSS, Geesthacht — ³Danish Polymer Centre, Risø National Laboratory, Roskilde, Denmark — ⁴Lehrstuhl für Makromolekulare Stoffe, Chemiedepartment, Technische Universität München, 85 747 Garching

Amphiphilic triblock copolymers are widely used as gel formers, e.g. in cosmetics. Poly(2-oxazoline) block copolymers constitute a new and versatile system and are promising candidates for the formation of micellar gels with chemically different types of micelles. This may be achieved by using triblock copolymers with blocks containing lipophilic, hydrophilic and fluorophilic side groups. Using small-angle neutron scattering with contrast matching, we could show that diblock copolymers with lipophilic and fluorophilic blocks and the same hydrophilic block do not form common micelles in aqueous solution. The cores of the micelles formed by copolymers with lipophilic blocks are spherical, whereas the ones from fluorophilic blocks are short cylinders, which is possibly due to the steric demands of the fluorophilic side chains forcing the polymer backbone to stretch. Triblock copolymers form gels above 10 wt-%. Their scattering can be described by a coexistence of spherical, lipophilic and elliptical, fluorophilic micellar cores, which are linked by the hydrophilic blocks. Thus, the system forms a multicompartment gel.

CPP 11.16 Tue 17:00 P3

Tuning the microstructure of polymer-metal nanocomposites prepared by pulsed laser deposition — ●JOHANNA RÖDER, JÖRG FAUPEL, and HANS-ULRICH KREBS — Institut für Materialphysik, Universität Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen

Nowadays polymer-metal nanocomposites have a wide range of applications. For instance metal clusters embedded in polymers possess interesting optical properties. Heading towards such new materials with tailored properties, it is important to understand and influence their microstructure. Here the samples were prepared in a one-step process by pulsed laser deposition, using poly (methyl methacrylate) (PMMA) as matrix. The embedded clusters were mainly characterized by TEM. The effects of polymer-cross-linking on the growth of Ag will be presented and discussed, as well as the microstructural changes after deposition of nucleation seeds in the form of less diffusing metals like Nb and Cu. The consequences of the different microstructures on the optical properties are shown.

CPP 11.17 Tue 17:00 P3

In-situ Monitoring of Pressure-Induced Aggregation of beta-Lactoglobulin — ●ALBERT BAARS¹, LESZEK KULISIEWICZ¹, RONALD GEBHARDT², WOLFGANG DOSTER², and ANTONIO DELGADO¹ — ¹Technische Universität München, Lehrstuhl für Fluidmechanik und Prozessautomation, D-85350 Freising — ²Technische Universität München, Physikdepartment E13, D-85747 Garching

At pressures up to 1 GPa, bovine beta-Lactoglobulin (B-Lg) in aqueous solution can undergo reversible and irreversible conformational changes, which lead to altered interactions between the dissolved protein molecules. This work investigates the impact of pressures up to 600 MPa on aqueous B-Lg solution by an in-situ rolling ball viscosimeter and by in-situ dynamic light scattering for mass fractions up to 6 % at 20 °C and pH 7. Between 0.1 and 100 MPa, the results reveal negligible changes in relative viscosity while in the range of 100 - 350 MPa the viscosity rises up to the twice of the initial value. At higher pressures only a slight increase appears. These findings can be deduced from aggregation of monomers and dimers to oligomers. Between 100 and 300 MPa an increase in hydrodynamic radius from 1.8 to 7.4 nm has been observed. In literature it is known that pressures higher than 100 MPa induces conformational changes of B-Lg protein. These lead to a reduction of negative surface charge due to the exposure of hydrophobic tryptophan residues to the solvent. In addition, the SH group from Cys 121 moves to the protein surface. This enables aggregation by formation

of hydrophobic and disulfide bonds. After pressure release, the latter are retained leading to an irreversible increase in relative viscosity.

CPP 11.18 Tue 17:00 P3

Suspensions with plastic flow behavior - relation between shear stress and first normal stress difference — ●DIMITER HADJISTAMOV — DECE GmbH, Helvetierstr.15, CH-4125 Riehen

Model suspensions with plastic flow behavior were rheologically investigated. The shear stress and simultaneously the first normal stress difference were measured during stressing experiments and following that a stress relaxation. We compared the flow and normal stress curves. The flow curve of a system with plastic flow behavior shows one or more yield stress regions, where the shear stress does not change with the shear rate. The shear stress rises continuously after the yield stress region with the shear rate. We found that the normal stress curve also exhibits a yield section - the yield normal stress region. The first normal stress decreases (contrary to the shear stress) at first after the yield normal stress region. The decrease of the normal stress can lead to negative values for the normal force. After them, the normal stress increases with the shear rate. It was established that it is possible to draw conclusion from the ratio between shear stress and normal stress about the strengthening of the structure of a suspension with plastic flow behavior.

CPP 11.19 Tue 17:00 P3

The diblock copolymer as an external field in A/B/A-B polymer mixtures — ●VITALIY PIPICH, DIETMAR SCHWAHN, and LUTZ WILLNER — Forschungszentrum Jülich GmbH, Institut für Festkörperforschung, Jülich, Germany

Ordering transitions in an A/B/A-B polymer mixture have been examined by small angle neutron scattering. The homopolymer blend PB/PS of critical composition was mixed with an increasing amount of the symmetric diblock copolymer PB-PS [PB and PS being polybutadiene and polystyrene, respectively] [1]. By deuteration of individual components we got blends with two scattering contrasts: (i) "bulk" contrast by deuteration the PB homopolymer and the PB-block of the copolymer, and (ii) "block" contrast, when only the PS-block was protonated. In particular for case (ii) we observed large-scale density fluctuations of the copolymer following a Q^{-3} scaling behavior. These density fluctuations were independent of temperature within the 3D-Ising ($\Phi_{DB} < 0.05$) and Brasovskii universality class ($\Phi_{DB} > 0.2$). However, within the Lifshitz universality class, e.g. $0.05 < \Phi_{DB} < 0.3$, the density fluctuations of the copolymer increased with decreasing temperature. Between $0.09 < \Phi_{DB} < 0.3$ the ordering of the copolymer occurred prior to the ordering of the homopolymers. So in a limited copolymer range a pre-ordered copolymer structure seemingly served as a template for the polymeric microemulsion and lamellar phase.

[1] V. Pipich, D. Schwahn, J. Chem. Phys. 123, 124904 (2005).

CPP 11.20 Tue 17:00 P3

Drying of polymer dispersions during film formation monitored via beam bending — ●KERSTIN VON DER EHE and DIETHELM JOHANNSMANN — Institute of Physical Chemistry, Clausthal University of Technology, Arnold-Sommerfeld-Strasse 4, 38678 Clausthal-Zellerfeld

Film formation from aqueous polymer dispersions takes place in several steps including loss of water, compactification of particles, and polymer interdiffusion. In the process, large in-plane stresses develop, which may induce cracking of the dry film. Large stresses are often encountered when the coating to be formed has a high mechanical modulus.

This work deals with polymer dispersions prepared via mini-emulsion polymerization. Mini-emulsion polymerization offers a good synthetic flexibility. In particular, nanocomposites can be created. By variation of surfactant concentration and time of sonication we obtain dispersions with different particle sizes. We work with dispersions of PBuMA, PMMA and poly(BuMA-co-MMA) with different solid contents.

For analyzing the behavior of the dispersions throughout film formation in regard to internal stresses we use a cantilever technique. [1] The films are prepared and dried on a flexible substrate fixed at one end. Bending of the substrate under stress is detected by a laser beam which is deflected from the free end of the substrate. With these experiments we find a dependence of the deflection on material parameters. The results are discussed in the frame of recent theoretical models of the film formation. [2]

References: [1] C. Peterson, C. Heldmann, D. Johannsmann, Langmuir 1999, 15, 7745 [2] A.F. Routh, W.B. Russel, Langmuir 1999, 15, 7762

CPP 11.21 Tue 17:00 P3

Melts of Reactively Compatibilized Blends of Polyamide 6 and Styrenic Polymers: Linear Viscoelasticity and Fractional Calculus — ●CHRISTIAN SAILER and ULRICH A. HANDGE — Institute of Polymers, Department of Materials, ETH Zürich, CH-8093 Zürich

In this study, we investigated the linear viscoelastic properties of reactively compatibilized blends of polyamide 6 and styrenic polymers in the molten state. Two blend systems were considered, i.e. blends of polyamide 6 (PA6) and acrylonitrile-styrene (SAN-K) and blends of PA6 and acrylonitrile-butadiene-styrene (ABS-K) which consisted of SAN-K and 10 wt.% of rubber particles. The compatibilizing agent was added to SAN-K and ABS-K and was capable of reacting with the amine end groups of PA6 in situ during melt blending. In linear viscoelastic shear oscillations we observed a complex low frequency dependence of the dynamic moduli for all blends. In contrast to the pure components the slopes of the $G'(\omega)$ and $G''(\omega)$ curves in the double-logarithmic plot were decreasing with decreasing frequency and the moduli exceeded the values of the components in the range of low frequencies. We analyzed the data by applying fractional differential models [1, 2]. Our analysis revealed that the data can be fitted by the model well over the whole frequency range.

[1] Chr. Friedrich, *J. Non-Newtonian Fluid Mech.*, **46** (1993) 307.

[2] H. Schiessel and A. Blumen, *J. Phys. A: Math. Gen.*, **26** (1993) 5057.

CPP 11.22 Tue 17:00 P3

Influence of pre-history and shear flow on the frequency dependent conductivity of carbon nanotube-filled polymers — ●INGO ALIG¹, SERGEJ M. DUDKIN¹, DIRK LELLINGER¹, SVEN PEGEL², and PETRA PÖTSCHKE² — ¹Deutsches Kunststoff-Institut, Schlossgartenstr. 6, D-64289 Darmstadt — ²Leibniz-Institut für Polymerforschung Dresden e.V., Hohe Str. 6, D-01069 Dresden

The influence of pre-history and shear response on AC conductivity of polymer-dispersed multi-walled carbon nanotubes (MWNT) are presented. Different composites of amorphous and crystalline polymers filled with different amounts of MWNT are investigated. The measurements are performed in a plate-plate geometry which allows simultaneous measurements of electrical and rheological properties. The conductivity spectra are recorded under non-isothermal conditions (melting, annealing, crystallization) and during isothermal relaxation after application of a steady state shear field. The measurements exhibit extraordinary changes in dielectric properties depending on mixing conditions, thermal history and/or external flow. Particularly, the changes in conductivity after transient shear indicate long-term relaxations in the conductive network formed by the nanotubes. The changes in AC conductivity are related to changes in (i) tube-polymer-tube interaction and (ii) tube orientation. The conductivity/permittivity spectra are discussed in the frame of percolation theory. In addition to the laboratory experiments, we will present results from in-line conductivity measurements during extrusion.

/1/ P.Pötschke, S.M. Dudkin, I. Alig, *Polymer* **44** (2003) 5023-5030

CPP 11.23 Tue 17:00 P3

Voiding - a way to increase the piezoelectric activity of polyamide 11 - films? — ●ALEXANDER KREMMER, WERNER WIRGES, PETER FRÜBING, and REIMUND GERHARD-MULTHAUPT — Institut für Physik, Universität Potsdam, Am Neuen Palais 10, 14469 Potsdam

After quenching from the melt and cold drawing polyamide 11 (PA11) - films form ferroelectric domains. The ferroelectric domains are oriented in the field direction by poling above the coercive field (75 MV/m) and the polymer becomes piezo- and pyroelectric. A remanent polarization of 50 mC/m² and a piezoelectric d_{33} coefficient of 4 pC/N are obtained. At room temperature the piezoelectric effect is relatively small compared with other ferroelectric polymers, however, it shows a better thermal stability. The orientation in the ferroelectric domains can be destroyed only through melting above 185 °C. The small piezoelectric effect is related to the high elastic modulus (2 GPa). Experiments are presented, which were performed in order to reduce the elastic modulus by voiding with supercritical CO₂. First the gas is dissolved in the polymer under high pressure (150 bar). Then the films are annealed at 170 °C in order to expand the gas rapidly and to stabilise the voids before the gas diffuses out of the film. The piezo- and pyroelectric properties are investigated.

CPP 11.24 Tue 17:00 P3

Investigation on the Molecular Mobility and Gas Transport Properties of Polymer/POSS Hybrid Materials — ●NING HAO, MARTIN BÖHNING, OLE HÖLCK, HARALD GOERING, and ANDREAS SCHÖNHALS — Bundesanstalt für Materialforschung, Unter den Eichen 87, D-12205 Berlin

Polymer based hybrid materials are prepared by blending polyhedral oligomeric silsesquioxanes (POSS) into different polymer matrices via a solution / film casting route. POSS can be regarded as a molecular silica nanoparticle. The property structure relationships of these nanocomposites are investigated by dielectric spectroscopy and gas transport measurements. As a main result POSS can be mixed homogeneously on a molecular level into the polymer matrix up to a limited concentration which depends on the organic substituents of the POSS component and the polymer matrix as well. For higher concentrations of POSS a phase separated structure with a POSS rich phase is observed. This structure influences strongly the gas transport properties of the nanocomposite materials

CPP 11.25 Tue 17:00 P3

Physical characterization of organometallic block copolymers: poly(styrene-b-ferrocenyldimethylsilane) / homo- polymer blends — ●JIANJUN XU^{1,2}, VASILIOS BELLAS¹, INGO ALIG², and MATTHIAS REHAHN^{1,2} — ¹Institut für Makromolekulare Chemie, TU Darmstadt, Petersenstr. 22, D-64287 Darmstadt — ²Deutsches Kunststoff-Institut, Schlossgartenstr. 6, D-64289 Darmstadt

Due to inclusion of iron atom in the chain extraordinary electrical, optical and magnetic properties are expected for polyferrocenyldimethylsilane copolymers. We focus here on polyferrocenyldimethylsilane (PFDMS) and polystyrene (PS) diblock copolymer, in which PFDMS is semi-crystalline and PS is amorphous. Synchrotron (SAXS, WAXS), rheological, DSC and dielectric experiments are combined to study phase structure, order-disorder and order-order transitions as well as crystallization of the PFDMS phase. From generalized phase diagram one can conclude that our system is in the weak segregation limit. Synchrotron X-ray experiments show spherical, cylindrical and lamellar morphologies in diblock copolymers blended with the homo polymers (PFDMS or PS) by varying the composition. The DSC experiments indicate the existence of confined crystalline structures. Dielectric relaxation experiments have been performed on doped and undoped samples in order to study conductivity in the organometallic block and polarization effects.

CPP 11.26 Tue 17:00 P3

Forces on driven colloids in polymer solutions — ●MATTHIAS KRÜGER^{1,2}, MARKUS RAUSCHER^{1,2}, and SIEGFRIED DIETRICH^{1,2} — ¹Max-Planck-Institut für Metallforschung, Heisenbergstr. 3, 70569 Stuttgart — ²Institut für Theoretische und Angewandte Physik, Pfaffenwaldring 57, 70569 Stuttgart

Dynamic density functional theory (DDFT) is a dynamic extension of the very successful equilibrium DFT to systems close to equilibrium. It allows to describe the collective dynamics of interacting Brownian particles at the microscopic level in terms of an evolution equation for the particle density. We extend the DDFT to include the effect of solvent flow. In Particular, we study the case of colloids driven through a polymer solution.

We observe accumulation of polymers in front of a driven colloid which gives rise to a friction additionally to the usual Stokes friction. We relate this friction to the diffusivity of a colloid in a polymer solution. We also compare our results to recent experiments measuring the force on a driven colloid in a polymer solution. Between two colloids moving side by side or behind each other, we find repulsive and attractive polymer induced interactions respectively.

CPP 11.27 Tue 17:00 P3

Dielectric heating of Inverse miniemulsions: size dependence on the absorption of microwave radiation — ●J TSUW¹, F KREMER¹, C HOLTZE², M ANTONIETTI³, R SIVARAMAKRISHNAN⁴, and K.D KRAMER⁴ — ¹Institute for Experimental Physics I, University of Leipzig, Linnéstraße 5, 04103, Leipzig, Germany — ²Experimental Soft Condensed Matter Group, 40 Oxford Street, Harvard University, Cambridge, MA 02138, U.S.A — ³Max Planck Institute of Colloids and Interfaces, Department of Colloid Chemistry, D-14424 Potsdam, Germany — ⁴Department of Physics, Free University of Berlin, Arnimallee, Berlin Dahlem, Germany

The absorption of microwave radiation in aqueous NaCl droplets is

analyzed in the frequency range 1MHz to 4GHz. The droplets were dispersed in a continuous oil medium characterized by a dielectric constant of 2.0 and a loss of less than 0.1. All miniemulsions investigated showed one dielectric loss peak, whose intensity and frequency position varied depending on the droplet size. The analysis of data is discussed in the context of Maxwell-Wagner polarization mechanism. The information obtained from this study not only allows the simple adjustment of heating rates (for example in microwave enhanced chemical reactions) by structural control in multiphase emulsions and dispersions, but also is relevant for the discussion of health impacts in high frequency telecommunication devices. References (1) J. Tsui et al. Dielectric heating of Inverse miniemulsions: size dependence on the absorption of microwave radiation (in preparation)

CPP 11.28 Tue 17:00 P3

Phase structures of oil continuous microemulsions towards new decontamination media — ●S. WELLERT¹, H. IMHOF¹, T. HELLWEG¹, M. DOLLE², H.-J. ALTMANN², and A. RICHARDT² — ¹TU Berlin, Stranski-Lab., Strasse des 17. Juni 112, D-10623 Berlin — ²Armed Forces Scientific Institute for Protection Tech., P.O.Box 1142, D-29623 Munster

Removal of chemical warfare agents from coated metal surfaces is an important issue in civil protection. In this purpose the German army uses a macroemulsion based on the technical surfactant Marlowet IHF in mixture with water, perchlorethylene and hypochlorite. Inherently, macroemulsions are unstable and therefore the formation of a microemulsion with the same surfactant is desirable. Microemulsions are macroscopically homogeneous and thermodynamically stable mixtures of water, oil and surfactants and exhibit various unique properties interesting for decontamination applications. Mixtures of water, perchlorethylene, hypochlorite, the emulsifier Marlowet IHF and the cosurfactant 2-propanol are under investigation in order to form oil continuous microemulsions. We present the phase behavior of the four-component system as well as different cuts through the phase tetrahedron containing stable one phase regions. Alternatively we used AOT instead of the established emulsifier. The identified stable one-phase regions were studied by dynamic light scattering to get knowledge about the formed microstructures of these microemulsions.

CPP 11.29 Tue 17:00 P3

Architectural influence on deformation and fracture properties of S-S/B-S triblock copolymers — ●ULRIKE STAUDINGER^{1,2}, BHABANI K. SATAPATHY^{1,2}, ROLAND WEIDISCH^{1,2}, ANDREAS JANKE², and KONRAD KNOLL³ — ¹Institute of Materials Science and Technology, Friedrich-Schiller-University Jena, Löbdergraben 32, D-07743 Jena, Germany — ²Leibniz-Institut für Polymerforschung Dresden, Hohe Str. 6, 01069 Dresden, Germany — ³BASF-AG, 67056 Ludwigshafen, Germany

The influence of molecular architecture on the deformation and fracture behaviour of triblock copolymers with two PS end blocks and random S/B middle block has been studied and the results have been correlated with their morphology. A triblock copolymer with short PS outer blocks and a S/B ratio of 1:1 in the middle block exhibits a wormlike structure and shows elastomeric behaviour. Increasing the soft phase content in the middle block to a S/B ratio of 1:2 results in an increased interaction parameter and thus to enhanced phase separation. The morphology changes into a lamellae structure leading to a distinct increase in strain, yield stress and Young's modulus. Increasing the PS outer block content up to 18 wt.-% also leads to lamellar morphology and a change to thermoplastic behaviour could be observed. The fracture toughness was evaluated using essential work of fracture method based on concepts of the Post-Yield Fracture Mechanics. With increasing PS content in the outer blocks the resistance against crack propagation increases. The fracture toughness is strongly increased in case of triblock copolymers with lamellae structure when compared to that of wormlike structure.

CPP 11.30 Tue 17:00 P3

Flow NMR of dispersed systems — ●ULRICH SCHELER and FRANK BAGUSAT — Leibniz Institute of Polymer Research Dresden, Hohe Strasse 6, D-01069 Dresden, Germany

Polymers and dispersions often exhibit non-Newtonian flow behaviour. The detailed investigation of this behaviour requires detailed and localized information, which is efficiently derived from a combination of NMR imaging and pulsed field gradient NMR, providing localized flow information. This is utilized to check the validity of assumption on the flow profile for the data analysis. NMR provides information on the fluid phase as opposed to most other methods. In addition to information

on density of the fluid phase (signal intensity), flow direction and velocity contrast in the fluid phase is generated by NMR parameters like relaxation times. This enables the selective investigation of different components in the fluid phase. Experiments are performed in Couette cell in a high-field NMR spectrometer. Variations of the inner cylinder permit the investigation of effects of local high shear. Examples are shown for a silica in water dispersion and oil in water emulsion.

CPP 11.31 Tue 17:00 P3

Self assembly in mixtures of surfactant and amphiphilic Poly(*p*-phenylenes): Rodlike structures — ●THOMAS HELLWEG¹, TOBIAS FÜTTERER¹, GERHARD FINDENEGG¹, and DIETER SCHLÜTER² — ¹TU Berlin, Stranski-Lab. (ER 1), Strasse des 17. Juni 112, 10623 Berlin — ²ETH Zürich

2,5-disubstituted poly(*p*-phenylenes) with one nonpolar substituent R1 and one polar substituent R2 on each monomeric unit represent an interesting class of amphiphiles in which the border between the hydrophilic and hydrophobic part of the molecule runs along its stiff backbone. We have studied the self-assembly of a poly(*p*-phenylene) oligomer, PP_{*n*} (*n*=12), with substituents R1= C₁₂H₂₅ and R2= -CH₂(OC₂H₄)₃OCH₃ in the pure state and in aqueous surfactant solutions, using light scattering, and SANS. This compound is soluble in aqueous solutions of nonionic surfactants such as e.g. C₈E₄, where it forms elongated stiff aggregates (contour length ca. 500 nm, diameter 5.5 nm). The ratio polymer to surfactant was found to be 1:3 in the mixed structures using SANS [1]. Dynamic light scattering data from the aqueous PP₁₂-C₈E₄ solution can be modelled by an intermediate scattering function for rod-like particle dynamics [2].

[1] T. Fütterer, Th. Hellweg, G. H. Findenegg, J. Frahn, and A. D. Schlüter; *Macromolecules* **38** (2005) 7451.

[2] T. Fütterer, Th. Hellweg and G. H. Findenegg; in: *Mesoscale Phenomena in Fluid Systems*, F. Case and P. Alexandridis (Hrsg.), ACS Symposium Series No. 861, (2003).

CPP 11.32 Tue 17:00 P3

Influence of molecular weight on rheological properties of linear symmetric S-(S/B)-S triblock copolymers — ●MAHENDRA THUNGA¹, ULRIKE STAUDINGER^{1,2}, BHABANI K. SATAPATHY^{1,2}, ROLAND WEIDISCH^{1,2}, and KONRAD KNOLL³ — ¹Leibniz Institute of Polymer Research, Hohe Str. 6, 01069 Dresden, Germany — ²Institute of Materials Science and Technology, Friedrich-Schiller-University Jena, Löbdergraben 32, 07743 Jena, Germany — ³BASF AG, D-67056 Ludwigshafen, Germany

The influence of molecular weight on morphology, rheology and mechanical properties of a symmetric linear S-S/B-S type triblock copolymer has been studied. The morphology reveals that the size of dispersed PS (hard) phase is narrowed down with the increase in molecular weight from 110 to 156 kg/mol. On further increasing the molecular weight to 200 kg/mol phase separation is observed with the formation of lamellar morphology. The rheological studies reveal that storage modulus and complex viscosity are strongly influenced by their relative molecular weights. An increase in molecular weight leads to an extended rubbery plateau and the terminal region is narrowed down. A transition from Newtonian to non-Newtonian flow in the low frequency regime could be observed with the increase in molecular weight along with an increase in the order-disorder transition temperature. DMA and DSC measurements reveal that the increase in the molecular weight from 165 to 200 kg/mol has led to two distinct transition points for PS rich phase and PB rich phase due to the macrophase separation.

CPP 11.33 Tue 17:00 P3

Thermal Patterning of a Critical Polymer Blend — ●ALBERT VOIT, ALEXEI KREKHOV, WOLFGANG ENGE, LORENZ KRAMER, and WERNER KÖHLER — Universität Bayreuth

The influence of inhomogeneous temperature fields on the demixing of a critical polymer blend has been investigated with the aim to control the spinodal demixing morphology. We have employed a focused laser beam to write spatial composition patterns into layers of the critical polymer blend poly(dimethylsiloxane)/poly(ethylmethyl siloxane) (PDMS/PEMS, Mw = 16.4/22.8 kg/mol) both in the one and in the two-phase region a few degrees above and below the critical temperature. Due to the critical divergence of the Soret coefficient, moderate temperature gradients are sufficient to induce composition modulations of large amplitude. In the two-phase regime the spinodal demixing pattern can be locally manipulated in a controlled way and the time evolution of

various patterns can be studied. 2D-simulations based on a modified Cahn-Hilliard equation are able to reproduce the essential spatial and temporal features observed in the experiments.

CPP 11.34 Tue 17:00 P3

Studies on the Interphase in PP-Glass Composites — ●HANNA M. BRODOWSKY and EDITH MÄDER — Leibniz-Institut für Polymerforschung Dresden, Hohe Str. 6, D-01069 Dresden

In composites, the interface between the components is essential for improving the mechanical properties. By using a suitable sizing (surface modification) of the fiber, the interface may be varied, e.g. by suppressing or promoting heterogeneous nucleation of a thermoplastic matrix. In the latter case, a three dimensional transcrystallized $\{\Delta q\}$ interphase $\{\Delta q\}$ with properties differing from those of the bulk matrix is formed.

Polypropylene-glass fiber composites with a number of different sizings and different PP chain lengths are prepared as single fiber model composites. These are studied in quasistatic or cyclic load tests. Static tests permit insights in the interfacial characteristics such as fracture energy release rate, shear strength and modulus. Cyclic tests on these model composites can be used to study the nature of dissipative processes and the damage behaviour. An AFM characterisation of the pulled out fibers provides supplementary information. Additionally, the dynamic behavior of bulk composites is characterized.

CPP 11.35 Tue 17:00 P3

Structure and dynamics of electrostatically interacting magnetic colloidal suspensions by means of static and dynamic x-ray scattering — ●TINA AUTENRIETH¹, JOACHIM WAGNER², AYMERIC ROBERT³, and GERHARD GRÜBEL¹ — ¹HASYLAB at DESY, Notkestrasse 85, 22607 Hamburg — ²Universität des Saarlandes, Saarbrücken — ³ESRF, Grenoble, France

A model system for complex liquids with dipolar interactions has been synthesized [1]. The particles consist of a magnetic cobalt ferrite core embedded in a silica shell and have a narrow size distribution. They interact due to the charged silica surface via a screened Coulomb potential in addition to the magnetic dipole-dipole interaction of the core. The colloidal suspension is strongly opaque and thus cannot be probed by visible light scattering techniques. Therefore both, the static and dynamic behaviour of such a concentrated, liquid-like ordered dipolar suspension are studied by means of Small Angle X-ray Scattering and X-ray Photon Correlation Spectroscopy without and in the presence of an external magnetic field [2]. The dynamics was probed over the Q-range of the static structure factor and shows even without magnetic field strong deviations from the Stokes-Einstein behaviour that can not be explained by the De-Gennes narrowing. The observed behaviour has to be attributed to indirect hydrodynamic interactions which are mediated by the suspending medium [3]. However, the hydrodynamic behaviour cannot be described by any of the available models for colloidal hydrodynamics. [1] T. Autenrieth et al., AOC 18, 520 (2004) [2] J. Wagner et al., JMMM 289, 54 (2005) [3] A. Robert et al., JCP 122, 084761 (2005)

CPP 11.36 Tue 17:00 P3

Free volume from positron lifetime spectroscopy and mechanical properties of EPDM rubber/SiO₂ nanocomposites — ●JAN KRUSE¹, RODRIGO LIMA DE MIRANDA¹, KLAUS RÄTZKE¹, MATTHIAS ADLER², DIRK W. SCHUBERT², and FRANZ FAUPEL¹ — ¹Lehrstuhl für Materialverbunde, Universität Kiel — ²Freudenberg Forschungsdienste KG, Weinheim

The addition of inorganic particles to a polymer matrix has a long tradition in polymer engineering. Decreasing their size to nanometre dimensions provides a high specific interaction surface and the possibility of a fine dispersion of the particles. In gas sealing applications, the particles might act as a permeation barrier by blocking diffusion paths (tortuosity). We have investigated EPDM rubber with up to 23 wt% nonfunctionalised SiO₂ nanoparticles. Positron annihilation lifetime spectroscopy (PALS) is a powerful tool to determine free volume from size dependent ortho-positronium lifetime. PALS shows just a slight decrease in free volume element size, but a linear decrease in free volume concentration (from o-Ps intensity) with filler amount. Dynamic mechanical thermal analysis (DMTA) was employed to observe the increase in elastic and damping modulus as well as the respective transition temperature.

CPP 11.37 Tue 17:00 P3

On the way to nano-porous polymer foams — ●FRANCISCO CAMACHO-GONZALEZ, JOHANN G. LEONHARTSBERGER, MARIO DANSACHMUELLER, SIMONA BAUER-GOGONEA, and SIEGFRIED BAUER — Soft Matter Physics, Johannes Kepler University, Altenberger Str. 69, A-4040 Linz, Austria

Electromechanical effects in polymers, like piezoelectricity and electrostriction are employed in transducers and photonics. With the formation of micron-sized voids, soft cellular polymers with huge piezoelectric effects and ferroelectric-like behavior were developed. Micron-sized voids are advantageous for transducer applications, but they prevent the materials to be used in photonics. For photonics applications it might be interesting to have soft polymers with voids in the submicron region. Amorphous polymers and elastomers were foamed under supercritical conditions of CO₂ at different temperatures. Transmission electron microscope (TEM) images show the formation of nano-voided structures in the polymer matrix when samples are saturated under optimal conditions. Saturation at higher temperatures lead to larger voids (in the micrometer range). Samples treated at lower temperatures show not much change in the matrix structure.

CPP 11.38 Tue 17:00 P3

Viscoelasticity of pericellular matrix gels — ●HEIKE BOEHM, CHRISTIAN H.J. SCHMITZ, RALF P. RICHTER, JOACHIM P. SPATZ, and JENNIFER E. CURTIS — Max-Planck-Institute for Metals Research, Department New Materials & Biosystems, and University of Heidelberg, Department of Biophysical Chemistry, Heisenbergstr. 3, D-70569 Stuttgart

Many mammalian cells surround themselves with a pericellular matrix (PCM), a highly hydrated polymer network connected to the cell membrane. The mechanical properties of the PCM are essential for cell proliferation and migration. The most vital component of this polymer network is hyaluronan, a long, unbranched polysaccharide. The viscoelasticity of the PCM is dynamically adjusted by the cell through the addition of glycoproteins called hyaladherins which crosslink or bind to the hyaluronan creating a stiffer network. The effect of most hyaladherins on hyaluronan networks has not yet been measured because the proteins are only available in such small volumes that established rheological techniques cannot be used. To bypass this difficulty, we perform one and two-point microrheological measurements by following the Brownian motion of embedded passivated particles in 20 μ l volumes. This technique enables the characterization of the shear modulus of well-defined hyaluronan networks, and the quantification of the effect of various hyaladherins for the first time. The results can subsequently be compared with measurements of the PCM on a living cell.

CPP 11.39 Tue 17:00 P3

Polymer-Induced Transient Networks in Water-in-Oil Microemulsions Studied by Dynamic Light Scattering — ●THOMAS BLOCHOWICZ, CHRISTOPH GÖGELEIN, and BERND STÜHN — Institute of Solid State Physics, TU-Darmstadt, 64289 Darmstadt

We study water-in-oil microemulsions, i.e. dispersions of water droplets coated with a monolayer of surfactant in a continuous oil phase. Of particular interest for the present work is the system consisting of water, n-decane and the anionic surfactant AOT. On addition of the amphiphilic triblock copolymer PEO(polyethylenoxide)-PI(polyisoprene)-PEO a transient network is formed. The dynamics of concentration fluctuations consisting of the translational diffusion of the droplets and the relaxation of the network are monitored with photon correlation spectroscopy. We mainly focus on the variation of the dynamic behavior as a function of two different parameters, namely the number of polymer molecules per droplet Z and the droplet volume fraction ϕ , which can be taken as a measure for the inter droplet distance. With increasing polymer content the dynamics of the system slows down and three different relaxation processes may be distinguished. We discuss the origin of the different relaxation modes. In particular it turns out that the intermediate relaxation mode may be suppressed by index matching the oil matrix and the PI block and that the network formation sensitively depends on the interdroplet distance.

CPP 11.40 Tue 17:00 P3

Diffusion of Block-Copolymer Micelles Close to the Water-Oil Interface — ●ANTONIO STOCO¹, STERGIOS PISPAS² und REINHARD SIGEL¹ — ¹Max-Planck-Institut of Colloids and Interfaces, D-14476 Golm — ²National Hellenic Research Foundation, Theoretical and Physical Chemistry Institute, 11635 Athens, Greece

The interaction of block copolymer micelles in water with a brush composed of the same block copolymer at the water-oil interface is investigated. For a concentration above the critical micelle concentration, the block copolymers adsorbed to interfaces coexists with block copolymer micelles in solution. Close to the interface, a modification of the micelle diffusion compared to the bulk behavior is expected because of changed friction and possible exchange processes. We built up an apparatus for light scattering with evanescent wave illumination of a liquid-liquid interface. In this special geometry, only a thin layer at the interface is illuminated, allowing for dynamic light scattering measurements close to the interface. In addition, ellipsometry measurements within the same apparatus give access to the interface profile. First results on polyisoprene-block-polyethyleneoxide polymers at to the water-dodecane interface are discussed.

CPP 11.41 Tue 17:00 P3

Tailoring the structure of hybrid organic-inorganic tetra and polyfunctional alco-oxo-titanium clusters in polystyrene —

●SONDES TRABELSI^{1,2}, GIULIA FORNASIERI^{3,4}, LAURENCE ROZES³, ANDREAS JANKE¹, AXEL MENSCH⁵, CLÉMENT SANCHEZ³, and MANFRED STAMM¹ — ¹Leibniz Institut für Polymerforschung Dresden e.V., Hohe Strasse 6, 01069 Dresden, Germany — ²Forschungszentrum Karlsruhe GmbH, Institute für Synchrotronstrahlung, ANKA, Hermann-von-Helmholtz-Platz 1, 76344 Karlsruhe, Germany — ³Laboratoire de Chimie de la Matière Condensée, UMR CNRS 7574, — ⁴Laboratoire de Chimie Inorganique, Institut de Chimie Moléculaire et des Matériaux d'Orsay (ICMMO), Bat 420 Université Paris-Sud 11, 91405 Orsay Cedex, France — ⁵Technische Universität, Dresden, Institut für Werkstoffwissenschaft, Helmholtzstraße 7, 01062 Dresden, Germany

Two types of Ti16O16(OEt)32-x(OPhCH=CH2)x cluster have been synthesized with different numbers of styrenic functional groups (i.e. tetra (x = 4) and poly (x = 16)) introduced on the surface of the cluster s core. Investigations combining small angle X-ray scattering (SAXS), transmission electro microscopy (TEM) and energy-filtering transmission electron microscopy (EFTEM) lead to a better understanding about the influence of the functionality s number on the structure of the hybrid nanomaterials. Compared to the tetra functional clusters the poly functional clusters were good dispersed in the hybrid even at very high content between 5 wt% and 10 wt%. Independently of the number of functionalities, three structural levels. The size of the aggregates has been reduced significantly by increasing the number of styrenic reactive groups.

CPP 11.42 Tue 17:00 P3

Analytical centrifugation to describe rheological behaviours of concentrated suspensions — ●TORSTEN DETLOFF, TITUS SOBISCH, and DIETMAR LERCHE — L.U.M. GmbH, Rudower Chaussee 29, 12489 Berlin, Germany

The flow behaviour of concentrated suspensions is mostly characterized by viscometric approaches. The interpretation of the results, especially at low shear rates, is often difficult due to sedimentation and particle migration within the viscometric gap. But studying separation processes can give information about the viscosity behaviour of such suspensions, because of the close connection between sedimentation kinetics and rheology. In this paper analytical centrifugation were used to determine the viscosity functions of spherical rigid particles in the nanometer range depending on volume concentrations between 5 and 47%. The measurement device - a multisample analytical centrifuge - LUMiSizer® (L.U.M. GmbH, Berlin Germany) employs the STEPTM-Technology (Space and Time resolved Extinction Profiles), which allows to measure the intensity of transmitted light as function of time and position over the entire sample length simultaneously. From this data the values of the flux density function at different initial volume concentrations were determined and a viscosity law as functions of volume concentration obtained by fitting. The approach was applied to spherical biological cells and silica particles.

CPP 11.43 Tue 17:00 P3

Dendrimer-Based Nanoassemblies: Insights from Small Angle Scattering Experiments — ●RALF KLEPPINGER — DSM Research

Highly branched macromolecules have found widespread applications in the growing field of nanomaterials. From an application point of view, hyperbranched systems (with less defined architecture) appear to be rather attractive candidates for bulk applications that allow tailoring of rheological properties. Dendrimer systems with their highly defined three-dimensional architectures on the other hand appear to be promising candidates in the field of biomedical materials where they have been proposed as new type of drug delivery systems. In any case, the investigation of such systems and in particular their complexes, represents a significant challenge. In this contribution we summarize results from small angle X-ray and -neutron scattering investigations that were performed on dendrimers and dendrimer-based complexes.

CPP 11.44 Tue 17:00 P3

Rigid Amorphous Fraction of Polymer Nanocomposites and Semicrystalline Polymers — ●ALBERT SARGSYAN¹, SELVIN THOMAS², ANDREAS WURM¹, SABU THOMAS², and CHRISTOPH SCHICK¹ — ¹aUniversity Rostock, Dept. Physics, Universitätsplatz 3, 18051 Rostock, Germany — ²Mahatma Gandhi University, School of Chemical Sciences, Kottayam, India

Very often semicrystalline polymers cause significantly smaller relaxation strength at glass transition than expected from the non-crystalline fraction. This observation could be explained by the introduction of a rigid amorphous fraction (RAF) which does not contribute to the heat of fusion or X-ray crystallinity nor to the relaxation strength at glass transition. The RAF is non-crystalline and in a glassy state above the common glass transition temperature. From heat capacity the temperature and time dependence of the RAF can be obtained. For PC, PHB and sPP it is possible to study the creation and disappearance of the RAF in situ during isothermal crystallization and on stepwise melting. A RAF can be detected for polymer nano-composites too. The approximate amount of the RAF was calculated taking into account the difference in Δc_p step between pure and filled polystyrene nano-composites. The solvents added as plasticizers haven't entered into the RAF even above the glass transition temperature (T_g). This gives the opportunity to create highly solvent resistant polymer nano-composites based on common polymers like polystyrene.

CPP 11.45 Tue 17:00 P3

Thermoplastic SBS nanocomposites based on brush coated silica microgels — ●LESZEK JAKUCZEK^{1,2} and JOCHEN GUTMANN^{2,3} —

¹Department of Polymer Engineering and Technology, Wrocław University of Technology, Wybrzeże Wyspińskiego 27, 50-386 Wrocław, Poland — ²Max Planck Institute for Polymer Research, Ackermannweg 11, D-55128 Mainz — ³Institute for Physical Chemistry, Johannes Gutenberg University, Welderweg 11, D-55099 Mainz

Physical modification of block copolymers enables the preparation of new types of materials exhibiting significantly improved mechanical and rheological properties. Especially well-defined nanofillers, with properties tailored at molecular level, are believed to be effective reinforcing agents, capable of meeting the expectations in new areas of application. One route leading to such nanocomposites is synthesis and incorporation of surface modified nanoparticles, like e.g. ultrafine polymer-grafted silica beads synthesized in emulsion. After surface modification via a grafting from ATRP synthesis, the resulting core-shell composites can be used in selective reinforcement of a chosen phase. Linear styrene-*b*-butadiene-*b*-styrene thermoplastic elastomer was modified with polystyrene-grafted organosilicon micro-gel particles. The state of filler dispersion and degree of grafting, morphology of the resulting nanocomposites, as well as their mechanical, rheological and thermal properties are examined using SEM, SAXS, GPC, DSC and dynamic thermomechanical analysis in order to provide information on interactions between filler and the modified matrix.

CPP 11.46 Tue 17:00 P3

Modification of the thermal properties of epoxies by anorganic nanoparticles — ●JÖRG BALLER^{1,2}, ROLAND SANCTUARY^{1,2}, MARTINE PHILIPP^{1,2}, RAVI BACTAVATCHALOU¹, and J. K. KRÜGER¹ —

¹Laboratoire Européen de Recherche Universitaire : Saarland-Lorraine-Luxembourg — ²Université du Luxembourg, Laboratoire de Physique des Matériaux, 162 a, avenue de la Faiencerie, L-1511 Luxembourg

Curing and polymerisation behaviour of epoxies filled with nanoparticles were investigated using Modulated Differential Scanning Calorimetry. Depending of the type of incorporated nanoparticles, important properties like relaxation behaviour and glass transition are considerably

modified. Comparison with results from viscosimetry and Brillouin scattering yields insights into the interaction between matrix and nanoparticles.

CPP 11.47 Tue 17:00 P3

Rheological properties of Carbon-nanofibre Reinforced Poly(ether ether ketone) Composites under Shear and Elongational Flow — •D.S. BANGARU SAMPATH¹, HOLGER RUCKDAESCHEL¹, JAN K.W. SANDLER¹, VOLKER ALTSTAEDT¹, and MILO S.P. SHAFFER² — ¹Polymer Engineering, University of Bayreuth, Universitaetsstrasse 30, 95447 Bayreuth, Germany — ²Department of Chemistry, Imperial College, London, Sw7 2A2, UK

The rheological properties of vapor grown carbon nanofibre (VGCNF) reinforced poly(ether ether ketone) (PEEK) are studied both under oscillatory shear as well as in uniaxial extension at 360 °C. The composites containing upto 15 wt% of carbon nanofibres are melt-blended in a Brabender co-rotating twin-screw extruder. It was shown that both the elastic moduli and the viscosity change with amplitude of oscillation and with the CNF concentration, respectively. The dynamic moduli and the viscosity were found to be increasing with increasing the CNF content. The composite with high fibre loading exhibits enhanced shear thinning. Furthermore, the linear viscoelastic data shows a transition to a solid like response at low frequency which indicates the so-called *percola-

tion threshold* appearing between 10 and 15 wt% of CNF. Interestingly, the melt elongational measurements show significant increase in melt strength, whereas the elongation at break remains unchanged upto 10 wt% CNF. We have shown that the addition of CNF can be significantly improve the foaming behaviour through its effect on the melt strength as well as extensibility.

CPP 11.48 Tue 17:00 P3

Non-linear rheological properties of fibrillar networks by self-organization — •MARTIN KÜHNE and CHRISTIAN FRIEDRICH — Freiburg Materials Research Centre (FMF) & Institute of Macromolecular Chemistry Albert-Ludwigs-University, Stefan-Meier-Str. 21, 79104 Freiburg, Germany

Dibenzylidene sorbitol (DBS) is known to gel in organic liquids and polymers by the formation of long fibres due to the self-organization of DBS molecules. We studied this process in detail for DBS organization in poly(propylene oxides) of different molecular weight. We report on the morphological as well as the linear and non-linear viscoelastic properties of these materials in the gel state. While the linear viscoelastic properties can be understood quantitatively on the basis of the "soft glassy materials" model, the non-linear properties are mainly determined by the damage of the fibre network.

CPP 12 POSTER Colloids, Nanoparticles and Self-Organizing Systems

Time: Tuesday 17:00–19:00

Room: P3

CPP 12.1 Tue 17:00 P3

Water density reduction at hydrophobic interfaces: a neutron reflectometry study — •MARCO MACCARINI¹, MICHAEL HIMMELHAUS¹, ROLAND STEITZ², MAXIMILIAN WOLFF³, and MICHAEL GRUNZE¹ — ¹Institut für Ang. Physikalische Chemie, Universität Heidelberg, Germany — ²Hahn-Meitner-Institut, Berlin, Germany — ³Institut Laue-Langevin, Grenoble, France

A close relationship exists between the structure of a liquid in the vicinity of a surface and the solvation force appearing between two surfaces immersed in the liquid. This relationship has important implications in the case of hydrophobic surfaces and water since the resulting force, the hydrophobic interaction, is responsible for key biological phenomena such as protein folding, self-assembling, colloids stability and membrane fusion. The origin of this interaction has still a number of unexplained features because the structure and the conformation of water molecules in the vicinity of hydrophobic surfaces are not fully understood. Theoretical studies (Lum 1999, Mamatkulov 2004) predicted a depletion layer, i.e. a reduced water density, near the hydrophobic surface/water interface. This extends to a thickness in the order of nm into the bulk water and is thermodynamically less stable than the vapor phase. In order to clarify the extension of the depletion layer and its dependence on some parameters like temperature, pH and electrolyte concentration, we performed neutron reflectometry on hydrophobic surfaces formed by the adsorption of alkanethiols self assembling monolayers (SAM) on gold surfaces in contact with water and non polar solvents.

CPP 12.2 Tue 17:00 P3

Interaction of a spherical particle with linear chains — •JAROSLAW KLOS — Faculty of Physics, A. Mickiewicz Univ., Umultowska 85, 61-614 Poznan, Poland

Linear polymers surrounding a hard sphere are simulated using the Cooperative Motion Algorithm on the face centered cubic lattice. The excluded volume condition is taken into account, and the properties of the chains are examined in two situations of: (i) free polymers, (ii) chains end-grafted onto the spherical surface ("hairy spheres"). In case (i) the size ratio $q=R/R_g$ of the sphere radius to the mean radius of gyration of the chains is considered the main parameter. The simulations indicate (1) a depletion layer in the neighborhood of the sphere, (2) an enhancement of the chain ends concentration at the particle surface, (3) an enhancement of the chain centers of mass concentration at some distance from the surface for large q , (4) a penetration of the centers of mass into the sphere for small q , (5) an orientation ordering of the chains in the region of interest. In case (ii) the simulations are performed in two extremes of the surrounding matrix: (a) the hairy spheres immersed in a pure solvent of single beads and (b) the hairy spheres in a melt of chains. The simulations indicate that (1) the concentration profiles of the end-grafted

chains under good solvent conditions are noticeably different from those calculated for the chains in a melt, (2) as the sphere radius increases, the monomer concentration profile changes from concave to convex (3) both the free ends and the centers of mass profiles are Gaussian-like, (4) depending on the position of the center of mass, both tangential and radial ordering of the polymers relative to the sphere are present.

CPP 12.3 Tue 17:00 P3

Surface Properties of Carbon Black Modified by Atmospheric Plasma — •GERALD J. SCHNEIDER¹, JOHANN VANCEA¹, ROBERT C. WEISS¹, ANDREAS WEIGERT¹, NURIA TRICÁS², and DIETMAR GÖRITZ¹ — ¹Institut für Physik, Universität Regensburg, 93040 Regensburg — ²Institut Quimic de Sarrià, Universitat de Barcelona, España

To study the interaction between polymer and carbon black the filler surface chemistry was modified by means of atmospheric plasma. The treated carbon black was characterized by small angle x-ray scattering. The scattered intensity was analyzed with regard to the fractal dimensions of surface and mass. X-ray photoelectron spectroscopy was used to analyze changes of the surface chemistry and scanning tunneling microscopy to detect changes of active sites on the surface.

CPP 12.4 Tue 17:00 P3

A fundamental measure free-energy functional for nonspherical particles — •HENDRIK HANSEN-GOOS^{1,2} and KLAUS MECKE³ — ¹Max-Planck-Institut für Metallforschung, Heisenbergstr. 3, 70569 Stuttgart — ²ITAP, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart — ³Institut für Theoretische Physik, Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen

In 1989, Y. Rosenfeld established his fundamental measure theory (FMT) free-energy functional for the hard-sphere fluid. The starting point for his derivation is an exact decomposition of the Mayer- f -bond in terms of convolutions of scalar and vectorial weight functions leading him to an excess free-energy function of scalar and vectorial weighted densities. Rosenfeld's free-energy has proved to describe very accurately inhomogeneous hard-sphere fluids and it is conveniently tractable computationally as only one-center convolutions are involved. Later on, a generalisation of his original FMT to nonspherical particles was given by Rosenfeld himself. Unfortunately, the theory does not show an isotropic-nematic transition as observed, e.g., for hard spherocylinders or ellipsoids. Other free-energy functionals that do predict an isotropic-nematic transition generally involve two-center convolutions and therefore demand more computational efforts. Starting from the exact expression for the Mayer- f -bond for convex particles we introduce an approximate decomposition leading us to a new free-energy functional for non-spherical particles. The functional is still based on one-center convolutions and can be shown to yield an isotropic-nematic transition for spherocylinders.

Strategies to enhance the agreement with simulation data are presented.

CPP 12.5 Tue 17:00 P3

Vibrational properties of ZnO and $Zn_{1-x}Mn_xO$ nanoparticles and ligand-nanoparticle interactions studied by Raman spectroscopy — ●M. SCHUMM¹, M. LENTZE¹, C. BARGLIK-CHORY², and J. GEURTS¹ — ¹Physikalisches Institut der Universität Würzburg, Am Hubland, 97074 Würzburg — ²Lehrstuhl für Silicatchemie, Universität Würzburg, Röntgenring 11, 97070 Würzburg

Nanostructured systems of the large bandgap semiconductor ZnO have attracted a great deal of attention in the recent past due to its special optical properties and various potential applications. Theoretical predictions of ferromagnetic behaviour at room temperature focused the interest among the group of diluted magnetic semiconductors on $(Zn,Mn)O$ nanostructures.

We report on a study of wet chemically synthesised ZnO and $(Zn,Mn)O$ nanoparticles (diameters 3-12 nm) by VIS micro- and Fourier Transform NIR Raman spectroscopy. Special attention was paid to properties of the binding between the ligands and the nanoparticle surface and to interactions between molecular vibrations of the ligands and the phonons of the nanocrystallites. Besides the verification of ligand binding to the particles' surface, ligand-induced strengthening of nanoparticle phonon modes and the formation of coupled modes between nanoparticle phonons and ligand vibrations were observed. Furthermore, the Raman spectra show confinement induced phonon peak shifting and broadening compared to the corresponding bulk material. Finally, for the $Zn_{1-x}Mn_xO$ nanoparticles the successful substitutional incorporation of Mn in the Zn sublattice was proven by its specific vibration modes in the Raman spectrum.

CPP 12.6 Tue 17:00 P3

Monitoring enzymatic degradation of polymeric nanoparticles with scattering methods — ●THOMAS SIEGEMUND^{1,2}, BERND-REINER PAULKE³, HERBERT SCHMIEDEL¹, NATALIE BORDAG², STEFFEN LINDERT¹, and WOLFGANG HÄRTIG² — ¹Universität Leipzig, Institut für Experimentalphysik I, Physik der weichen Materie, Linnéstraße 5, 04103 Leipzig — ²Universität Leipzig, Paul-Flechsig-Institut für Hirnforschung, Jahnallee 59, 04109 Leipzig — ³Fraunhofer Institut für angewandte Polymerforschung, Geiselbergstraße 69, 14476 Potsdam

Nanoparticles can be used as carriers for the delivery of drugs. We prepared nanoparticles as carriers for the model drug thioflavin T that binds Alzheimer's disease related fibrillar amyloid β -peptides in the brain. These polymer colloids are composed of a polystyrene core and a degradable poly(butyl-2-cyanoacrylate) shell with diameters from 60 to 170 nm. The enzymatic degradation of core-shell nanoparticles, as required in vivo, was observed after their treatment with porcine liver esterase, a non-specific esterase, and basic/acidic hydrolysis in vitro. Shells of nanoparticles were dose-dependently degraded while their polystyrene cores remained intact. We applied light scattering and neutron scattering as useful tools to monitor the particle diameters and to evaluate details of the degradation process, especially the degradation-dependent changes in the neutron scattering-length density profile. The degradation speed was studied at different temperatures as function of nanoparticle, enzyme and salt concentration at fixed pH. Deviations from Michaelis-Menten behavior are discussed within a simple model.

CPP 12.7 Tue 17:00 P3

Novel Metal Cages from Bionanoparticle Templates — ●GÜNTHER JUTZ, ANNE HORN, NATHALIE MOUGIN, and ALEXANDER BÖKER — Lehrstuhl für Physikalische Chemie II, Universität Bayreuth, 95440 Bayreuth, Germany

In the presented project we make use of the well-defined composition and structure of the cowpea mosaic virus (CPMV). We use this plant virus as a template for the production of monodisperse, well defined nanoparticles and nanocapsules. We followed this aim with different approaches. After the incubation of the aqueous virus solution with a metal salt under reductive conditions either a homogenous coating or the deposition of distinct nanoparticles onto the capsid has been observed by TEM, SEM and AFM. Another approach uses the well defined surface chemistry of the virus for the site specific decoration of the capsid with nanoparticles. To achieve this, preformed, monofunctionalized nanoparticles can be covalently bound to the capsid. To broaden the range of nanoparticles that can be attached to the virus, it was modified with different chelating ligands that promote binding of metal cations and

serve as heterogeneous nucleation sites for the site specific in-situ growth of nanoparticles. Characterization of the ligand modified virus and the composite particles has been performed using FPLC, SPR, TEM, SEM and AFM.

CPP 12.8 Tue 17:00 P3

Modeling of anisotropic silica clusters — ●GERALD J. SCHNEIDER and DIETMAR GÖRITZ — Institut für Physik, Universität Regensburg, 93040 Regensburg

The mechanical properties of elastomers can be improved by adding precipitated silica. The hierarchical structure of this colloidal filler consists of primary particles, having typical diameters of about 20 nm. During an agglomeration process clusters are formed, which are build up from these primary particles. Regarding the mechanical properties of elastomers, structural changes of silica clusters due to external forces are of interest. These rearrangement during deformation can be studied by means of small-angle scattering experiments. To describe quantitatively the experimental results we introduce a new model, based only on the mathematics of fractals, which is able to predict experimental scattering patterns. With the help of experimental data the usability of the theory will be demonstrated.

CPP 12.9 Tue 17:00 P3

The scattering from thin, lamellar diblock copolymer films in the distorted-wave Born approximation — ●CHRISTINE M. PAPANAKIS¹, P. BUSCH², M. RAUSCHER³, D.-M. SMILGIES², and D. POSSELT⁴ — ¹Physikdepartment E13, TU München, James-Frank-Str. 1, D-85747 Garching — ²Cornell University, Ithaca NY, USA — ³MPI für Metallforschung und Universität Stuttgart — ⁴Roskilde University, Denmark

Grazing-incidence small-angle X-ray scattering (GISAXS) of thin films of diblock copolymers reveals information about the ordering and preferential orientations of the phase-separated microdomains within the films. The grazing-incidence geometry enhances the surface sensitivity; however, the scattering cannot be described any more with a simple kinematic theory, as in transmission small-angle scattering.

We have calculated the scattering cross-section in the framework of the distorted-wave Born approximation, a dynamical scattering theory. We treat the case of thin films of lamellar diblock copolymers, where the orientation of the lamellae is either perpendicular or parallel to the film interfaces and compare the predictions to experimental results from thin films of poly(styrene-*b*-butadiene) diblock copolymers. For perpendicular lamellae, Bragg rods are found, which are extended along the film normal, whereas for parallel lamellae, intensity maxima appear along the film normal. The positions of these maxima can be explained by accounting for refraction at the film surface and reflection at the film-substrate interface.

CPP 12.10 Tue 17:00 P3

pH-Responsive mixed Blockcopolymer/Surfactant Aggregates — ●THOMAS HELLWEG¹, GUILLERMO ORTOS GIL¹, and HELMUT SCHLAAD² — ¹TU Berlin, Stranski-Lab. (ER1), Strasse des 17. Juni 112, 10623 — ²MPI-KGF, 14424 Potsdam

Amphiphilic block copolymers can self-assemble into various ordered mesophases. The symmetry and stability of the microstructure depends intimately on chain size and chemistry as well as physical variables such as temperature. The present work is related to the study of three Poly(styrene)-Poly(L-lysine) diblock copolymers in aqueous surfactant and organic solvents, by Dynamic Light Scattering and Atomic Force Microscopy. The study is focussing on the following points: the characterization of the structures in solution, their stabilization using surfactants, the random coil- α -Helix transition in the polypeptide block and the influence of added substances on the system. The results show: the affinity of each polymer to the solvent depends strongly on the block length ratio. The pH induced transition from the random coil to α -helix seems to be between 10-11 and induces a significant decrease in the translational diffusion coefficient. The addition of water or benzoic acid to the organic solutions induces structural changes.

CPP 12.11 Tue 17:00 P3

Control of forces in aqueous wetting nanofilms — ●KATARZYNA CIUNEL¹ and REGINE V. KLITZING² — ¹Stranski-Laboratorium, TU Berlin, Str. d, 17. Juni 112, D-10623 Berlin — ²Institut für Physikalische Chemie, CAU Kiel, Ludewig-Meyn-Strasse 8, D-24118 Kiel

The (de)stability and functionality of thin liquid films plays an important role for processes in technical applications, like foaming, emulsifica-

tion and flotation. 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 (disjoining pressure vs. film thickness) and it is measured by varying the outer pressure in a so-called thin film pressure balance. The approach of a solid substrate to one film interface (wetting film: air/water/solid) changes the drainage behaviour with respect to a free-standing film (foam film). In order to modify the interactions between the fluid and the interface in a wetting film the solid surface is pre-coated with polyelectrolytes of different charge and viscoelasticity. The air/water interface is varied by the adsorption of different amphiphiles. The results give a clear evidence for negative charges at the free air/water interface.

CPP 12.12 Tue 17:00 P3

Is the radial breathing mode really radial? — •M. MOHR, M. MACHÓN, and C. THOMSEN — Institut für Festkörperphysik, TU Berlin, Hardenbergstr. 36, 10623 Berlin

The diameter-dependent radial breathing mode (RBM) plays a key role in the characterization of single-walled nanotubes. This mode is often assumed to be purely radial. *Ab initio* calculations of the phonons have shown the existence of a non-radial component which is small but has important effects, e.g. in the electron-phonon coupling.¹ A simple geometrical model based on symmetry considerations shows similar results.² We demonstrate with an independent variational approach that the RBM is not radial and study the dependence of the non-radial component on diameter and chirality.

[1] M. Machón *et al.* Phys. Rev. B **16** 035416 (2005)

[2] M. Damnjanović *et al.*, J. Phys.: Condens. Matter **16** (2004) L505

CPP 12.13 Tue 17:00 P3

Electric fields effects in thin films of symmetric diblock copolymers — •XIULI JIANG¹, THOMAS GUTBERLET², MUKUL GUPTA², THOMAS GEUE², and THOMAS THURN-ALBRECHT¹ — ¹Department of Physics, Martin-Luther-University, Halle, Germany — ²Laboratory for Neutron Scattering, ETH Zürich & PSI, Villigen, Switzerland

Due to their potential use as nanostructure templates, it is of significant interest to control the orientation and order of the microstructure of block copolymers by means of external fields. Using neutron reflectivity, diffuse scattering and small angle scattering we analysed the microstructure of a lamellar diblock copolymer under competing influences of interfacial interactions and an electric field standing perpendicular to the surface of the film. While the electric field tends to align the lamellar normal to the substrate, interfacial interactions favour an alignment parallel to the film. In this situation a field, too weak to overcome the interfacial interactions which is typically limited to a range of about lamellar periods, leads to a reduction of the defects at the boundaries between domains of different orientations, and in consequence to a complete alignment of the microphase structure parallel to the substrate. Otherwise, due to the confinement the torque exerted by the electric field leads only to a small increase of the mosaicity of the sample, which is reflected by a considerable increase in the diffuse scattering signal. Finally a field of several ten kV/mm is necessary to align the central part of the film with boundary layers parallel to the interfaces remaining even at these high fields.

CPP 12.14 Tue 17:00 P3

Electric Field induced Effects on the Microdomains in Concentrated Block Copolymer Solutions — •KRISTIN SCHMIDT¹, HEIKO SCHOBERTH¹, THOMAS M. WEISS², VOLKER URBAN³, PETER LINDNER⁴, ALEXANDER BÖKER¹, and GEORG KRAUSCH¹ — ¹Lehrstuhl für Physikalische Chemie II, Universität Bayreuth, D-95440 Bayreuth, Germany — ²European Synchrotron Radiation Facility (ESRF), F-38043 Grenoble, France — ³Oak Ridge National Laboratory (ORNL), Oak Ridge, TN-37831, USA — ⁴Institut Laue Langevin (ILL), F-38043 Grenoble, France

We investigate the microscopic mechanism of reorientation of concentrated block copolymer solutions exposed to an electric field by time-resolved synchrotron small-angle X-ray scattering (SAXS). As a model system, we use a lamellar polystyrene-*b*-polyisoprene block copolymer dissolved in toluene. The underlying mechanism at the level of individual macromolecules is studied by small-angle neutron scattering (SANS). Depending on the electric field strength we observe a decrease of the lamellar distance of lamellae orientated parallel to the E-field. Through the parallel orientation of the lamellar plane, the polymer backbones orient perpendicular to the E-field lines. We therefore expect that the

diblock chains exhibit a certain degree of stretching. Hence, we study the single-chain form factor of the copolymer exposed to an electric field.

In addition, we observe an influence of the electric field on the order disorder temperature and phase separation in our block copolymer solutions. We found a significant shift in T_{ODT} at moderate field strengths. For further investigations we study this effect by birefringence.

CPP 12.15 Tue 17:00 P3

Analysis of Self Assembled Monolayers (SAMs) on metallic substrates by — •P. ANGELOVA¹, M. GENSCHE², K. HINRICHS², K. KOSTOVA¹, and D. TSANKOV¹ — ¹Institute of Organic Chemistry, Bulgarian Academy of Sciences, Acad. G. Bonchev Str. Bl. 9, 1113 Sofia, Bulgaria — ²ISAS-Institute for Analytical Sciences, Department Berlin, Albert Einstein Str. 9, 12489 Berlin, Germany

Long-chain alkanethiols and disulfides tend to adsorb onto metallic surfaces and to form closely packed and well ordered monomolecular films. Besides adsorption, the self-assembly also includes spontaneous self-organization of the molecules constituting the film, mostly by means of van der Waals interactions. Essential role in forming highly ordered films has the type of the molecules which affects the intermolecular distance and the degree of orientation. Newly synthesized para-substituted benzyl esters of 16-mercaptohexadecanoic acid, containing NO₂, CN, OCH₃ and Cl as substituents were prepared as SAMs on different metallic substrates (Au, Ag, Pd) and investigated by IR ellipsometry. The specific stretching vibrations of the indicator groups were used for identifying of the film orientation. Particularly useful were the stretching vibrations of the NO₂ group and the respective optical simulations are presented. As input data for the simulations served vibrational parameter derived from previously investigated Langmuir-Blodgett films. The determination of thickness and dependence of the ellipsometric spectra on the average orientation of the vibrational transition moments of the NO₂ groups in the films with aligned molecules is addressed.

CPP 12.16 Tue 17:00 P3

Essential Parameters of PS-*b*-P4VP Nanotemplates Development for Applications — •YIMING SUN¹, RADIM KRENEK¹, GANNA GORODYSKA¹, ALEXANDER SIDORENKO², and MANFRED STAMM¹ — ¹Leibniz-Institut für Polymerforschung e.V., Dresden, Germany — ²Bell Labs, Lucent Technologies, Murray Hill, USA

Block copolymer nanotemplates demonstrate a cheap and prospective way for nanodevices requiring regular patterns of closely packed asymmetric nanodomains (nanowires) of various materials on various substrates. Many application based on electrodeposition or PVD of metals and their alloys, electrochemical polymerization and other kinds of loading can be taken into account. Here we deal with essential parameters for the nanotemplate deposition improving ordering and varying periodicity of the nanotemplates. The nanotemplates are based on self-assembly of poly(styrene-*block*-4-vinylpyridine) (PS-*b*-P4VP) with low molar mass additive 2-(4-hydroxyphenylazo)benzoic acid (HABA). Various morphologies may be formed, depending on ratio of molecular weights of the blocks, with a characteristic scale of nanodomains of about 10 nm. We show that ordering of patterns may be improved by a combination of slow vapour annealing and low roughness of substrates (ITO glass, Si and mica). Variation of periodicity was studied in respect to stoichiometric ratio of HABA in the assembly.

CPP 12.17 Tue 17:00 P3

Controlled Surface Design of Nanoparticles via Switchable Polymer Brushes — •NIKOLAY HOUBENOV¹, SERGIY MINKO², ALEXANDER SIDORENKO³, PETRA UHLMANN¹, and MANFRED STAMM¹ — ¹Leibniz-Institut fuer Polymerforschung Dresden e.V., Germany — ²Clarkson University Potsdam, New York — ³Bell Labs, Lucent Technologies, Murray Hill, USA

Switchable multicomponent grafted polymer films (polymer brushes) can be successfully used to control the spatial position of nanoparticles of various size and nature. We applied different methods for creating surface patterns, as adsorption via dynamic wetting (by settling the substrates at different angles) of 10-100 nm charged latex particles, or plasma deposition of golden clusters (2-5 nm total film thickness), on stimuli responsive polymer brushes. It was shown, that via controlled surface arrangement, one is able to create long-ranged arrays of nanoparticles, with a characteristic lateral distance, which is a function of the physical-chemical properties of the particles and the polymer brushes. Changing the chain conformation of the grafted PAA-P2VP, PI-P2VP or PS-P2VP brush-like layers by external stimuli, we observed a disarrangement at the particles

stripes location from a range of few nanometers to sub-microscopic scale. Such an altering of the quality of the surrounding medium creates a memory effect on the material surface by continuous revealing or concealing (replacing) the particles (clusters).

CPP 12.18 Tue 17:00 P3

Importance of boundary conditions for fluctuation forces between colloids — ●HARTWIG LEHLE^{1,2} and MARTIN OETTEL^{1,2} — ¹Max Planck Institut für Metallforschung, Heisenbergstraße 3, 70569 Stuttgart — ²ITAP, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart

We consider rotationally symmetric colloids trapped at a fluid interface and subjected to thermal movement. Due to the constraints the colloids impose on the spectrum of the capillary waves the free energy becomes dependent on colloid-colloid separation leading to a thermal Casimir force. The free energy is calculated in a functional integral approach. We present two distinct schemes to calculate the partition function elucidating the importance of the various boundary-type dependent contributions to the Casimir force. The long-range behaviour of the Casimir force can be expressed in terms of multipole interactions of auxiliary “charge fields” on the colloids. The resulting force is shown to be long-range, $F \sim -1/(d \log(d))$ in the case of fixed colloids and a pinned contact line. If the colloid position or the contact line are also fluctuating, additional competing terms induce a cancellation of the leading terms. For a pinned contact line and fluctuating colloid heights the leading contribution to the interaction is of dipole-dipole ($\sim -1/d^4$), for a fluctuating contact line of quadrupole-quadrupole ($\sim -1/d^8$) character.

CPP 12.19 Tue 17:00 P3

Effects of the bead-surface interaction on the restricted rotational dynamics of nonrigid immobilized macromolecules. — ●ALEXANDER UVAROV and STEPHAN FRITZSCHE — Universität Kassel, D-34132 Kassel, Germany

Many problems in biophysics involve the rotational motion of macromolecules which immersed in solution. Well-known examples refer to dielectric relaxation, nuclear magnetic relaxation as well as to the depolarization of the fluorescence light. During the past decade, therefore, a large number of experiments and dynamic simulations (DS) have been carried out in order to describe the rotational properties of biomolecules. Apart from free macromolecules in solution, some experiments also concerned the restricted mobility of macromolecules which are immobilized on a surface and which are interpreted in terms of their molecular subsystems, the so-called *beads* of the macromolecule [1].

In the present contribution, we explore the question of how the bead-bead as well as bead-surface interaction affects the (restricted) rotational diffusion of molecules immobilized at a surface. Making use a recently derived Diffusion equation [1], we performed detailed computations for the orientational correlation functions and the rotational diffusion coefficient of the macromolecule for several types of the bead-bead and bead-surface interaction potentials. Results from our theory will be compared with other computations including the Brownian DS of the macromolecule [2].

[1] A. Uvarov and S. Fritzsche, *J. Chem. Phys.* **121**, 6561, (2004)

[2] B. Carrasco, G. de la Torre, *Biophys. Journal* **75**, 3044, (1999).

CPP 12.20 Tue 17:00 P3

Experimental and theoretical investigation of vibrational modes in ringing gels — ●ERIK JÄRMSTORP, BARBARA DROSSEL, and RUDOLF FEILE — Institut für Festkörperphysik, Technische Universität Darmstadt, Hochschulstr., 64289 Darmstadt

Ringing gels exhibit a strong acoustic emission of sound waves when they are excited by knocking onto the containers they were prepared in. This distinguishes them from other gels, which do not show this ringing sound. To start a detailed investigation of the physical basis of the phenomenon we have investigated the vibrational modes of silica gels which show this ringing behaviour. Experimentally, we have developed a non-contact method using the reflection of a laser beam to study the oscillatory motion of the gel surface within a cylindrical container. This method allows a clear separation of gel modes from other acoustic emissions caused by the specific excitation process (knocking) and the experimental set-up which was not possible in former experiments [1]. We were also able to study the time development of the gelation process. Theoretically, we solved the wave equation of motion for vector displacements of volume elements according to the boundary conditions for the experimental set-up in cylindrical symmetry. The results are compared with a scalar ansatz presented in [1], and are discussed in respect to

the experimental results. The results from the gelation experiments are compared with different models for the microscopic processes involved in the gelation.

[1/ C. Sinn, *J. Non-Cryst. Solids* **347**, 11-17 (2004)

CPP 12.21 Tue 17:00 P3

Brillouin and ultrasonic study of the gelation of ringing silica gels — ●BENJAMIN DÖNIGUS, ANDREAS KÖHLER, OLIVER MESETH, and RUDOLF FEILE — Institut für Festkörperphysik, Technische Universität Darmstadt, Hochschulstr. 8, 64289 Darmstadt

Ringing gels are distinguished from other gels by a strong acoustic emission of sound waves excited by knocking onto the containers they were prepared in [1]. Brillouin and ultrasonic experiments were performed on the influence of the microscopic network formation on the elastic properties of the bulk gel during the gelation and further aging process. We find a reduction of the speed of sound when the gelation proceeds. The decrease of the sound velocity is compared with existing theoretical predictions [2,3]. Additionally, both experimental methods indicate a two-step process in the gelation.

[1/ C. Sinn, *J. Non-Cryst. Solids* **347**, 11-17 (2004), and references therein

[2/ M.A. Biot, *J. Acoust. Soc. Am.* **28**, 168 (1956); **28**, 179 (1956); *J. Appl. Phys.* **33**, 1482 (1962)

[3/ D. L. Johnson, *J. Chem. Phys.* **77**, 1531-1539 (1982)

CPP 12.22 Tue 17:00 P3

Structure and dynamics of confined charged colloids — ●MADELEINE KITTNER¹ and PD DR. RER. NAT. SABINE KLAPP^{1,2} — ¹TU Berlin, Theoretische Chemie - Stranski-Lab, Strasse des 17. Juni 135, 10623 Berlin — ²TU Berlin, Theoretische Physik, Hardenbergstr. 36, 10623 Berlin

We investigate the structure and dynamics of charged colloids confined by two plane-parallel repulsive walls (slit pore), using Molecular Dynamics Simulations (MD) in a canonical ensemble. The colloidal system is described by a purely repulsive soft-sphere-Yukawa potential, that involves only the screened spherical macromolecules. The range of repulsion is controlled by the Yukawa parameter κ which, in real systems, is determined by the ionic strength or the charge density.

Our MD results show that an increase of the repulsion range (i.e., decrease of κ) yields an increase of the components of the pressure tensor, particularly in the direction normal to the walls. This is consistent with the behavior of the density profiles, which are highly structured for small κ especially in narrow pores. On the other hand, considering the translational dynamics parallel to the walls, we observe that decrease of the range of repulsion leads to decreasing pore-averaged diffusion constants. We also investigate the inhomogeneity of the dynamics induced by the layer formation.

CPP 12.23 Tue 17:00 P3

Self-Assembly of Inorganic and Biological Nanoparticles at Fluid Interfaces: Kinetics and Structure Formation — ●SERGEJ KOUTOUZOV, GÜNTHER JUTZ, MICHAELA HOFFMANN, and ALEXANDER BÖKER — Lehrstuhl für Physikalische Chemie II, Universität Bayreuth, 95440 Bayreuth, Germany

We report on the self-assembly processes of photoluminescent CdSe nanoparticles and fluorescently labeled CPMV bionanoparticles at oil/water liquid interfaces and their ability to stabilize so-called Pickering emulsions. The adsorption kinetics and particle density at the interface were followed by the changes in interfacial tension during the particle segregation to the interface using a pendant drop tensiometer. In addition, we monitored the increase in luminescence or fluorescence light emission from the interface via 2-dimensional spectroscopy, which allows for a time resolved direct determination of the particle concentration gradient at the interface. Concentration as well as size dependence of the nanoparticle diffusion to the interface was investigated using the above mentioned methods. Finally, the morphology of the resulting aggregates was investigated using TEM.

CPP 12.24 Tue 17:00 P3

Capillary-induced interactions between colloids at an interface — ●MARTIN OETTEL^{1,2}, ALVARO DOMINGUEZ³, and SIEGFRIED DIETRICH^{1,2} — ¹MPI für Metallforschung, Heisenbergstr. 3, 70569 Stuttgart, Germany — ²ITAP, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart — ³Física Teórica, Universidad de Sevilla, Apartado 1065, 41080 Sevilla, Spain

Within a general framework we study the effective, deformation-induced interaction between two colloids trapped at a fluid interface. For mechanically non-isolated systems, the effective interaction is logarithmic in the separation d , for isolated systems it follows a shorter-ranged power-law. As an application, we consider the interface deformation owing to the electrostatic field of charged colloids. Both the attractive, effective interaction and the direct electrostatic repulsion decay as d^{-3} . An attractive minimum in the total potential at intermediate separations is possible only for large enough colloidal charges.

CPP 12.25 Tue 17:00 P3

Luminescence of $ZnMnP_2O_7$ clusters in powders of KBr — ●OLGA GOMENYUK¹, SERGIY NEDILKO¹, IRYNA NEDEYLKO¹, OLEXANDER SLEPTSOV¹, VASIL SCHERBATSII¹, NADIJA ANTRAPTEVA², VOLODYMYR BOJKO², and NADIJA TKACHOVA² — ¹Taras Shevchenko Kyiv National University, Department of Physics., 2, block 1, Acad. Glushkova ave., Kyiv 03680, Ukraine — ²National Agriculture University, Geroiv Oborony st., 8, Kyiv 03041, Ukraine

Diphosphates of divalent metals (zinc, manganese) are the object of interest as multifunctional materials. The contents of cations in solid solutions, their physical, e.g. optical and luminescent properties are determined by the composition of initial reagents. Mentioned compounds were synthesized by precipitation of the suitable cations. Luminescence properties were investigated in the spectral region from 50 to 1100 nm at 4.2, 10, 77 and 300 K temperatures using visible, ultraviolet and vacuum ultraviolet (synchrotron) radiation for excitation of luminescence. Structure and peak positions of the luminescence bands depend on the samples temperature and excitation wavelength. The bands were considered as caused by both inner transitions in manganese ions, recombination of the self trapped excitons and emission of defects. Dependences of the luminescence intensity on the composition of the mentioned phosphates and their content in KBr are analyzed. Experiments with of synchrotron radiation use were done at SUPERLUMI, HASYLAB, Germany.

CPP 12.26 Tue 17:00 P3

The x-ray small angle scattering setup at beamline 9 at the synchrotron source DELTA, University of Dortmund: Measurements on Lysozyme solutions — ●CHRISTOF KRYWKA¹, CHRISTIAN STERNEMANN¹, NADEEM JAVID², ROLAND WINTER², and METIN TOLAN¹ — ¹Institute of Physics / DELTA, University of Dortmund, D-44221 Germany — ²Institute of Chemistry, University of Dortmund, D-44221 Germany

The physical and chemical properties of proteins are influenced by their aqueous microenvironment. Dynamics of folding and aggregation processes play an important role in conformational diseases (e.g. Alzheimer, Parkinson). It was shown that the latter processes are in fact influenced by the type and concentration of cosolvents. As a part of our immune system Lysozyme breaks carbohydrate chains, destroying the structural integrity of bacteria cell wall. Small-angle X-ray scattering (SAXS) measurements on aqueous solutions of Lysozyme were performed in a wide range of concentrations and in presence of different types of cosolvents, typical for conditions where unfolding sets in within cells. We determined the effects of cosolvents on the unfolded state structures and aggregated structures. From the measured structure factors information about the structure of the hydration shell and, for the higher concentrated samples, information about the intermolecular interaction potential can be obtained.

CPP 12.27 Tue 17:00 P3

Absorption spectra for light-harvesting systems using non-Markovian as well as modified Redfield master equations — ●M. SCHRÖDER, M. SCHREIBER, and U. KLEINEKATHÖFER — Institut für Physik, Technische Universität Chemnitz, 09107 Chemnitz

Circular aggregates are studied to model the B850 ring of bacteriochlorophylls within the LH2 complex of purple bacteria. The spectral density which describes the coupling strength and frequency dependence of the interaction between the ring system and the environment has recently been determined by ab initio calculations [1]. Starting with a quantum master equation one can develop a formula for the frequency-domain absorption spectra [2]. Often one decouples the population dynamics from that of the coherences (secular approximation) and neglects memory effects (Markov approximation) in this procedure. Here we will investigate these approximations in some more detail as well as the influence of the form of the spectral density and static disorder using Monte Carlo methods. The calculations will be made using a numerical de-

composition of the spectral density and different formalisms to treat the memory effects: time-local and time-nonlocal approaches as well as the modified Redfield method [3].

- [1] A. Damjanović, I. Kosztin, U. Kleinekathöfer, and K. Schulten, Phys. Rev. E **65**, 031919 (2002).
 [2] F. Neugebauer, D. Malzahn, and V. May, Chem. Phys. **201**, 151 (1995).
 [3] W.M. Zhang, T. Meier, V. Chernyak, S. Mukamel, J. Chem. Phys. **108**, 7763 (1998)

CPP 12.28 Tue 17:00 P3

Characterization of Short-lived Radicals of Purine Bases in Aqueous Solution by Magnetic Resonance — ●ALEXEY KIRYUTIN^{1,2}, KONSTANTIN IVANOV², and HANS-MARTIN VIETH¹ — ¹Department of Physics, Free University of Berlin, Arnimallee 14, D-14195 Berlin, Germany — ²International Tomography Center of SB RAS, 630090, Institutskaya 3a, Novosibirsk, Russia

The structure of nucleotide radicals and their properties can be examined by the effects of chemically induced dynamic nuclear polarization (CIDNP) created in reversible photoreactions between nucleotides and suitable organic dye molecules. The CIDNP spectra with microsecond time resolution were obtained in photoreactions between purine bases and several dyes. Usually radical reactions such as protonation, deprotonation and termination occur on the microsecond time scale. The intensity and sign of the CIDNP at the aromatic protons of adenosine 5'-monophosphate and guanosine 5'-monophosphate (AMP, GMP) was studied depending on the dye and pH value of aqueous solution. From the shape of CIDNP spectra different nucleotide radicals were identified. For GMP and AMP the CIDNP was measured at variable magnetic field (0-7 T). From simulation of these field dependencies g-factors of the short-lived neutral, anionic and cationic forms of the nucleotide radicals were determined. These results contribute to the understanding of radical formation of nucleotides. In addition, the use of CIDNP effects for studying the structure of nucleic acids and the mobility of their bases will be discussed.

CPP 12.29 Tue 17:00 P3

Electron and Hydrogen Transfer Reactions in the Photolysis of Aromatic Amino Acids Studied by CIDNP — ●KARSTEN MIESEL and HANS-MARTIN VIETH — Department of Physics, Free University of Berlin, Arnimallee 14, D-14195 Berlin, Germany

The near UV photolysis of N-acetyl tyrosine (NATyrOH) and N-acetyl tryptophan (NATrpH) in aqueous solutions was investigated by field dependent chemically induced dynamic nuclear polarisation (FD-CIDNP) and its time dependence in high magnetic field (TR-CIDNP). For both amino acids, ionisation is most efficient in basic solutions yielding a solvated electron (e^-_{aq}) and the amino acid radicals NATyrO• and NATrpH•+. As the primary event, monophotonic ionisation occurring from singlet excited precursors is identified, leading to a characteristic maximum in their CIDNP field dependencies. Simulations of the field dependencies allowed the determination of g-factors of the amino acid radicals. Concomitantly, some side reactions were investigated, such as decarboxylation and the formation of L-DOPA in the photolysis of tyrosine. The radical precursors are identified and a reaction scheme is presented. The observation of strong ¹H-CIDNP on the solvent peak (HDO) in the photolysis of NATyrO⁻ is attributed to H-transfer between the o-benzosemiquinone radical and NATyrO•, and subsequent deprotonation of NATyrOH. An equivalent mechanism is proposed to occur in the photolysis of NATrpH.

CPP 12.30 Tue 17:00 P3

Secondary Structure Analysis of Synthetic Spider Silk Proteins by Fourier Transform Infrared Spectroscopy — ●MICHAEL TAMMER¹, PATRICK KÖLSCH¹, UTE SLOTTA², THOMAS SCHEIBEL², and FRIEDRICH KREMER¹ — ¹Universität Leipzig, Institut für Experimentelle Physik I, Linnestr. 5, 04103 Leipzig — ²Lehrstuhl für Biotechnologie, Technische Universität München, Lichtenbergstr. 4, 85747 Garching

Silk fibers produced by spiders for their web are extremely thin, lightweight, extendible and very strong. The combination of strength and stretchiness of this material gives a toughness comparable to that of high-tensile steel. Therefore several attempts has been done so far to produce artificial fibres spun from dope solutions composed of genetically modified natural proteins, designer proteins or protein-plastic blends.

In the contribution synthetic silk constructs based on the primary

structure elements of the garden spider's (*Araneus diadematus*) major dragline silk proteins ADF-3 and ADF-4 are investigated by polarized FTIR spectroscopy. Thin films were prepared by spincoating a protein solution with one or more components forming a silk dope. IR spectra of these films and after solvent treatment with methanol or potassium phosphate were recorded. By analyzing the amide I absorbance band the secondary structure for the proteins of all samples are deduced. The treatment was found to emphasize beta-sheet conformations at the expense of alpha-helix and turn structures.

CPP 12.31 Tue 17:00 P3

Electron and Hydrogen Transfer Reactions in the Photolysis of Aromatic Amino Acids Studied by CIDNP — ●KARSTEN MIESEL and HANS-MARTIN VIETH — Department of Physics, Free University of Berlin, Arnimallee 14, D-14195 Berlin, Germany

The near UV photolysis of N-acetyl tyrosine (NATyrOH) and N-acetyl tryptophan (NATrph) in aqueous solutions was investigated by

field dependent chemically induced dynamic nuclear polarisation (FD-CIDNP) and its time dependence in high magnetic field (TR-CIDNP). For both amino acids, ionisation is most efficient in basic solutions yielding a solvated electron (e^-_{aq}) and the amino acid radicals NATyrO• and NATrph•+. As the primary event, monophotonic ionisation occurring from singlet excited precursors is identified, leading to a characteristic maximum in their CIDNP field dependencies. Simulations of the field dependencies allowed the determination of g-factors of the amino acid radicals. Concomitantly, some side reactions were investigated, such as decarboxylation and the formation of L-DOPA in the photolysis of tyrosine. The radical precursors are identified and a reaction scheme is presented. The observation of strong ^1H -CIDNP on the solvent peak (HDO) in the photolysis of NATyrO⁻ is attributed to H-transfer between the o-benzosemiquinone radical and NATyrO•, and subsequent deprotonation of NATyrOH. An equivalent mechanism is proposed to occur in the photolysis of NATrph.

CPP 13 POSTER New Experimental Techniques

Time: Tuesday 17:00–19:00

Room: P3

CPP 13.1 Tue 17:00 P3

Measurements of interfacial viscoelasticity with the quartz crystal microbalance: influence of acoustic scattering from a small crystal-sample contact — ●ALEXANDER MARTIN KÖNIG, MATHIS DÜWEL, BINYANG DU, MIRIAM KUNZE, and DIETHELM JOHANNSMANN — Institute of Physical Chemistry, Clausthal University of Technology, Arnold-Sommerfeld-Str. 4, D-38678 Clausthal-Zellerfeld

We discuss the influence of the limited contact size on measurements of high-frequency interfacial viscoelasticity performed with a combination of the quartz crystal microbalance (QCM) and the Johnson-Kendall-Roberts (JKR) apparatus. In this instrument, a sphere-plate contact is established between an elastomeric lens and a quartz resonator. The analysis is carried out in the frame of the sheet-contact model, which states that the shift of resonance frequency and bandwidth both are proportional to the contact area as long as the contact area is much smaller than the crystal itself. In particular, the ratio of the shift in bandwidth and the shift in frequency (termed D-f ratio) is predicted to be constant and independent of geometry. However, the experiment does show a slight increase of the D-f ratio with contact radius when the contact radius is comparable to the wavelength of sound inside the crystal. This effect can be explained by acoustic scattering.

CPP 13.2 Tue 17:00 P3

High sensitiv AC chip calorimetry for nanogram samples — ●H. HUTH, A. MINAKOV, and C. SCHICK — University of Rostock, Institute of Physics, Universitätsplatz 3, 18051 Rostock, Germany

The combination of silicon technology and calorimetry opens up new possibilities. Thin film calorimeter allow heating and cooling at rates up to 10.000 K/s. For several fast crystallizing polymers it is possible to prevent crystallization on cooling totally and to reach the amorphous glassy state. But often one would prefer to measure thermal properties of small samples at or at least close to thermodynamic equilibrium. This can be achieved by a combination of chip calorimetry and AC calorimetry at slow scanning or at constant bath temperature. The frequency chosen provides a well defined time scale of the experiment. A direct comparison with results from other dynamic methods like dielectric spectroscopy is possible. Based on a differential AC-calorimeter we show an improved experimental setup combining the advantages of the different methods already described. Not only a high sensitivity in the pico Joule per Kelvin range is achieved but AC measurements at relative high frequencies are possible too. As another application the combination of both methods is possible where one can prevent crystallization by very fast cooling before following of the crystallization at temperatures below the maximum crystallization temperature using the AC measurement technique. The AC technique allows the investigation of crystallization at very slow rates not easy achievable by fast scanning also in thin films of semicrystalline polymers. Measurements on small samples of semicrystalline polymers are presented.

CPP 13.3 Tue 17:00 P3

The role of heat conducting walls in transient grating experiments — ●MARIANNE HARTUNG and WERNER KÖHLER — Physikalisches Institut, Universität Bayreuth

Laser-induced dynamic gratings are frequently employed for the measurement of heat conduction, Fickian diffusion and thermodiffusion in simple liquids and polymer solutions. We have analyzed experimentally and theoretically the systematic errors, which are caused by departures from one-dimensional heat conduction and diffusion. While the measured thermal diffusivities possibly have to be corrected for systematic errors, non one-dimensional mass diffusion has no effect on the experimentally determined mass and thermal diffusion coefficient.

M. Hartung, W. Köhler, Eur. Phys. J. E 17, 165 (2005)

CPP 13.4 Tue 17:00 P3

Ultra-fast scanning calorimetry of Poly(butylene terephthalate) — ●ALEXANDER MINAKOV^{1,2} and CHRISTOPH SCHICK² — ¹Natural Science Research Center, A.M. Pokhrov General Physics Institute, Vavilov st. 38, 119991 Moscow, Russia — ²University of Rostock, Department of Physics, Universitätsplatz 3, D-18051 Rostock, Germany

Ultra-fast scanning calorimetry (including controlled ultra-fast cooling) was applied to study crystallization and melting-reorganization processes in 40 ng Poly(butylene terephthalate) (PBT) sample at the scanning rates up to 100000 K/s. We have found that the cold crystallization cannot be completely prevented in such sample even at the rates ca. 1000 K/s. The totally amorphous PBT sample can be obtained only at the rates ca. 10000 K/s. The melting-reorganization process was observed as follows. The sample was molten up to 350K with the rate 1000 K/s and cooled down to crystallization temperature with the same rate. The crystallization at 100 C, 130 C and 150 C was performed (3 min was enough for complete crystallization). Then the sample was cooled down to 24 C with the rate 1000 K/s. Next the melting-recrystallization curves were measured at the heating rates in the range 1000 - 40000 K/s. In the first case, the reorganization cannot be totally prevented even at 20000 K/s. We have found that few milliseconds were enough for recrystallization during fast heating after melting. In the sample crystallized at 130 C the recrystallization was prevented completely at the rate 10000 K/s, and at 5000 K/s in the sample crystallized at 150 C. We have found that 1 ms was not enough for reorganization in this case.

CPP 13.5 Tue 17:00 P3

Dynamic Structure Factor of Different Systems of Polymers — ●MICHAEL STRAUCH and EKKEHARD STRAUBE — Martin-Luther-Universität Halle-Wittenberg, Fachbereich Physik, Fachgruppe Theoretische Physik, Von-Seckendorff-Platz 1, D-06120 Halle (Saale)

In this poster we present our investigations concerning the dynamic structure factor $S_q(t)$ in different systems of polymer chains.

In a first step, we have calculated the dynamic structure factor for a chain with randomly distributed friction coefficients ξ_i and spring constants k_i , thus generalising the result of the well-known ROUSE model. In the more general case, the analysis can only be done numerically.

Furthermore, we have considered a network of polymer chains. In this

case, one expects a finite value of $S_q(t)$ for large times because the correlations between the chain segments do not completely vanish.

Finally, we compare our results with those of DE GENNES where the chain dynamics are basically described as a purely longitudinal diffusion along the chain.

CPP 13.6 Tue 17:00 P3

New fast calorimeter for intermediate scanning rates — ●SERGEY ADAMOVSKY and CHRISTOPH SCHICK — Universität Rostock, Institut für Physik, Universitätsplatz 3, 18051 Rostock

For thermal measurements there are very sensitive differential scanning calorimeters available. The problem is that only relatively slow processes can be studied using a commercial device: heating rates of more than 300 K/min (5 K/s) are hardly reachable. On the other side, ultra-fast calorimetry was developed in the last years. These devices are suitable for very small samples and their heating rates only start at about 100K/s. So there was a gap from 5 K/s to 100 K/s. To cover this middle-range a new calorimeter was developed. The sensor is a 0.15 mm thick glass slide (a microscope cover slip was used); a Ni-heater and a Cu-Constantan (Type "T") thermocouple were deposited on the glass. The sensor is connected to a computer-controlled amplifier.

Application of the calorimeter for polymer materials is presented. Drying and solidification of modern paints as well as crystallization study of polymeric materials are presented.

CPP 13.7 Tue 17:00 P3

Pyroelectric tomography: Non-destructive 3D mapping of polarization profiles in poled polyvinylidene fluoride copolymer sensor cables — ●ROSaura FLORES SUÁREZ, MICHAEL WEGENER, WERNER WIRGES, and AXEL MELLINGER — Department of Physics, University of Potsdam, Am Neuen Palais 10, 14469 Potsdam

The copolymers of polyvinylidene fluoride (PVDF) with trifluoroethylene are very attractive for sensor applications because they do not need to be stretched in order to become piezoelectric and may therefore be directly coated onto substrates or wires. P(VDF-TrFE) sensor cables may be used in such applications as traffic control or intruder monitoring in which their flexibility and rigidity as well as their rather high load tolerance are essential. In the present work, 3D polarization profiles in poled P(VDF-TrFE) sensor cables (diameter approx. 1.1 mm, thickness of the active layer approx. 200 μm) were measured by means of the focused thermal-pulse (TP) method [1] with a lateral resolution of 44 μm . The relatively high data acquisition speed allowed the recording of up to 2 kPixels of in-plane data. The investigated sensor cables included samples poled with an industrial 4-needle corona setup, as well as samples poled under laboratory conditions using a single needle at voltages of -25 kV and -60 kV under different atmospheres (air and SF₆, respectively). By studying the polarization "footprints" of the corona needles, optimum poling geometries could be deduced.

[1] A. Mellinger, R. Singh, M. Wegener, W. Wirges, R. Gerhard-Multhaupt and S. B. Lang, Appl. Phys. Lett. **86**, 082903 (2005).

CPP 13.8 Tue 17:00 P3

High NA UV digital in-line holography — ●MARTINA SCHÜRMAN¹, HANS JÜRGEN KREUZER², MICHAEL GRUNZE¹, and AXEL ROSENHAHN¹ — ¹Angewandte Physikalische Chemie, Universität Heidelberg, 69120 Heidelberg — ²Department of Physics and Atmospheric Science, Dalhousie University, Halifax, Nova Scotia B3H 3/5, Canada

Holography is a lensless imaging technique with intrinsic three-dimensional properties. The radial divergence of spherical waves enables the acquisition of a magnified image of the sample. Unlike conventional microscopy, the method does not require lenses. The achievable resolution thus only depends on the wavelength of the light and the detection angle. With short wavelengths tiny objects can therefore easily be resolved. For the first time, UV laser light and a high numerical aperture setup were used in order to holographically enlarge transparent and opaque particles and characterize their imaging properties. Furthermore, fibroblast cells were imaged in order to explore future applications in biology. As the presence of the reference wave introduces the third dimension, first experiments demonstrating the three dimensional nature of the method are also shown. All results are compared to images obtained by conventional light microscopy.

CPP 13.9 Tue 17:00 P3

Imaging of surface and in depth modification of Polybutadiene (PBD) and silane-linked Polyethylenimine (PEI) films — ●MARTIN MICHEL¹, THORSTEN ANDRES¹, THORSTEN MEYER², BERND ZIMMERMANN², MANFRED NEUMANN², and ULRICH HEINZMANN¹ — ¹Molekül- und Oberflächenphysik, Fakultät für Physik, Universität Bielefeld — ²Elektronenspektroskopie, Fachbereich Physik, Universität Osnabrück

We present the characterization of surface-structured thin Polybutadiene (PBD) and Polyethylenimine (PEI) films by Atomic Force Microscopy (AFM) and Imaging Ellipsometry. The surfaces of those 70 nm thin films were modified by a plasma modification process, using square meshes as "in contact masks". To investigate the resulting structures we performed AFM and Imaging Ellipsometry. In contrast to AFM, Imaging Ellipsometry enabled imaging of "in depth" modifications of our surface structures. Such "in depth" modifications were also investigated in branched and unbranched silane-linked organic layers of PEI. Additionally both the PBD and PEI films have been characterized by X-Ray Photoelectron Spectroscopy (XPS). The experimental results will be presented in detail.

CPP 13.10 Tue 17:00 P3

Torsional Quartz Crystal Resonators Contacting the Sample Face-On: Technical Aspects and Application to the Film Formation Process — ●ALEXANDER MARTIN KÖNIG, BINYANG DU, and DIETHELM JOHANNSMANN — Institute of Physical Chemistry, Clausthal University of Technology, Arnold-Sommerfeld-Str. 4, 38678 Clausthal-Zellerfeld

Traditional AT-cut quartz crystal resonators operating in MHz range are extensively used to explore the interfacial properties of coatings. However, the penetration depth of the shear wave emanating from AT-cut resonators typically is hundreds of nanometers, limiting their applicability to thicker coatings. X-cut torsional resonator-operating in kHz range provide for a complementary approach. Here, the penetration depth is hundreds of micrometers. We report on the use of torsional resonators only contacting the sample across the front face of the cylinder. As we show, the equations for the analysis of AT-cut resonator measurements can be used in the same way for torsional resonators operated in this mode. In particular, the experimental results show that the Sauerbrey equation also holds for torsional resonators. This finding turns them into suitable devices for investigating the film-formation process. By varying the concentration of the colloidal dispersions and controlling the evaporation rate of the solvent, different mechanisms of film-formation were observed. The mechanism of film formation can be inferred from the evolution of frequency and bandwidth as a function of time. The film is formed via wet-sintering for slow evaporation, while for fast evaporation the film is formed via dry-sintering.

CPP 13.11 Tue 17:00 P3

Spectroscopic Ellipsometric Light Scattering: a Tool for the Detection of Anisotropic Layers on the Interface of Colloidal Particles — ●ARNE STARK¹, ANDREAS ERBE² und REINHARD SIGEL¹ — ¹Max-Planck-Institut of Colloids and Interfaces, D-14476 Golm — ²University of Leeds, Leeds, UK

The sensitivity of ellipsometric light scattering (ELS) to anisotropy is demonstrated by model calculations and experiments on lipid vesicles. ELS is the combination of light scattering with the polarization optics and nulling scheme of an ellipsometer. Similar to reflection ellipsometry it is sensitive on interface layers, however not on flat interfaces but at the interface of colloidal particles to the surrounding solvent. The presented model calculations based on Mie theory indicate a change of the information content with varying wavelength. In addition, a strong effect of the layer anisotropy on the signal is found. Experiments on lipid vesicles confirm the significant effect of anisotropy. We were able to determine the optical anisotropy of these vesicles. From this, it is possible to estimate the average tilt angle of the lipid chain in the vesicle.

CPP 13.12 Tue 17:00 P3

Interfacial strength of the contacts between glass spheres and a solid surface investigated by torsional and thickness-shear quartz resonators — ●BINYANG DU, ALEXANDER MARTIN KÖNIG, and DIETHELM JOHANNSMANN — Institute of Physical Chemistry, Clausthal University of Technology, Arnold-Sommerfeld-Str. 4, 38678 Clausthal-Zellerfeld

A torsional quartz resonator and a thickness-shear quartz resonator were used to study the interaction between a monolayer of glass spheres

and the resonator surface. The glass sphere induces a negative or a positive frequency shift, depending on the mass of the sphere m_s , the spring constant of the sphere-plate contact, κ_s , and the frequency of the resonator ω . This behaviour can be explained by the "Mass-Spring-Model".

[1] The sphere is considered as a second small resonator with a resonance frequency $\omega_s = (\kappa_s/m_s)^{1/2}$. For $\omega_s \gg \omega$, the spheres are rigidly attached to the crystal and behave like a Sauerbrey film. The frequency shift is negative. In the opposing limit of $\omega_s \ll \omega$, inertia holds the spheres in place. The sphere-plate contact increases the overall stiffness of the composite resonator and therefore increases the resonance frequency in proportion to the spring constant. Employing both thickness-shear resonators and torsional resonators and varying the sphere size, different regimes were mapped out. Interestingly, varying humidity of the environment changes κ_s as well as ω_s , leading to a cross-over from positive frequency shift to negative frequency shift. The results indicate that quartz resonators can probe interfacial capillary aging.

[1] G. L. Dybdal, Journal of Applied Physics 58, 2789 (1985)

CPP 13.13 Tue 17:00 P3

New methods for the characterisation of orientation in thin polymer films and application to light-induced anisotropy —

•CHRISTOPH JUNG¹, JOACHIM STUMPE², OLGA KULIKOVSKA², EMIEL PEETERS³, and BIANCA VAN DER ZANDE³ — ¹Lehrstuhl EPIV/ Prof. Dr. J. Köhler, University of Bayreuth, Universitätsstr. 30, 95447 Bayreuth, Germany — ²Fraunhoferinstitute of Applied Polymer Research, Geiselbergstr. 69, 14476 Potsdam, Germany — ³Philips Research Laboratories, Prof. Holstlaan 4, 5656 AA Eindhoven, The Netherlands

The recently developed method of Immersion Transmission Ellipsometry (ITE, patent pending) allows to fully characterise the absolute 3D refractive indices and the thicknesses of anisotropic films, which are thinner than the wavelength of the probing light, with high accuracy. The three-dimensional properties of anisotropic thin films are important for the display technology and optical data storage, predominantly. In addition, the method of waveguide spectroscopy is refined to explore the tilt gradient of thicker films in its profile. Different biaxial, tilted and

splayed films were generated by photo-orientation and photoalignment in the bulk of photochromic and liquid crystalline polymer films and subsequently characterised.

[1] C. C. Jung and J. Stumpe; Immersion transmission ellipsometry (ITE): a new method for the precise determination of the 3D indicatrix of thin films, Appl. Phys. B, 80, 231-238 (2005).

[2] C. C. Jung, J. Stumpe, E. Peeters, B. M. I. van der Zande; Novel way for Full Characterisation of Splayed Retarders using Wentzel-Kramers-Brillouin Method, Jpn. J. Appl. Phys., 44, 4000-4005 (2005).

CPP 13.14 Tue 17:00 P3

In situ study on the mechanisms of living polymerization via small angle neutron scattering and 1H NMR — •AIZHEN NIU¹, JOERG STELLBRINK¹, JUERGEN ALLGAIER¹, LUTZ WILLNER¹, DIETER RICHTER¹, BERND W. KOENIG², ROLAND P. MAY³, and L. J. FETTERS⁴ — ¹Institute für Festkörperforschung, Forschungszentrum, Jülich GmbH, 52425 Jülich, Germany — ²IBI-2, Forschungszentrum, Jülich GmbH, 52425 Jülich, Germany — ³Institute Lau-Langevin, F-38042, Grenoble, Cedex 9, France — ⁴School of Chemical and Biomolecular Engineering, Cornell University, Ithaca, NY 14853-5201

In this work for the first time a combined 1H-NMR and small angle neutron scattering in situ study of the anionic polymerization was performed. Both initiation and propagation phases were explored. This combined technique allows the structural and kinetic characteristics to be accessed and cross compared. The smaller aggregates contain most of the reacted monomer. Their structure changes from high functionality wormlike chains at early stages of the reaction to star-like aggregates where the crossover occurs at a degree of polymerization of 40. 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. The period when initiation and propagation occurred simultaneously was found to consist of three regimes where the initiation rate increased with time, the aggregation states of the living chains are decreasing with increasing rate.

CPP 14 Polymer Crystallization

Time: Wednesday 14:00–15:30

Room: ZEU Lich

CPP 14.1 Wed 14:00 ZEU Lich

Deformation and Fracture Mechanisms in Semicrystalline Polymers as revealed by Microfocus Synchrotron X-ray Scattering —

•NIKOLAOS ZAFEIROPOULOS¹, RICHARD DAVIES², CHRISTIAN RIEKEL², YONGFENG MEN³, JENS RIEGER³, and MANFRED STAMM¹ — ¹Leibniz-Institut für Polymerforschung Dresden, Hohe Strasse 6, 01069, Dresden — ²European Synchrotron Radiation Facility, BP 220, F-38043 Grenoble Cedex, France — ³BASF Aktiengesellschaft, Polymer Physics, 67056 Ludwigshafen, Germany

The fracture properties of polymers are one of the key parameters that define their service life and limit their applications. One of the most interesting and important questions is how the molecular architecture and the structure of polymers at nano-length scales influence their fracture properties. X-ray scattering is a powerful means of probing bulk structures at the nanometer scale. It can therefore provide a wealth of information relating to such structure-property relationships. In the present study, synchrotron radiation microfocus small and wide angle X-ray scattering is used to investigate the fracture mechanisms ahead of a crack tip in situ with the application of load, and the damage area ahead and around the crack tip post mortem, in isotactic polypropylene and high density polyethylene samples of different thermal histories. The results revealed that significant cavitation develops in the damage area at the plastically deformed region beyond the crack tip, and inside the damage zone rod and platelet-shaped cracks/voids are formed (as revealed by SAXS), accompanied by martensitic crystal transformations or the formation of a conformationally disordered phase (as revealed by WAXS).

CPP 14.2 Wed 14:15 ZEU Lich

What happens to entanglements during polymer crystallization? —

•HENDRIK MEYER — Institut Charles Sadron, CNRS UPR 22, 67083 Strasbourg, France

We developed a simplified polymer model which appeared to be very efficient for the study of polymer crystallization from the dense melt using molecular dynamics simulations [1]. Chain-folded lamellae were obtained

starting from the isotropic melt with chains of N=400 monomers corresponding to 10-12 entanglement lengths. The thickness of the lamellae decreases with crystallization temperature as observed in experiments. We now reanalyzed the obtained configurations with a primitive path analysis [2] to quantify the entanglement length of the chains. We find that for fast crystallization, the entanglement length remains almost unchanged. For slower crystallization, in particular above the temperature where homogeneous nucleation of crystals was observed, some disentanglement occurs, and the entanglement length increases by about 50%. This means that the majority of entanglements is still present. They must be in the amorphous zones where the entanglement density thus increases.

[1] H. Meyer and F. Müller-Plathe, J. Chem. Phys. 115 (2001) 7807; Macromolecules 35 (2002) 1241.

[2] R. Everaers et. al., Science 304 (2004) 823.

CPP 14.3 Wed 14:30 ZEU Lich

Nanotomography of Semicrystalline Elastomeric Polypropylene

— •MECHTHILD DÖRING, NICOLAUS REHSE, CHRISTIAN DIETZ, SABINE SCHERDEL, and ROBERT MAGERLE — Chemische Physik, TU Chemnitz, D-09107 Chemnitz

Semicrystalline polymers contain nanometersized crystallites embedded in a matrix of amorphous material. The form and the arrangement of the crystallites determine the properties of the materials considerably. We use Nanotomography to image the three-dimensional structure of semicrystalline elastomeric polypropylene. The method is based on scanning probe microscopy imaging and subsequent etching of the sample surface layer by layer. Our aim is to automate the method as far as possible, to analyse different polymers, and to study the relations between structure and properties of the materials. Furthermore, the spatially complex structures are quantitative characterized with modern image analysis techniques.

CPP 14.4 Wed 14:45 ZEU Lich

Thin Films of Crystalline Diblock Copolymers — ●C. PAPANAKIS¹, I. BOTIZ², G. REITER², and C. DARKO¹ — ¹Physik Department E13, Technische Universität München, James-Frank Str. 1, 85748 Garching — ²Institut de Chimie des Surfaces et Interfaces, CNRS, Mulhouse, France

In thin films of diblock copolymers having one crystallizing block, a number of surface structures have been observed, e.g. edge-on or flat-on lamellae with high persistence lengths, spirals and dendrites, allowing the structuring of organic surfaces on a large range of length scales. The crystallization growth process in thin films of lamellar poly(styrene-*b*-ethyleneoxide) diblock copolymer was followed by in-situ optical microscopy. Using grazing-incidence small-angle X-ray scattering (GISAXS) and grazing-incidence X-ray diffraction (GIXD), we investigate the orientation of the mesoscopic structures with respect to the substrate as well as the orientation of the crystalline chains with respect to lamellar interfaces. This information on the structure inside the film is compared to the surface texture obtained by atomic force microscopy

with the focus on the effect of crystallization temperature.

CPP 14.5 Wed 15:00 ZEU Lich

Understanding polymer crystallization: a personal resumee — ●GERT STROBL — Institut für Physik, Albert-Ludwigs-Universität, 79104 Freiburg

New findings during the last decade have triggered a reconsideration of the foundations of polymer crystallization. The expansion of knowledge is due to the introduction of novel techniques - in-situ atomic force microscopy, high speed calorimetry, combination of standard techniques in simultaneous runs, or the use of new evaluation procedures in scattering experiments - which is demonstrated by a selection of important and clear-cut experimental results. The lecture points at some straightforward conclusions and presents a new thermodynamic scheme developed on the basis of the observations.

— 15 min. break —

CPP 15 Dynamics and Diffusion

Time: Wednesday 14:00–15:00

Room: ZEU 114

CPP 15.1 Wed 14:00 ZEU 114

Anomalous diffusion in short chain polymer melts — ●M. ZAMPONI¹, A. WISCHNEWSKI¹, M. MONKENBUSCH¹, L. WILLNER¹, B. FARAGO², and D. RICHTER¹ — ¹Forschungszentrum Juelich, 52425 Juelich, Germany — ²Institut Laue-Langevin, 38042 Grenoble, France

The dynamics of linear polymer chains in the melt depends strongly on the chain length: Short unentangled chains perform free Rouse motion, long chains are confined by mutual entanglements. In the reptation model these topological constraints are described by a virtual tube which follows the primitive path of the observed test chain. However, this definition means that a test chain with a length in the order of one entanglement distance can not be captured in a tube, even if the matrix chains are much longer than the test chain.

We report on a systematic neutron spin echo study of different binary polyethylene blends. The measured dynamic structure factor of short test chains of various lengths (below or about the entanglement length) in a long chain matrix shows significant deviations from the expected Rouse behavior pointing to the fact that the short labelled chains are subject to topological constraints. Also anomalous behavior in the time dependence of the center of mass mean squared displacement was found showing a clear subdiffusive regime. Blends of short unentangled chains in a matrix of the same length still show discrepancies: Although the segmental diffusion shows Rouse behavior, again anomalous behaviour of the c.o.m. diffusion is found. These deviations may be explained by taking intermolecular interactions as discussed by Guenza [M.Guenza, *Macromolecules* 35, 2714 (2002)] into account.

CPP 15.2 Wed 14:15 ZEU 114

Diffusion processes in binary fluid mixtures in confined geometries. — ●JOCHEN SOMMERFELD and MARTIN SCHOEN — Stranski-Laboratorium für Physikalische und Theoretische Chemie, Sekretariat C 7, Technische Universität Berlin, Strasse des 17. Juni 135, 10623 Berlin

By means of molecular dynamics (MD) simulations we study the dynamical properties of binary fluid mixtures confined by planar substrates. Molecules of fluid mixtures interact through Lennard-Jones(12,6) potentials. Interactions between fluid particles and the wall substrates are described by Lennard-Jones(10,4) potentials. Thus we can explore both symmetric and asymmetric mixtures by choosing the depth of potentials $\{\epsilon_{AA}, \epsilon_{BB}, \epsilon_{AB}\}$ and energetic preference of one kind of fluids by substrates (i.e., the selectivity of the substrates). We calculate transport coefficients using the Green-Kubo relations (i.e., integrating of time correlation functions). We focus on the calculation of diffusion coefficients, both self-diffusion coefficients D_{AA} and D_{BB} and interdiffusion coefficient D_{AB} , and the self-part of the intermediate scattering function $F_s(k, t)$ depending on the distance between substrates, selectivity of the walls, and the Lennard-Jones parameters of the two kinds of particles. The effect of phase separation on calculated quantities will be analyzed.

CPP 15.3 Wed 14:30 ZEU 114

Diffusion of dye molecules through nanoporous TiO₂ networks — ●M. DÜRR, M. OBERMAIER, A. SCHMID, A. YASUDA, and G. NELLES — Materials Science Laboratory, Sony Deutschland GmbH, D-70327 Stuttgart

Nanosize-structured materials with their unique physical and chemical properties are recently attracting a growing interest. For many applications, diffusion of molecules in solution through such nanoporous materials can be of great importance, e.g. for the sensitization of nanoporous TiO₂ when used in dye-sensitized solar cells. To quantify the influence of the nanoporous TiO₂ network on the diffusion of both Ru-complexed bipyridine dye molecules as well as porphyrin molecules, we investigated the diffusion limitations to the adsorption of dye molecules on the surface of the TiO₂ nanoparticles. A simple model is shown to be capable of reproducing the uptake curves obtained by means of optical absorption spectrometry for materials with different porosity and average size of the nanoparticles. The effective diffusion constants are found to be reduced by up to 3 orders of magnitude in the porous layers when compared to diffusion in the pure solvent. Depending on the strength of the interaction between the dye molecules, two different modes of diffusion limitation can be distinguished. In the case of porphyrin molecules, the $\pi - \pi$ - interaction energy was determined.

CPP 15.4 Wed 14:45 ZEU 114

Molecular view of a colloidal gelation — ●SYLVIE ROKE — Max-Planck Institute for Metals Research, Heisenbergstr. 3, Stuttgart, Germany

Many colloidal particles are coated physically or chemically by adsorption with a thin outer layer. Often this layer serves different purposes, such as shielding van der Waals interactions, providing so-called steric stabilization and/or to passivate surface states. If molecular transitions take place in the layer, as a function of temperature, pressure or solvent composition, dramatic changes in collective particle behaviour may result.

So far, particle properties have only been studied experimentally by techniques that lack molecular interface specificity. As a result, the molecular surface properties of the colloids that can affect the particle interaction have never been investigated directly.

We have used the recently developed technique vibrational sum frequency scattering to obtain molecular information about octadecyl-coated silica particles dispersed in n-hexadecane that undergo a gelation. The interface molecules are completely disordered in fluid suspension at high temperatures and become ordered prior to gel formation at lower temperatures. The appearance of interfacial order is accompanied by the liberation of heat and densification, and results in increased van der Waals forces between the particles leading to gelation. On a timescale of days the interface becomes completely ordered, which can affect aging in such gels.

CPP 16 Electronic Structure and Spectroscopy II

Time: Wednesday 14:00–17:30

Room: ZEU 160

CPP 16.1 Wed 14:00 ZEU 160

Statistics of low energy weakly localized Frenkel exciton levels in one-dimensional disordered systems — ●MARIUSZ BEDNARZ — Abteilung Theoretische Physik, Universität Ulm, Albert-Einstein-Allee 11, 89069 Ulm, Germany

A novel approach to probe the statistics of low energy levels of weakly localized Frenkel states in one-dimensional disordered systems will be shown. We analyze theoretically the spectral dynamics of excitons caused by the vibration-assisted hopping over localized states. The Pauli master equation is used as a tool to describe exciton hopping. Exciton fluorescence under very narrow spectral excitation conditions, resonant with the absorption band, is put forward to uncover the regularities of the exciton spectral dynamics. Under such conditions the fluorescence spectra are composed of a narrow peak at the excitation energy and a red shifted wing. This spectral structure has a simple explanation within the framework of the band-edge local level structure which has been proven to exist in the low-energy tail of the density of exciton states. The narrow peak results from the localized exciton states (mostly with large oscillator strength) created by the pump, while the wing is formed due to possible hopping of initially created excitons to the lower energy localized states, occurring within the same localization segment as well as between different ones. We show in a very detailed manner how the statistics of low energy levels can be extracted from the wing of such spectra at zero Kelvin. The effect of the localization due to spatial correlation of molecular energetic disorder on the energy level statistic also will be shown.

CPP 16.2 Wed 14:15 ZEU 160

Double-Pole Approximation in Time-Dependent Density Functional Theory — ●H. APPEL¹, E.K.U. GROSS¹, and K. BURKE² — ¹Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, D-14195 Berlin-Dahlem, Germany. — ²Department of Chemistry and Chemical Biology, Rutgers University, 610 Taylor Rd, Piscataway, NJ 08854.

A simple approximate solution of the TDDFT response equations is the single pole approximation (SPA). By relating the poles of the Kohn-Sham (KS) response function to the poles of the true interacting response function, SPA provides additive shifts that correct the KS excitation energies towards the true excitations of the system. In the present work [1] we have extended the SPA to the case of two strongly coupled poles. The analysis provides a variety of new results beyond those of SPA. Most importantly, one can determine the regimes where SPA fails and provide corrections in that case. In addition corrections to oscillator strengths become accessible by using the double-pole approximation (DPA). Within the DPA we show that in certain regimes the coupling between poles can cause a transition to vanish entirely from the optical spectrum. DPA has recently been successfully applied to core-hole interaction in the X-ray absorption spectroscopy of 3d transition metals [2].

[1] Double-Pole Approximation in Time-Dependent Density Functional Theory, H. Appel, E.K.U. Gross, K. Burke, cond-mat/0510396

[2] Measuring the kernel of time-dependent density functional theory with X-ray absorption spectroscopy of 3d transition metals, A. Scherz, E.K.U. Gross, H. Appel, C. Sorg, K. Baberschke, H. Wende, and K. Burke, Phys. Rev. Lett., in print.

CPP 16.3 Wed 14:30 ZEU 160

ESR-Imaging including Conduction Electron Drift Velocity Measurement — ●MALTE DRESCHER¹, NOAM KAPLAN², and ELMAR DORMANN¹ — ¹Physikalisches Institut, Universität Karlsruhe(TH), D-76128 Karlsruhe, Germany — ²Racah Institute of Physics, Hebrew University, Jerusalem, Israel

This contribution presents the results on ESR-imaging via temperature dependent pulsed X-band ESR focussing on quasi one-dimensional organic conductors, where due to their long T_2 -time constants even pulsed conduction electron spin resonance and a resolution better than $10\mu\text{m}$ is possible. Additionally to depicting spin densities we succeeded in spatially resolved determining dynamic properties, e.g. spin-spin-, spin-lattice-relaxation, spin diffusion coefficient or phase transition temperatures.

Since flow measurement is an established tool in NMR-imaging, the possibility of performing ESR experiments on conduction electrons allows in principle to determine the electron spin drift velocity for given electric

current. An appropriate pulsed gradient and current ESR detection scheme was developed and the first successful experiment of detecting the phase shift in the ESR-signal induced by an applied electrical current was performed. The ohmic correlation is demonstrated in a range of more than $\pm 250\text{mA}$ in crystals exhibiting a cross-sectional area of less than 1mm^2 and a maximum drift velocity of $0.3 \frac{\text{m}}{\text{s}}$ was found in the metallic phase of a radical cation salt.

CPP 16.4 Wed 14:45 ZEU 160

Multielectron Vibrational States in α -Helical Polypeptides — ●DMITRY TSIVLIN and VOLKHARD MAY — Institut für Physik, Humboldt Universität zu Berlin, Newtonstr. 15, D-12489 Berlin

Studies of amide vibrations in α -helical polypeptides attracted much interest due to the mechanism of self-trapping of vibrational excitation, originally proposed by Davydov. Recently, it became possible to observe the self-trapped states in α -helices by using femtosecond infrared pump-probe spectroscopy [1].

Since for the amide vibrational states the so-called nonadiabatic limit is reached [2], theoretical description of the system requires a quantum treatment of the high-frequency amide mode coordinates as well as the coordinates of the polypeptide lattice. In the present work, by employing a multielectron expansion of the model Hamiltonian an accurate quantum-dynamical description of vibrational states formed by amide C=O and N-H stretching modes of α -helix is presented [3]. Using the multiconfiguration time-dependent Hartree method, linear and pump-probe infrared absorption spectra are calculated by numerical time-propagation of the exciton-chain vibrational wavefunction. Formation of self-trapped exciton states is discussed within the adiabatic exciton approximation and within the full quantum approach. Interpretation of the infrared pump-probe experiments for α -helical polypeptides and for peptide model crystals is proposed [1,2].

[1] J. Edler et al., Phys. Rev. Lett. **93**, 106405 (2004)

[2] D.V. Tsivlin, V. May, and H.-D. Meyer, J. Chem. Phys., submitted

[3] D.V. Tsivlin and V. May, Chem. Phys. Lett. **408**, 360 (2004)

CPP 16.5 Wed 15:45 ZEU 160

The electronic structure of liquids studied by resonant X-ray emission (RXES) and X-ray absorption spectroscopy (XAS) in the soft X-ray range — ●OLIVER FUCHS¹, L. WEINHARDT¹, F. MAIER¹, E. UMBACH¹, M. BÄR², T. HOFMANN², J. WHITE², V. MAREPALLY², C. HESKE², M. ZHARNIKOV³, M. GRUNZE³, and J.D. DENLINGER⁴ — ¹Exp. Physik II, Uni Würzburg — ²Dept. of Chem., Univ. of Nevada, Las Vegas — ³Angew. Physikal. Chemie, Uni Heidelberg — ⁴ALS, Berkeley

The investigation of liquids by means of soft x-ray techniques is a technically challenging task since it requires a third-generation synchrotron source combined with a high-efficiency grating spectrometer, and a wet cell with an ultra-thin window separating the liquid from ultra-high vacuum. With our flow-through wet cell we have investigated the electronic structure of various liquids including H_2O , D_2O , NaOH, NaOD, ethanol, acetic acid, and various aqueous solutions. The spectra reveal details on the hydrogen bonding network of water and its temperature dependence. The investigation of aqueous solutions reveals on the one hand the effect of the solutes on the hydrogen bonds of water, and on the other hand the influence of the hydration shell on the electronic structure of the solutes. Moreover, molecular dynamics within the time scale of the core hole lifetime (a few femtoseconds) leads to isotope effects in both, RXES and XAS spectra, and can be described by theoretical molecular dynamics simulations.

CPP 16.6 Wed 16:00 ZEU 160

Reduction of Noble Metal Ions to Metal Nanoparticles on J-Aggregates — ●STEFAN KIRSTEIN¹, HANS V. BERLEPSCH², CHRISTOPH BÖTTCHER², DÖRTHE M. EISELE¹, and ANNA BURMISTROVA¹ — ¹Humboldt University of Berlin — ²Free University, Berlin

Cyanine dye molecules and their J-aggregates are well known to serve as sensitizers for photo induced electron transfer processes. Technically, this feature is utilized in photographic films where dyes are adsorbed at silver halide crystals which is reduced to elementary silver by an electron transfer from the photoexcited dye. Here, the same mechanism is used

to grow silver nanoparticles at the surface of tubular J-aggregates form AgNO_3 salt solutions.

The amphiphilic tetrachlorobenzimidacarbocyanine dye molecule C8S3 (amphipipe) forms tubular J-aggregates in aqueous solutions with a uniform diameter of 17 nm and lengths of over 100 μm . The addition of noble metal salts (Na_2PdCl_4 or AgNO_3) to a solution of C8S3 aggregates leads to the formation of metal nanoparticles at the surface of the dye aggregates. The particles are observed by cryo-TEM and also by AFM for aggregates adsorbed at solid surfaces. The particles are rather uniform in size with a mean diameter of a few nanometer and distributed along the aggregate surface. In parallel to the growth of the particles a dramatic quenching of the aggregate fluorescence is observed. Therefore, the growth of the metal nanoparticles is explained by a photoexcited electron transfer process from the J-aggregates to the metal ions. A systematic study of this process for AgNO_3 will be presented.

CPP 16.7 Wed 16:15 ZEU 160

Torsional Potentials for the Ground and Excited State of Bithiophene Calculated by Time-dependent Density Functional Theory — ●WICHARD J.D. BEENKEN¹, SEBASTIAN WESTENHOFF², and TÖNU PULLERITS³ — ¹Technische Universität Ilmenau, FG Theoretische Physik I, Postfach 100565, D-98684 Ilmenau — ²University of Cambridge, Optoelectronics Group, Cavendish Laboratory, CB3 0HE, UK — ³Lunds Universitet, Kemisk Fysik, Box 124, SE-22100 Lund

We have studied bithiophene by time-dependent density functional theory. In particular we have analyzed the dependence of singlet excitation energies and transition dipoles on the torsional angle between the two thiophenyl groups. The torsional spectrum has been computed quantum-mechanically as well as semi-classically in order to understand, how this influences the broadening of absorption and luminescence spectra. We discuss the general consequences for the spectral broadening, Stokes shift and energy relaxation in poly-thiophenes, in particular, how torsional disorder effects the absorption and photoluminescence spectra. Furthermore, such results are necessary input parameters for molecular dynamics. In particular for simulation of polythiophenes in the excited state reliable data are rare. We will show some exemplary simulations.

CPP 16.8 Wed 16:30 ZEU 160

Optical Absorption and Energy Transport in Dendrimers — ●CHRISTOPH SUPRITZ¹, PETR CHVOSTA², and PETER REINEKER¹ — ¹Department of Theoretical Physics, University of Ulm, 89069 Ulm — ²Department of Macromolecular Physics, Faculty of Mathematics and Physics, Charles University, Prague

Dendrimers are highly branched polymers which are expected to be useful, for example, as efficient artificial light harvesting systems (like in photosynthesis) in nano-technological applications. It is generally assumed that inside dendrimers energy is transported via Frenkel excitons, but at the moment it is not clear whether this energy transport occurs in a coherent (wavelike) manner or via an incoherent hopping process. In our model we take into account the exciton phonon interaction by introducing a heat bath that interacts with the exciton in a stochastic manner. In this way we can describe the coupled coherent and incoherent exciton transport inside dendrimers and calculate their linear optical absorption spectra in the framework of linear response theory. To mimic the influence of a reaction center (like in photosynthesis) on energy transport, we attach a sink to the dendrimer through which excitons can be taken out of the system. We present these results for a number of different dendrimer types.

CPP 16.9 Wed 16:45 ZEU 160

Optical absorption of various linear and cyclic thiophene based π -conjugated polymers — ●MARIUSZ BEDNARZ and PETER REINEKER — Abteilung Theoretische Physik, Universität Ulm, Albert-Einstein-Allee 11, 89069 Ulm, Germany

Recently, using thiophene based repeat units, the first series of fully conjugated macrocyclic structures: cyclo(thiophene-diacetylenes) and cyclo[n]thiophenes were synthesized (P. Bäuerle et al.). Such structures together with various series of linear oligothiophenes with controlled chain length exhibit an interesting relation between their absorption spectra. In particular, there is a clear relation between the peak position of the oligothiophenes and cyclothiophenes: the spectrum for the cyclothiophene with a given size corresponds to an oligothiophene chain of about half the length. The absorption spectra of such linear and cyclothiophenes show a systematic red shift with increasing number of thiophene units. In the present contribution, we will address an approach, based on the Frenkel exciton Hamiltonian, which describes the observed red shift tendency and the relationship between cyclothiophenes and corresponding oligothiophenes. Detailed study of the microscopic parameters depending on various side- and end-groups attached to the bare thiophene chains will be given. Also we show that cyclo(thiophene-diacetylenes) can be described as a fully conjugated system with very interesting manifestation of the cyclic symmetry as a Davydov components in the case of very small rings. It will be shown that diacetylene units embedded into thiophene cyclic structures can be described as another chromophore with larger $\pi - \pi^*$ transition than thiophene units itself.

CPP 16.10 Wed 17:00 ZEU 160

Amplified Spontaneous Emission of Cross-linkable Conjugated Polymers in Multilayer Devices — ●BODO WALLIKEWITZ, DIRK HERTEL, and KLAUS MEERHOLZ — Universität zu Köln, Luxemburgerstrasse 116, 50939 Köln

Although the performance of polymer and small organic light emitting diodes (OLEDs) has made tremendous progress over the past decade, electrically pumped organic laser diodes as an advanced application remain a challenge. To achieve lasing optical gain manifested by for instance amplified spontaneous emission (ASE) is mandatory. We investigated for the first time ASE properties, gain and loss of cross-linked conjugated copolymers. Cross-linkable materials offer the advantage of solution processing of thick multilayer devices, essential for future electric driven organic lasers. Furthermore we studied the influence of chromophore type and chromophore concentration on the ASE threshold, optical gain and loss. We obtained low thresholds below 5 $\mu\text{J}/\text{cm}^2$, high gain above 33 cm^{-1} and low losses below 5 cm^{-1} . These are very low thresholds, even for conventional conjugated polymers described in the literature. Thick hole transport layers (HTL) are necessary to enable ASE and optimize mode confinement in the emitter material on quenching electrodes. We restored the properties of neat polymer films on electrodes by using a thick, cross-linked HTL in between. The threshold is minimized by optimizing the refractive index of HTL, HTL thickness and polymer thickness. Furthermore, electrical properties of HTLs and efficiencies of thick multilayer OLEDs are presented and discussed.

CPP 16.11 Wed 17:15 ZEU 160

Watching protons tunnel: Nuclear momentum distributions from electronic structure calculations — ●DANIEL SEBASTIANI — MPI Polymerforschung; Ackermannweg 10; 55128 Mainz

We present first-principles electronic structure calculations of nuclear momentum densities $\rho_n(\mathbf{p}) = |\Psi_n(\mathbf{p})|^2$ (where $\Psi_n(\mathbf{p})$ is the nuclear vibrational wavefunction in momentum representation). Experimentally, the momentum distributions $\rho_n(\mathbf{p})$ are directly accessible through neutron Compton scattering methods. Our computational technique can be applied to complex hydrogen bonded systems (molecules or condensed phases). We illustrate its potential by describing the tunneling-induced ferroelectric phase transition in potassium dihydrogen phosphate (KDP). The results are in very good agreement with experiment.

CPP 17 Thin Films and Surfaces II

Time: Wednesday 15:45–17:30

Room: ZEU Lich

CPP 17.1 Wed 15:45 ZEU Lich

Self assembly of diblock copolymers on patterned substrates: A Single Chain in Mean Field simulation study — ●KOSTAS DAOULAS¹, MARCUS MUELLER¹, MARK STOYKOVICH², SANG-MIN PARK², YIORYOS PAKAKONSTANTOPOULOS², JUAN DE PABLO², and PAUL NEALEY² — ¹Institut fuer Theoretische Physik, Georg August Universitaet, D37077 Goettingen — ²Department of Chemical and Biological Engineering, University of Wisconsin, Madison, WI 53706-1691

The implementation of a recently developed Single Chain in Mean Field (SCMF) method is presented, to study the self assembly of a lamella-forming ternary blend of a diblock-copolymer with its respective homopolymers on periodically patterned substrates. The pattern consists of square arrays of spots preferentially attracting one component and the structure of the assembled blend is investigated as a function of pattern dimensions and film thickness. The SCFM simulations show that the blend morphology closely follows the pattern at the substrate forming a quadratically perforated lamella (QPL). Depending on the pattern dimensions, the QPL is connected to the film free surface either through cylindrical-like necks or lamellae-like domains, resulting in a bicontinuous morphology. The theoretical predictions concerning the structure observed on the free surface of the film are in accordance with experimental data obtained for the same systems.

CPP 17.2 Wed 16:00 ZEU Lich

Nanoaggregates on surfaces structured by nanolithography — ●MAIK VIELUF, HARALD GRAAF, and CHRISTIAN VON BORCZYKOWSKI — Optische Spektroskopie und Molekülphysik, Institut für Physik, Technische Universität Chemnitz, 09107 Chemnitz

For detailed investigations of single nanoaggregates a suppression of the interaction among the aggregates is necessary. Such suppression can be reached by fixing the aggregates to a structured surface with a certain distance between the structures. We report on a structuring on nanometer scale by local anodic oxidation of self-assembled monolayers by atomic force microscopy (AFM). The oxide structures are selectively chemically modified to achieve functionalized nanostructures. These functionalized nanostructures are used to bind semiconductor or metal nanoparticles or supramolecular structures. Such structures are investigated by confocal microscopy to evaluate the optical properties.

CPP 17.3 Wed 16:15 ZEU Lich

A combinatorial study on gradient noble metal / polymer blend multilayers — ●STEPHAN V. ROTH¹, HARALD WALTER², RALPH DOMNICK³, CHRISTIAN SCHROER¹, MARION KUHLMANN¹, RAINER GEHRKE¹, and PETER MÜLLER-BUSCHBAUM⁴ — ¹HASYLAB at DESY, Notkestr. 85, D-22603 Hamburg — ²CSEM SA, Badenerstrasse 569, CH-8048 Zürich, Switzerland — ³identif GmbH, Ulrich-Schalk-Str. 3 D-91056 Erlangen — ⁴TU München Physik Department LS E13, James-Franck-Str. 1, D-85748 Garching

Nanostructuring of thin noble metal films is of utmost importance for many technological and biophysical areas, e.g. anti-counterfeiting and DNA scanning [1]. Usually a multilayer geometry is chosen consisting of noble metal layer / polymer / substrate. The optical properties of such multilayer systems depend crucially on the structure and morphology of the noble metal layer. It is determined by key parameters like deposition method or noble metal-polymer interaction affecting the self-assembly of the metal atoms. We advanced two-fold: Firstly, as polymer layer we chose a blend of deuterated polystyrene (dPS) and polyisoprene (PI). Secondly we installed a gradient in mass thickness of the noble metal layer during evaporation. To obtain information for combinatorial libraries microbeam grazing incidence small-angle x-ray scattering (μ GISAXS) allowing to scan such gradients is excellently suited [2]. We present a combinatorial study on a gold and copper gradient multilayers.

[1] G. Bauer et al., *Nanotechnology* **14**, 1289 (2003)[2] S.V. Roth et al., *Appl. Phys. Lett.* **82**, 1935 (2003)

CPP 17.4 Wed 16:30 ZEU Lich

Electrical Detection and Characterization of Self-Assembled Polyelectrolyte Multilayers by a Silicon-on-Insulator based Thin Film Resistor — ●PETRA A. NEFF¹, ALI NAJI², REGINE VON KLITZING³, and ANDREAS R. BAUSCH¹ — ¹Lehrstuhl für Biophysik - E22, Technische Universität München, Germany — ²Physik Department - T37, Technische Universität München, Germany — ³Institut für Physikalische Chemie, Christian-Albrechts-Universität Kiel, Germany

The build up of polyelectrolyte multilayers (PEMs) was observed by a silicon-on-insulator (SOI) based thin film resistor. Although the structural properties of polyelectrolyte multilayers have been extensively studied, a detailed understanding is still lacking. The layer-by-layer deposition of the polycation poly(allylamine hydrochloride) (PAH) and the polyanion poly(styrene sulfonate) (PSS) results in defined potential shifts, which decrease with the number of layers deposited. We model the response of the device assuming electrostatic screening of polyelectrolyte charges by mobile ions within the PEMs. The screening length κ^{-1} inside the PEMs was found to be increased compared to the value corresponding to the bulk solution. Furthermore the partitioning of mobile ions between the bulk phase and the polyelectrolyte film was employed to calculate the dielectric constant of the PEMs and the concentration of mobile charges.

CPP 17.5 Wed 16:45 ZEU Lich

Modulation of physico-chemical surface properties of binary polyelectrolyte brushes and its influence on protein adsorption — ●PETRA UHLMANN, NIKOLAY HOUBENOV, NINA BRENNER, and MANFRED STAMM — Leibniz Institute of Polymer Research, Hohe Strasse 6, D-01069 Dresden

Binary brushes constituted from two incompatible polymers can be used in the form of ultrathin polymeric layers as a versatile tool for surface engineering to tune physico-chemical surface characteristics as wettability, surface charge, chemical composition or morphology, and furthermore to create responsive surface properties. Mixed brushes of oppositely charged polyelectrolytes are representing a special case of responding surfaces which are sensitive to changes of the pH value in aqueous environment. The polyelectrolyte brushes used were composed of the two oppositely charged polyelectrolytes poly(2-vinylpyridine) (P2VP) and polyacrylic acid (PAA) and the in-situ properties and surface characteristics, as surface charge, surface tension, extent of swelling of these brush layers are described. To test the behaviour of the polyelectrolyte brushes when coming into contact with biosystems, protein adsorption experiments with globular model proteins were performed at different pH values and salt concentrations of the buffer solutions. The influence of the pH value and the buffer salt concentration on the adsorbed amount, the structure of the protein layers and the interfacial tension during protein adsorption as well as the protein adsorption mechanism in reference to recently developed theories about protein adsorption on polyelectrolyte brushes will be discussed.

CPP 17.6 Wed 17:00 ZEU Lich

Experimental determination of the coverage-height dependence of self-assembled monolayers during film formation — ●AHMED ABD EL MONEM¹, JANA WEHRMEISTER², MARK HELM², and MICHAEL HIMMELHAUS¹ — ¹Angewandte Physikalische Chemie, Universität Heidelberg, Im Neuenheimer Feld 253, 69120 Heidelberg — ²Institut für Pharmazie und molekulare Biotechnologie, Universität Heidelberg, Im Neuenheimer Feld 364, 69120 Heidelberg

So far, the adsorption kinetics of Self Assembled Monolayers (SAM) of alkanethiols on the coinage metals has been extensively studied. A lot of theoretical and experimental work has been done to evaluate the adsorption rate and layer thickness. However, measurements of the adsorption kinetics have been found to depend strongly on the method applied according to the physical transducer mechanism used to trace surface adsorption, such as the change in the dielectric properties of the interface or the alteration of surface state density. In this work, we present a novel approach, which combines linear and nonlinear optical techniques, i.e. spectral ellipsometry and optical second harmonic generation, to acquire such different information during the adsorption process of alkanethiols on gold independently. Accordingly, by observing the adsorption of different alkanethiols (C4, C12, C18) in-situ the differences between the two methods could be clarified. Preliminary experiments carried out on

the adsorption of alkanethiol-terminated polyethylene glycol demonstrate the potential of the method for the determination of the coverage-height dependence of surface-grafted polymer brushes, which is particularly important for direct comparison with theoretical predictions.

CPP 17.7 Wed 17:15 ZEU Lich

Irreversible adsorption of tethered chains at substrates. Monte Carlo Study. — ●RADU DESCAS^{1,2}, JENS-UWE SOMMER², and ALEXANDER BLUMEN¹ — ¹Theoretische Polymerphysik, Universität Freiburg, Hermann-Herder-Strasse 3, D-79104 Freiburg, Germany — ²Institut de Chimie des Surfaces et Interfaces, 15, rue Jean Starcky, F-68057 Mulhouse Cedex, France

We study using the bond fluctuation model the irreversible adsorption of single chains grafted with one end to the surface [1]. While the reversible adsorption involves equilibrium states [2,3], the irreversible adsorption implies non-equilibrium ones. We find that the adsorbate's

growth is dominated by the zipping of monomers according to their order along the chain. The time of adsorption $t(M)$ as a function of the number M of adsorbed monomers follows a power law; M^α with $\alpha > 1$. We introduce a two-phase model, in which the chain is described by an adsorbate portion and a corona. According to our model the adsorption can be viewed as consisting in a main stage, during which single monomers attach to the surface through zipping, and a late stage, in which the corona collapses on the surface. We find that α is given by $\alpha = 1 + \nu$, where ν is the Flory exponent, and study the time evolution of various density profiles.

[1] R Descas, J. -U. Sommer and A. Blumen, submitted.

[2] R Descas, J. -U. Sommer and A. Blumen, J. Chem. Phys. 120, 8831, (2004).

[3] R Descas, J. -U. Sommer and A. Blumen, J. Chem. Phys. 122, 134903, (2005).

CPP 18 Polymer Materials II

Time: Wednesday 15:45–17:15

Room: ZEU 114

CPP 18.1 Wed 15:45 ZEU 114

Thiol molecules can build up far more than a monolayer: Substrate-Consuming Metal-Organic Layers (SCMOLs) — ●STEFAN WALHEIM¹, MATTHIAS BARCZEWSKI^{1,2}, BIRGIT RIEDEL¹, JOCHEN GEERK³, ALFRED BLASZCZYK¹, MARCEL MAYOR^{1,4}, and THOMAS SCHIMMEL^{1,2} — ¹Institute for Nanotechnology, Forschungszentrum Karlsruhe, 76021 Karlsruhe (Germany) — ²Institute of Applied Physics, University of Karlsruhe, 76131 Karlsruhe (Germany) — ³Institute for Solid-State Physics, Forschungszentrum Karlsruhe, 76021 Karlsruhe (Germany) — ⁴Chemistry Department, University of Basel, 4056 Basel (Switzerland)

A novel procedure for the self-assembly of metal-organic layers is described. These layers grow from metal substrates. The organic (thiol)-molecules gradually combine with the metal atoms of the substrate to build up an optically transparent metal-organic solid. The metal atoms are essentially consumed during the growth process. For this reason we call these layers - which can reach thicknesses up to 1 micron - Substrate-Consuming Metal-Organic Layers (SCMOLs). Rutherford Back-Scattering (RBS), Small Angle X-Ray Scattering (SAXS) and Atomic-Force Microscopy (AFM) were applied to gather information about the growth behaviour and the morphology of this nano-structured material. This opens perspectives towards the development of a new type of self-assembled thin solid films with possible applications, e. g. for novel procedures of constructive lithography.

[1] S. Walheim, M. Barczewski, A. Blaszczyk, M. Mayor, Th. Schimmel, Patent application: DE 102005025693.7 (2005)

CPP 18.2 Wed 16:00 ZEU 114

Optical or electrical poling of azo-dye layers — ●ANSGAR DRAUDE¹, SVEN VERPOORT¹, RAFAEL MEINHARDT¹, HILMAR FRANKE¹, and ROGER A. LESSARD² — ¹Fachbereich Physik / Angewandte Physik, Universität Duisburg-Essen, Lotharstr. 1, D-47048 Duisburg, Germany — ²COPL, department de physique, génie physique et optique, Université Laval, Québec, Canada G1K7P4

Polycrystalline films of the azo-material DR1 have been investigated. After evaporation on glass substrates the molecules are randomly orientated.

The molecules can be reoriented using different technics. Optically transparent regions may be formed either by light exposure using the Trans-Cis photo-isomerization (optical poling) or by an electrical Corona (electrical poling). The optical anisotropy has been measured by the angular dependence of the absorption-coefficient.

Stable holographic gratings may be recorded as well in the randomly oriented as in the pre-oriented regions. Measuring the topology (AFM or profilometer) indicates a relation between orientational order and material flow.

CPP 18.3 Wed 16:15 ZEU 114

Flexible ferroelectret field-effect switches — ●INGRID GRAZ¹, MARTIN KALTENBRUNNER¹, CHRISTOPH KEPLINGER¹, REINHARD SCHWÖDIAUER¹, SIEGFRIED BAUER¹, STEPHANIE LACOUR², and SIGURD WAGNER² — ¹Soft Matter Physics, Johannes Kepler University, Altenberger Str. 69, A-4040 Linz, Austria — ²Department of Electrical Engineering, Princeton University, Princeton NJ, 08544, USA

Ferroelectrets are internally charged cellular polymers with engineered macroscopic dipoles formed on the internal surfaces of the voids. The strong piezoelectricity of ferroelectrets results in large external electric fields when the mechanical stress acting on the ferroelectret changes. The generated electric field can be used to alter the conductance of the source-drain channel of thin film field-effect transistors (ferroelectret-field effect transistor). We have prepared flexible ferroelectret field-effect switches made of cellular polypropylene films and amorphous silicon thin film transistors. Single element piezoelectric switches, pressure sensors and microphones are demonstrated, which may easily be scaled up to large area, flexible transducer arrays.

CPP 18.4 Wed 16:30 ZEU 114

Thermoplastic Elastomers with Piezoelectric Properties — ●TORSTEN FINNBERG, REZA GHAHARY, and BERND-JOACHIM JUNGNIKEL — Deutsches Kunststoff-Institut, Schlossgartenstrasse 6, 64289 Darmstadt, Germany

The strong piezoelectricity of some polymers results from a favorable combination of permanent polarisation and deformability. The latter may be enhanced by inserting the polarized entities in an elastomeric matrix. We have synthesized thermoplastic elastomers based on poly (ethyl acrylate), PEA, and polyamide-11, PA-11, with a PA-11 content of 30 wt-%. The PA-11 should contribute the ferroelectric polarization, and the PEA ensures the rubber-like elasticity. Due to the low dielectric strength of that material, poling was possible only up to 30 MV/m, and the resulting polarization was caused by dipole orientations in the amorphous phase and the surface of the crystalline phase of the PA-11 rather than being a real ferroelectric remanent polarization. The polarization was nevertheless stable and lead to a quasistatic piezoelectric coefficient of about 1 pC/N. That value exceeded that of about 0.4pC/N of the pure PA-11 as prepared at the same conditions. The results prove that the balance between polarization and deformability in piezoelectric polymers may be shifted to the latter with gain - or at least without loss - in performance but leading to a piezoelectric material with interesting mechanical properties.

CPP 18.5 Wed 16:45 ZEU 114

Spatially Inhomogeneous Polarization Switching in Poly(Vinylidene Fluoride) Observed with Focused Thermal Pulses — ●AXEL MELLINGER, MARCO SCHREIBER, MICHAEL WEGENER, and WERNER WIRGES — Department of Physics, University of Potsdam, Am Neuen Palais 10, 14469 Potsdam

Poly(vinylidene fluoride) and its copolymer with trifluoroethylene are well-known ferroelectric polymers, with numerous applications for piezo- and pyroelectric transducers. However, the dynamics of the electrical poling process is still the subject of intense investigation. Recent progress in the non-destructive, three-dimensional mapping of space-charge and polarization profiles with thermal pulses [1] allows the spatially resolved imaging of the polarization switching process as the material is subjected to periodic electric fields at mHz frequencies. The polarization maps with a lateral resolution of 50 μm and a near-surface depth resolution of better than 0.4 μm reveal a highly inhomogeneous switching, with a partial pinning of the polarization in a 1 μm surface layer.

[1] A. Mellinger, R. Singh, M. Wegener, W. Wirges, R. Gerhard-

Mulhaupt and S. B. Lang, Appl. Phys. Lett. **86**, 082903 (2005).

CPP 18.6 Wed 17:00 ZEU 114

Insulating to semi-metallic transition of different polymers under low-energy ion bombardment — ●Y. KOVAL, M. S. ALAM, and P. MÜLLER — Physikalisches Institut III, Universität Erlangen-Nürnberg, Erwin-Rommel Str. 1, 91058 Erlangen, Germany

It is well known that bombardment of polymers with high-energy ions can transform them from an insulating to a conducting state. On the

other hand, low-energy ions are considered to be not suitable for this type of transformation. However, we have found that low-energy ions can be successfully used for a conducting layer formation. Depending on treatment conditions, the conduction mechanism in such layers can vary from hopping of charge carriers to semi-metallic behavior. The ultra-small thickness of the conducting layer together with the semi-metal type of conductance can be interesting for polymer electronics technology. Several polymers were investigated in various regimes of low-energy ion bombardment. We present a summary of our recent results.

CPP 19 SYMPOSIUM Functional Organic Thin Films I

Time: Thursday 09:30–12:30

Room: ZEU Lich

Invited Talk

CPP 19.1 Thu 09:30 ZEU Lich

Electronic structure of hybrid interfaces for polymer-based electronics — ●WILLIAM R. SALANECK — Department of Physics, IFM, Linköpings Universitet, S-581 83 Linköping, Sweden

Conjugated polymers are currently used in organic molecular and polymer based electronics. The interface between the organic material (molecular or polymeric) and inorganic electrode materials controls a great deal of the interfacial charge transfer characteristics. In Linköping, studies of molecular modification of energy level alignment at hybrid interfaces have been carried out for many years. Molecular adsorption may be used to control interfacial electronic parameters almost as-desired for applications in molecular and polymer based electronic applications. The characterization of the electronic structure of the interface between spin-coated polymer films and metallic substrates (the device fabrication mode), is often carried out using photoelectron spectroscopies. Several examples of recent work on the molecular modification of hybrid interfaces, carried out in Linköping, will be presented. In addition, some very recent results on fast charge transfer at hybrid interfaces, studied by variations on UPS, will be discussed.

CPP 19.2 Thu 10:00 ZEU Lich

Optimized hole injection with strong electron acceptors at organic-metal interfaces — ●NORBERT KOCH¹, STEFFEN DUHM¹, ANTIJE VOLLMER², ROBERT L. JOHNSON³, and JÜRGEN P. RABE¹ — ¹Humboldt-Universität zu Berlin, Institut f. Physik, Newtonstr. 15, 12489 Berlin — ²BESSY GmbH, 12489 Berlin — ³Universität Hamburg, Institut f. Experimentalphysik, 22761 Hamburg

The energy level alignment at interfaces between three electroactive conjugated organic materials and Au was systematically varied by adjusting the pre-coverage of the metal substrate with the electron acceptor tetrafluoro-tetracyanoquinodimethane (F4-TCNQ). Photoelectron spectroscopy revealed that electron transfer from Au to adsorbed F4-TCNQ was responsible for lowering the hole-injection barrier by as much as 1.2 eV. This novel interface modification scheme is independent of the charge transfer complex formation ability of the organic materials with the electron acceptor.

CPP 19.3 Thu 10:15 ZEU Lich

Interaction of Me atoms with thin organic films: In (Sn, K)/CuPc — ●OLGA MOLODTSOVA¹, VICTOR ARISTOV^{1,2}, VICTOR ZHLIN², DENIS VYALIKH³, and MARTIN KNUPFER¹ — ¹Leibniz IFW Dresden, Germany — ²ISSP, RAS Chernogolovka, Russia — ³IFF, TU Dresden, Germany

Among the Organic Molecular Thin Film Crystals the family of the phthalocyanines (Pc*s) plays an important role and many researchers pay attention to this materials. In the present investigation we have focused on the evolution of the electronic structure of CuPc films during metal deposition and on interactions during this process. The measurements were performed by means of high-resolution photoemission electron spectroscopy, core-level and valence-band, and using synchrotron-radiation facility. In particular we have found, that e.g. the In deposition onto CuPc films is characterized by two stages of the In/CuPc interface formation. The first stage takes place until a nominal In coverage of 6 Å and is characterized by strong diffusion of the In atoms into the organic film. In atoms occupy sites close to the pyrrole nitrogens, strongly interact and transfer negative charge to CuPc. This stage comes to the end when a stoichiometry of In₂CuPc is reached. The second stage begins just after the first is completed, at about 7 Å: on top of the In₂CuPc compound a metallic indium film is formed. This behavior will be compared with

formation of Sn (K)/CuPc interfaces.

CPP 19.4 Thu 10:30 ZEU Lich

Self consistent theory of charge carrier injection at the metal-organic interface — ●FREDERIK NEUMANN, YURI GENENKO, CHRISTIAN MELZER, and HEINZ VON SEGGERN — Institute of Materials Science, Darmstadt University of Technology, Petersenstraße 23, D-64287 Darmstadt, Germany

The effect of the injection barrier on charge transport plays an important role in understanding and development of organic electronic devices. In previous studies this effect was considered in the special cases of low and high injection barriers.

The focus of the present study is on the development of an injection model which incorporates space charge effects. The challenge of this task is the problem of self-consistency. The amount of injected charge carriers injected per unit time strongly depends on the barrier height, while at the same time the electrostatic potential generated by the injected charge modifies the height of the injection barrier itself.

Here a self-consistent model of the injection process on metal/organic interfaces is presented. This model requires a proper description of both, the organic and the metal side of the interface.

To describe the metal a DOS of quasi-free electrons is chosen. The description for the organic semiconductor is based on a gaussian DOS. Since charge transport in organic semiconductors occurs by hopping of charge carriers between localized states, we introduced the concept of a mobility edge and a field dependent mobility. The resulting differential equations are solved in a self-consistent manner by introducing continuity of the electrochemical potential and electric displacement.

— 15 min. break —

Invited Talk

CPP 19.5 Thu 11:00 ZEU Lich

Fast and stable integrated polymer circuits — ●WALTER FIX — PolyIC GmbH & Co KG, Guenther-Scharowsky-Str. 1, 91052 Erlangen, Germany

Printed electronics based on polymer transistors will enable the availability of electronics on nearly every product. This will create a new electronics revolution, not by replacing standard electronic based on silicon, but it will enable the realization of electronic intelligence to products, where there is no electronics today. This includes low cost radio frequency identification (RFID) applications, e.g. as a substitute of the optical barcode, as well as smart objects and electronics for flexible displays. This is possible due to the new polymer electronics technology, PolyIC combines soluble electronic polymer materials with high volume printing processes to achieve low cost, high volume printed electronics. Recent results on our technology as well as our roadmap towards printed electronics products will be presented, including fast and stable circuits as well as RFID Tags working at 13.56 MHz.

CPP 19.6 Thu 11:30 ZEU Lich

Full-Organic and Highly Efficient Top-emitting PIN-OLEDs for Display Applications — ●MICHAEL HOFMANN¹, THOMAS STÜBINGER¹, PHILIPP WELLMANN¹, MARTIN VEHSE¹, JAN BIRNSTOCK¹, ANSGAR WERNER¹, JAN BLOCHWITZ-NIMOTH¹, and QIANG HUANG² — ¹Novaled GmbH, Tatzberg 49, 01307 Dresden, Germany — ²TU Dresden, George-Bähr-Straße 1, 01069 Dresden, Germany

The next generation of active matrix displays is going to incorporate bright top-emitting organic LEDs. The top-emission design with high aperture ratio of 70% is favourable, because bottom emitting OLEDs

suffer from the area occupation of advanced driving circuitry in the back-plane. The concept of doped charge transport layers will easily enable the implementation on TFT-substrates. Furthermore, the approach ensures low operating voltage and high power efficiency over a large brightness range. Additionally, doped OLEDs can be adapted to a variety of electrode materials.

Essential requirements for OLED applications on reflective substrates are summarized. Performance and emission characteristics as well as lifetime data of full-organic OLED-stacks using molecular p- and n-doped transport layers are presented. In order to improve the quality of OLED-devices, thin film simulation tools are applied to study the influence of organic layer thicknesses and optical properties of both the top-most semi-transparent electrode and the reflective bottom contact. Microcavity effects are revealed and light outcoupling means are proposed.

CPP 19.7 Thu 11:45 ZEU Lich

Full-Color Polymer OLED Displays and White Solid-State-Lighting Devices Fabricated by Direct Lithography — ●ANNE KÖHNEN¹, MALTE GATHER¹, KLAUS MEERHOLZ¹, AURÉLIE FALCOU², and HEINRICH BECKER² — ¹Institut für Physikalische Chemie, Luxemburgerstr. 116, Köln 50939, Germany — ²Merck OLED Materials GmbH, Industrial Park Höchst, F 821, 65926 Frankfurt/Main, Germany

We report on a full color passive matrix display fabricated by a three step direct photo-lithography process. The device consists of parallel stripes of red, green and blue emitting conjugated polymers which are sandwiched between a transparent anode and a metal cathode in passive matrix geometry. The photo-activated oxetane-based crosslinking reaction which was used to pattern the emissive layers had no negative effect on the device performance. Each pixel in the final device can be addressed separately and covers an area of 0.3 mm². Pictures and animations were readily displayed on the panel using a commercially available passive matrix driver.

The color coordinates of the red (0.68,0.32), green (0.29,0.59) and blue (0.17,0.20) emitting polymers are well saturated and in good agreement with the PAL color standard for display applications. Colors within this triangle were accessible by adjusting the intensity of the primaries.

Due to the high efficiency of the device we also discuss application of the display as a solid-state white-light or mood-light source. The emission profile can be accurately adjusted to coincide with the white point or with any other color. At a brightness of 400 Cd/m² the power efficacy for white light (CIE=0.33,0.33) reaches 2.5 lum/W.

CPP 19.8 Thu 12:00 ZEU Lich

Large area polymer OLEDs for lighting — ●CHRISTOPH GÄRDITZ^{1,2}, DIRK BUCHHAUSER^{1,3}, RALPH PÄTZOLD¹, OLIVER WEISS^{1,4}, JOACHIM WECKER¹, and ALBRECHT WINNACKER² — ¹Siemens AG, CT MM 1, Günther-Scharowsky-Str. 1, 91058 Erlangen, Germany — ²Department of Materials Science VI, University Erlangen-Nuremberg, Germany — ³Department of Experimental Physics, University of Freiberg, Germany — ⁴Department of Materials Science, Technical University of Darmstadt, Germany

CPP 20 SYMPOSIUM Microfluidics I: Boundary conditions, manipulation, and transport

Time: Thursday 09:30–12:30

Room: ZEU 160

Invited Talk

CPP 20.1 Thu 09:30 ZEU 160

Interplay of slip and viscoelasticity in dewetting of thin liquid films — ●MARKUS RAUSCHER^{1,2}, ANDREAS MÜNCH³, BARBARA WAGNER⁴, and RALF BLOSSEY⁵ — ¹Max-Planck-Institut für Metallforschung, Heisenbergstr. 3, 70569 Stuttgart — ²Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart — ³Institut für Mathematik, Humboldt Universität Berlin, 10099 Berlin — ⁴Weierstrass Institut für Angewandte Analysis und Stochastik, Mohrenstr. 39, 10117 Berlin — ⁵Interdisciplinary Research Institute, c/o IEMN Avenue Poincaré BP 60069, F-59652 Villeneuve d Ascq, France

The dynamics of dewetting thin liquid films and the resulting film morphologies have been topic of intense research and great progress (experimental and theoretical) has been made. In particular the influence of the interplay between the rheology of the liquid and the slip at the liquid-substrate interface on the shape of dewetting fronts has been discussed in great detail.

We discuss the dewetting dynamics of thin slipping viscoelastic and

Newtonian films in hydrodynamic thin film models based on generalized Maxwell and Jeffreys models. Depending on the ratio of slip length to film thickness one obtains different slip regimes and different thin film models. For weak slip with slip lengths smaller than the film thickness our model predicts dewetting fronts which decay towards the resting film in an oscillatory fashion, independent of the rheological properties of the fluid. But strong slip can lead to monotonically decaying fronts even for Newtonian fluids, as confirmed by recent experiments.

CPP 19.9 Thu 12:15 ZEU Lich

New highly conductive formulation of PEDOT:PSS - a substitute of ITO for OLED anodes — ●KARSTEN FEHSE¹, KARSTEN WALZER¹, GUFENG HE¹, MARTIN PFEIFFER¹, KARL LEO¹, WILFRIED LÖVENICH², and ANDREAS ELSCHNER² — ¹Institut für Angewandte Photophysik, TU Dresden, D-01062 Dresden, Germany — ²H.C. Starck GmbH, Central Research and Development Division, c/o Bayer AG, Bldg. B 202, D-51368 Leverkusen, Germany

Standard organic light emitting diodes (OLEDs) emit through a transparent and electrically conductive substrate. Indium tin oxide (ITO) is usually used for this purpose. Due to increasing costs of ITO, we suggest the use of a polymer instead, which carries out both hole transport and injection. The OLED itself is based on a stack of small molecules with doped transport layers. We use a new highly conductive formulation of PEDOT:PSS with a conductivity of 500 S/cm, that provides a smooth and electrically suitable substrate for the OLED stack. We discuss both fluorescent and phosphorescent monochromatic OLEDs based on such a formulation which achieve good efficiencies. The OLEDs made thereon will be compared with devices of similar stack on ITO.

CPP 20.2 Thu 10:00 ZEU 160

Polymer melts slip over solid surfaces: Experimental studies of the slip length — ●RENATE FETZER¹, MARKUS RAUSCHER², and KARIN JACOBS¹ — ¹Dept. of Experimental Physics, Saarland University, D-66123 Saarbrücken, Germany — ²MPI for Metal Research, D-70569 Stuttgart, Germany

We present a novel method to assess the slip length and viscosity of thin films of highly viscous Newtonian liquids. We quantitatively analyze dewetting fronts of low molecular weight polystyrene melts on Octadecyl-

(OTS) and Dodecyltrichlorosilane (DTS) polymer brushes. Using a thin film (lubrication) model derived in the limit of large slip lengths, we can extract slip length and viscosity of films with thicknesses between 50 nm and 230 nm and temperatures above the glass transition. We find slip lengths from 100 nm up to 1 micron on OTS and between 300 nm and 10 microns on DTS covered silicon wafers. The slip length decreases with temperature. The obtained values for the viscosity are consistent with independent measurements.

CPP 20.3 Thu 10:15 ZEU 160

Single Molecule Diffusion in Confined Liquids under Shear — ●ARNE SCHOB and FRANK CICHOS — Photonics and optical materials, Institute of physics, TU Chemnitz, 09107 Chemnitz

The liquid-solid boundary is of fundamental importance for microfluidics, chromatography, lubrication and many other applications. Accessing the details and especially the molecular dynamics in this boundary region, however, involves a number of difficulties due to the fact that liquids dynamics varies on a length scale of a few nanometers. We present for the first time experiments that are based on the tracking of single dye molecules in liquid films confined in a surface forces apparatus. Our setup allows to follow molecular motion in liquid films of a few nanometer thickness and under applied shear flow. Employing a new method of single molecule diffusion analysis, we are able to separate the imposed shear velocity from the single molecule diffusion with an extremely high accuracy. Shear displacements of 8 nm within 15 ms can be detected even though diffusional displacements are at least by one order of magnitude larger. The studies on confined films of tetrakis(2-ethylhexoxy)silane demonstrate, that down to a film thickness of 10 nm no change in the effective viscosity of the liquid at the solid boundary occurs. Contrary to recent literature reports, no dependence of the diffusion constant on the shear rate is found.

CPP 20.4 Thu 10:30 ZEU 160

Factors affecting the determination of hydrodynamic slip by using the colloidal probe technique — ●ELMAR BONACCURSO, BENOIT SEMIN, and SVETLANA GURYIANOVA — Max-Planck-Institut für Polymerforschung

Recently, new insight has been gained in describing the boundary condition for the flow of a liquid on a solid, especially in microfluidic devices and other types of highly confined geometries. There is experimental evidence that the no-slip boundary condition, as usually applied for modeling macroscopic fluid flows, may break down at the nanometer scale, and that it might be replaced by a partial-slip boundary condition. One of the experimental techniques able to reveal the occurrence of slip at this scale is the colloidal probe technique: a micron-sized, spherical bead is attached to an atomic force microscope cantilever and pushed towards a solid, flat surface in the liquid which is tested. By measuring the interaction between sphere and surface, one can indirectly infer the velocity of the liquid at the boundary. Here we present a number of factors which affect such a measurement, thus allowing to determine/exclude the presence of slip and eventually helping to quantify it.

— 15 min. break —

Invited Talk

CPP 20.5 Thu 11:00 ZEU 160

Sorting in Structured Microfluidic Devices — ●ALEXANDRA ROS¹, JAN REGTMEIER¹, THANH TU DUONG¹, and DARIO ANSELMETTI² — ¹Bielefeld University, Experimental Biophysics and Applied Nanoscience, Universitätsstr. 25, 33615 Bielefeld, Germany — ²Bielefeld University, Fakultät für Physik, D-33615 Bielefeld

Suitably tailored microfluidic devices open access to unexpected dynamics and migration phenomena for colloidal particles and molecules. Recently, absolute negative mobility, i.e. the motion opposite to a net acting force, was observed in a lab-on-a-chip for colloidal particles [1]. This non-equilibrium effect is based on Brownian motion and non-linear dynamics induced by microstructuring. Exploiting the sensitive dependence of this paradoxical effect on basic particle properties, we demonstrate the simultaneous migration of two different species of alike-charged particles into opposite directions. The application of this new migration phenomenon for the separation or sorting of biomolecules, cell compounds and cells will be discussed.

[1] A. Ros, R. Eichhorn, J. Regtmeier, T. Duong, P. Reimann, D. Anselmetti, *Nature* **436**, 928 (2005)

CPP 20.6 Thu 11:30 ZEU 160

Modeling particle motion in structured microfluidic devices — ●RALF EICHHORN and PETER REIMANN — Universität Bielefeld, Fakultät für Physik, D-33615 Bielefeld

The motion of a colloidal particle in a structured microfluidic system under the influence of externally applied electric fields is modelled, including electroosmotic and electrophoretic effects as well as thermal fluctuations. The theory is applied to a microfluidic lab-on-a-chip known to exhibit absolute negative mobility [1] (i.e. net motion opposite to the net acting force) and predicts that two different species of like-charged particles may simultaneously migrate into opposite directions for suitable electric driving fields.

[1] A. Ros, R. Eichhorn, J. Regtmeier, T. Duong, P. Reimann, D. Anselmetti, *Nature* **436**, 928 (2005)

CPP 20.7 Thu 11:45 ZEU 160

Fluid transport in microchannels induced by high frequency travelling electric waves — ●MAIKA FELTEN¹, MAGNUS JÄGER², PETER GEGGIER², and CLAUS DUSCHL¹ — ¹Fraunhofer-Institut für Biomedizinische Technik, Invalidenstraße 42, 10115 Berlin — ²Universität des Saarlandes, Ensheimer Straße 48, 66386 St. Ingbert

Presently, the handling of fluid volumes in the nanoliter range suffers from a lack of suitable pumping methods. This severely limits the impact of lab-on-chip applications in biotechnology and cell biology. For the creating of a fluid flow in microchannels, we use a combination of temperature fields and high-frequency electric fields that act on the fluid. The temperature field induces inhomogeneities of the permittivity and / or conductivity of the medium. Together with the electric field, this creates volume charges in the liquid bulk which in turn interact with the electric field. To induce a certain flow direction, the electric potential is applied as a sinus-shaped wave travelling parallel to the channel axis. The use of temperature fields is a versatile method to control the fluid flow. For this reason, we combine temperature fields generated by the Ohmic heating due to the electric field with external heating sources like Peltier elements and laser light. By these means, we are able to generate a directed net fluid flow but also highly complex streaming patterns. These streaming patterns can be used to mix tiny volumes in a laminar flow or to accumulate nanoparticles in stationary vortices.

CPP 20.8 Thu 12:00 ZEU 160

Lattice Boltzmann studies of chaotic flows in microchannels — ●FATHOLLAH VARNIK and DIERK RAABE — MPI fuer Eisenforschung, Max-Planck Strasse 1, 40237 Duesseldorf

Via lattice Boltzmann simulations, it is shown that a qualitative change in flow properties may be triggered by a variation of the wall roughness/geometry alone. In particular, a transition from a steady flow toward an unsteady chaotic flow is observed as the roughness height in increased in shark teeth channels. Similar observations are also made for a random distribution of obstacles along the channel underlining the generality of the observed transition.

We focus on the impact of various roughness parameters on the transition showing that it is not the roughness height alone which determines the onset of flow instability. Rather, it is the combined effect of the roughness height- and wave length which is essential. In particular, by an increase of the roughness wave length, it is possible to trigger flow instability even if the roughness height is reduced.

In view of increasing number of potential applications of chaotic flows in civil engineering, environmental industry (e.g. solution recovery) as well as in the medical science (e.g. enhanced chaotic mixing in microchannels), the results of our studies may find a wide range of applications as they open an alternative way for tuning flow properties, namely via an appropriate channel design.

CPP 20.9 Thu 12:15 ZEU 160

Vibration dynamics of a bubbly fluid in a channel — ●ARTHUR STRAUBE¹ and SERGEY SHKLYAEV² — ¹University of Potsdam, Am Neuen Palais 10, PF 601553, D-14415 Potsdam — ²Department of Mathematics, Technion – Israel Institute of Technology, 32000 Haifa, Israel

We study the behavior of a bubbly fluid in a long channel subjected to small amplitude, high frequency oscillation. Bubbly medium dynamics is described in terms of an averaged model [1]. Evolution of a quiescent liquid with the uniform distribution of bubbles in the channel subjected to transversal vibration is chosen as the initial state. It is demonstrated that the behavior of small bubbles in the channel can be controlled: depending on the vibration frequency, bubbles either migrate to the boundaries

of the layer or accumulate into one or more steady stripes parallel to the boundaries; the characteristic width of the stripes depends on the diffusion of the bubbles. We perform a linear stability analysis and prove that such structures are stable up to some critical intensity of vibration

action. To understand the dynamics of the system beyond this threshold the full nonlinear system is analyzed numerically.

[1] A.V. Straube, D.V. Lyubimov, S.V. ShklyaeV, Averaged dynamics of two-phase media in a vibration field, submitted to Phys. Fluids.

CPP 21 SYMPOSIUM Functional Organic Thin Films II

Time: Thursday 14:00–17:00

Room: ZEU Lich

Invited Talk

CPP 21.1 Thu 14:00 ZEU Lich

Recent Advances in Charge Transport in Organic Field effect Transistors — ●ANANTH DODABALAPUR, LIANG WANG, LAWRENCE DUNN, and DEBARSHI BASU — Microelectronics Research Center, The University of Texas at Austin

This presentation will focus on two recent advances in studying charge transport in organic thin-film field-effect transistors with pentacene active semiconductor layers. With the help of electron-beam lithography we have fabricated transistors with short channel lengths. This, combined with careful surface treatments to improve hole injection, has enabled the fabrication of devices which are not seriously injection limited with channel lengths in the range between 250 nm and 5 microns. The electric-field dependence of carrier mobility has been measured in the range $10^4 - 6 \times 10^5$ V/cm and between 60-300 K by analyzing the transistor DC characteristics. The field dependence of the mobility more closely follows a Frenkel-type dependence than a polaronic dependence.

A new method to measure charge carrier mobility in organic field-effect has been developed in which the drift mobility of injected carriers (generated with a step voltage pulse) is measured. This permits the measurement of the velocity and mobility of the fastest carriers. The mobility evaluated in this manner is generally found to be higher than that obtained by the conventional technique based on an analysis of DC currents in a transistor. Extensions of our new method to measure the distribution of velocities or mobilities will also be described.

CPP 21.2 Thu 14:30 ZEU Lich

Ambipolar charge transport in the blend system $C_{60}/CuPc$ — ●ANDREAS OPITZ, MARKUS BRONNER, and WOLFGANG BRÜTTING — Experimental Physics IV, University of Augsburg, 86135 Augsburg, Germany

In recent years, large progress has been made in the realization of electronic circuits based on organic field-effect transistors (OFETs). However, these circuits as being built-up of unipolar (mostly p-type) OFETs only, have a number of drawbacks. To overcome them, recently, ambipolar OFETs have been suggested as a first step towards complementary organic circuits.

In this work we are analysing the ambipolar charge transport in blend systems of small organic molecules. These mixed layers are prepared by co-evaporation of n-conducting fullerene (C_{60}) and p-conducting copperphthalocyanine (CuPc) on pre-structured TFT-substrates. It was found that the electrical characteristics (e.g. mobilities of holes and electrons) depend strongly on the composition of the blend and on the preparation conditions like substrate treatment and substrate temperature during the evaporation. The preparation parameters act on the film morphology analysed by scanning force microscopy and on the electrical properties of the films. We further demonstrate ambipolar and complementary inverters with these materials as a basic constituent of more complex organic electronic circuits. Comparison with simulations based on an analytical model [1] shows that asymmetric mobilities and threshold voltages have to be avoided to reduce shifts in the inverter transfer curves.

[1] R. Schmechel et al., *J. Appl. Phys.* **98** (2005) 084511.

CPP 21.3 Thu 14:45 ZEU Lich

Inversion layer formation in organic field-effect devices — ●THOMAS LINDNER¹, GERNOT PAASCH¹, and SUSANNE SCHEINERT² — ¹IFW Dresden — ²TU Ilmenau

One of the challenges for polymer electronics is the realization of complementary circuits (CMOS) requiring both *n*- and *p*- channel transistors on the chip. Depositing both an electron-conducting and a hole-conducting organic material is technologically cumbersome. Only recently both *n*- and *p*- channels have been achieved in the same material. The problems to create both accumulation and inversion layers in the same material have been attributed to the difficulty to engineer the metallic source/drain contacts for efficient injection of both electron and holes, and also to the fact that the electron and hole mobilities differ (often) by

several orders of magnitude. Although the formation of inversion layers has been well understood in microelectronics, it has to be studied anew, since the mobility and the intrinsic density are many orders of magnitude lower. An analytical estimate of the relation between three relevant characteristic times reveals the peculiarities occurring in the organics. Detailed insight is obtained from a numerical simulation study for MOS capacitors and transistors of different design. Both the design and the source/drain contact properties influence the formation of the inversion layer and the occurrence of hysteresis effects significantly.

CPP 21.4 Thu 15:00 ZEU Lich

Field Effect Transistors and Space Charge Limited Currents on Perylene Single Crystals — ●G. ULBRICHT¹, J. SMET¹, A. TRIPATHI², J. PFLAUM², and K. VON KLITZING¹ — ¹Max Planck Institute for Solid State Research, 70569 Stuttgart — ²Universität Stuttgart, 3. Physikalisches Institut, 70550 Stuttgart

To understand the fundamental charge carrier transport in organic semiconductors, research on single crystals is necessary. Perylene is a well studied organic semiconductor and known to show high mobilities in time of flight experiments at low temperatures. We are studying Perylene single crystals by measuring space charge limited currents (SCLC) and field effect transistors (FETs). In the SCLC sandwich geometry, the crystals show exceptionally low trap densities down to $3 \cdot 10^{12}$ cm⁻³ as well as a distinct hysteretic behaviour. The latter helps to interpret the SCLC data significantly, in particular while contacts are not ideal. FETs were fabricated on the surface of Perylene crystals and characterised down to 180 K. Only hole conduction was observed. With as-prepared contacts, we calculated from the FET characteristics a lower limit of the mobility of about 10^{-5} cm²/Vs. Clear signs for the existence of significant contact barriers motivated us to explore different electrode materials and fabrication methods. We show that contact barriers can be significantly reduced by annealing source and drain electrodes after deposition. This does not change the threshold field of about $7 \cdot 10^7$ V/m, but raises the lower limit of the hole mobility measured by 2-point FET characteristics up to $1.3 \cdot 10^{-3}$ cm²/Vs. Supported by the DFG (Sm64/4, Pf385/2)

CPP 21.5 Thu 15:15 ZEU Lich

Light responsive ambipolar organic field-effect transistor based on amorphous thin films — ●TOBAT P. I SARAGI, IRINA SUSKE, KRISTIAN ONKEN, THOMAS FUHRMANN-LIEKER, and JOSEF SALBECK — Macromolecular Chemistry and Molecular Materials, Department of Science and Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), University of Kassel, Heinrich-Plett-Strasse 40, D 34109 Kassel, Germany.

In this contribution we demonstrate an ambipolar behavior of new spiro-linked compound. We used a field-effect transistor method to show the ambipolar behavior. Both p- and n-type transistor characters can be observed in our experiment. Surprisingly, both transistor characteristics are significantly enhanced as light used as additional control parameter. This effect makes the material is interesting for photosensor or other promising application. The change of drain current vs. drain voltage and drain current vs. gate voltage curves under illumination are presented and discussed as well. Moreover, the optical, thermal, surface morphology and electrochemical properties are presented and discussed as well.

— 15 min. break —

CPP 21.6 Thu 15:45 ZEU Lich

The realization of a defect-free pentacene based organic semiconductor diode: dominance of n-conduction — ●CARSTEN BUSSE¹, LARS RUPPEL¹, ALEXANDER BIRKNER¹, GREGOR WITTE¹, CHRISTOF WÖLL¹, and GERNOT PAASCH² — ¹Lehrstuhl für Physikalische Chemie I, Ruhr-Universität Bochum, 44780 Bochum, Germany — ²Leibnitz Institute for Solid State and Materials Research IFW Dresden, 01171 Dresden, Germany

We have fabricated an organic diode based on a defect-free organic semiconductor with two tunneling electrodes: Pentacene was deposited on an Au(111) surface, which was modified by an insulating self-assembled monolayer (SAM) of alkanethiols. High-resolution STM-data reveal the formation of virtually perfect pentacene islands. Using the tip of an STM and the Au-substrate as a pair of electrodes, we investigated the transport characteristics of this organic diode as a function of thickness of the pentacene layers and of temperature. In addition, the interface dipole at the pentacene / Au+SAM electrode was varied by changing the endgroups of the alkanethiols (-CH₃, -CF₃, -COOH). The results demonstrate that the transport properties are controlled by the built-up of a region with space-charge limited current just below the tip. The temperature dependence indicates that at room temperature and below the current in this model device is due to band-like transport. In addition, n-type behavior is seen in contrast to the commonly observed p-type behavior for polycrystalline pentacene.

CPP 21.7 Thu 16:00 ZEU Lich

How single conjugated polymer molecules respond to electric fields — ●F. SCHINDLER¹, J. M. LUPTON¹, M. J. WALTER¹, U. SCHERF², and J. FELDMANN¹ — ¹Photonics and Optoelectronics Group, Physics Department, LMU München — ²FB Chemie, Universität Wuppertal

For a microscopic understanding of the operation principle of optoelectronic devices based on organic thin films, such as polymeric light-emitting diodes, it is imperative to investigate the role of external electric fields (EFs) on the single molecule level. Single molecule fluorescence spectroscopy is a versatile tool for studying the intrinsic properties of individual chromophores which constitute the photophysical entity of a conjugated polymer (CP) molecule [1]. Here, we present the first report on how EFs influence the emission of single chromophores at low temperatures. Surprisingly, we observe a linear Stark effect which originates from a permanent polarisation of the π -electron system [2]. This can be thought of in terms of an effective dipole, which is averaged out in the ensemble but nevertheless sensitively controls bulk effects. The effective dipole orientation with respect to the backbone is identified for different CPs and provides direct insight into the intrinsic internal EFs acting on the single chromophore. These fields lead to charge conjugation symmetry breaking of the π -electron system and naturally bear substantial implications for the use of conjugated polymers in functional organic thin films.

[1] F. Schindler et al., PNAS 101, 14695 (2004)

[2] F. Schindler et al., Nature Mat. (in press)

CPP 21.8 Thu 16:15 ZEU Lich

Energy transfer between zinc-phthalocyanine and CdSe/ZnS nanocrystals for sensitizing organic photovoltaics — ●ROBERT KOEPPE, ANITA FUCHSBAUER, SHENGLI LU, and NIYAZI SERDAR SARICIFTCI — Linz Institute for Organic Solar Cells (LIOS), Altenbergerstr. 69, A-4040 Linz, Austria

Zinc-phthalocyanine (ZnPc) and C60 is a material combination for the manufacturing of high efficiency thin film organic solar cells [1]. The low absorption coefficient of both materials around 500nm light wavelength where the solar photon flux has its maximum is a loss mechanism leading to a low quantum efficiency in this range. A Förster energy transfer from a donor absorbing in this wavelength range onto the ZnPc molecule is proposed. As a model system we investigate CdSe/ZnS core-shell nanocrystals as energy transfer donor together with ZnPc as acceptor. In a bilayer configuration we see strong quenching of the nanoparticle luminescence in dependence on the size of the organic ligand shell around the nanocrystals. This distance dependence indicates an effective energy transfer between the nanocrystals and the ZnPc film. [1] D. Wöhrle, D. Meissner, Adv. Mater., 3, 129 (1991)

CPP 21.9 Thu 16:30 ZEU Lich

Impedance spectroscopy on organic semiconductors for solar cell application — ●MARTIN KNIPPER¹, JÜRGEN PARISI¹, and VLADIMIR DYAKONOV² — ¹Energy and Semiconductor Research Laboratory, Department of Physics, University of Oldenburg, 26111 Oldenburg, Germany — ²Faculty of Physics and Astronomy, University of Würzburg, Am Hubland, 97074 Würzburg, Germany

Impedance spectroscopy is a powerful tool for studying the electrical transport properties of bulk heterojunction solar cells. The photovoltaic absorber consist of a mixture of poly(3-hexylthiophene) (P3HT) and [6,6]-phenyl-C₆₁-butyric acid methyl ester (PCBM), sandwiched between a transparent indium tin oxide (ITO) front electrode and a metal (Au or Al) back electrode as well as a polymer buffer layer (PEDOT:PSS). We look at the individual material components as well as the composites with and without the PEDOT:PSS interfacial layer. It allows us to investigate the internal device structure, the behaviour of the interfacial layer and the metal/P3HT junction. For the various devices we find different equivalent circuit diagrams. Upon varying the thickness of the semiconductor layer, it is aimed to discriminate bulk and surface effects, in order to improve the preparation process of the composite absorber. From this measurements we found an ϵ_r of 3 for the P3HT and one of 3.4 for the PCBM:P3HT bulk heterojunction.

CPP 21.10 Thu 16:45 ZEU Lich

Optimising Polythiophene based bulk heterojunction solar cells reaching 5% power conversion efficiency — ●HARALD HOPPE, TOBIAS ERB, and GERHARD GOBSCH — Institute of Physics, Ilmenau Technical University, Weimarer Str. 32, 98693 Ilmenau, Germany

State of the art plastic solar cells reaching power conversion efficiencies of 5% are reported. These solar cells are based on the poly(3-alkyl)thiophene-fullerene bulk heterojunction system, exhibiting a relatively low fullerene content. To obtain the optimum balance between charge generation and transport, the film thickness of the photoactive layer was varied. Morphological factors for reaching efficient and stable devices are discussed.

CPP 22 SYMPOSIUM Microfluidics II: Soft objects in flow, open geometries

Time: Thursday 14:00–17:00

Room: ZEU 160

Invited Talk

CPP 22.1 Thu 14:00 ZEU 160

Confinement and manipulation of single molecules in micro- and nanochannels — ●PETRA SCHWILLE, FEDOR MALIK, PETRA S. DITTRICH, and MADHAVI KRISHNAN — Institute for Biophysics, Biotechnology Center, Technical University Dresden

Micro- and nanofluidic structures are ideally suited to observe and manipulate minute amounts of biomolecules under close-to-native conditions without tedious and error-prone immobilization to surfaces. In particular, soft polymer structures such as PDMS can be easily adapted to host several manipulation steps, e.g. for solution mixing and cell or

particle sorting on one chip, and at the same time allow to analyze the solution by high resolution optics such as single molecule fluorescence spectroscopy. We discuss several successful and promising microfluidic applications, such as for enzyme kinetics, particle sorting, and the design of a chip allowing for the generation of $\sim 5\mu\text{m}$ sized homodisperse droplets that contain the reaction mixture for cell-free protein expression, as a basic model for what could be developed into artificial cells.

Recently, we devised a strategy to quantitatively study the translocation of DNA binding proteins, such as helicases, restriction endonucleases and exonucleases at the single molecule level by scaling down the structure sizes to nanochannels whose dimensions approach the persistence

length of DNA (50-60 nm). The method is based on the entropic stretching of DNA in confined structures, and the subsequent application of fluorescence techniques such as bright field fluorescence microscopy and/or Fluorescence Correlation Spectroscopy to quantify transport coefficients of enzymes that translocate along the DNA backbone

CPP 22.2 Thu 14:30 ZEU 160

Dynamics and Formation of Actin Bundles in Extensional Flow — ●DAGMAR STEINHAUSER, SARAH KÖSTER, and THOMAS PFOHL — Max-Planck-Institut für Dynamik und Selbstorganisation, Bunsenstrasse 10, 37073 Göttingen

We are interested in the dynamics of biopolymers under extensional flow and the formation of condensed structures, bundles and networks, induced by inter-chain and intra-chain linker molecules. In particular the bundling behavior of actin filaments in presence of actin binding proteins (e.g. α -actinin) or multivalent ions is considered. Actin filaments as well as their bundles and networks are visualized in continuous flow by stroboscopic laser light illumination. Using a hydrodynamic focusing device we are able to observe the evolution of the bundling of individual filaments. A detailed analysis of the fluctuations of the formed bundles leads to information about their stiffness in dependence on the number of actin filaments.

CPP 22.3 Thu 14:45 ZEU 160

Electrophoretic mobility of DNA from Lattice Boltzmann simulations — ●SANDEEP TYAGI¹ and CHRISTIAN HOLM^{1,2} — ¹Frankfurt Institute for Advanced Studies, Max-von-Laue-strasse 1, D-60438 Frankfurt am Main, Germany — ²Max-Planck-Institut für Polymerforschung, Ackermannweg 10, D-55128 Mainz, Germany

We investigate the electrophoretic motion of DNA of various length under the influence of an applied DC electric field in the bulk and under confinement. The simulation method uses an implicit solvent model with an effective dielectric permittivity, but includes both long range hydrodynamic and full electrostatic interactions. The DNA is treated via a semi-flexible bead-spring model. The charged "beads" on the DNA and the associated free counterions are frictionally coupled to the solvent using a lattice Boltzmann solver due to Ahlrichs and Dünweg (J. Chem. Phys., Vol. 111, 1999). This efficient technique that scales linearly with the number of particles is demonstrated to produce experimentally known results for the dependence of the electrophoretic mobilities of DNA on the degree of polymerization. Chain conformations of DNA and the corresponding counterion distribution around the chains at various externally applied electric fields are probed. We also discuss the extension of this technique for studying electrophoretic motion of charged objects in slit-pore including dielectric boundaries.

CPP 22.4 Thu 15:00 ZEU 160

Freely suspended actin cortex models in a controlled microfluidic environment — ●TAMAS HARASZTI^{1,2}, SIMON SCHULZ^{1,2}, WOUTER ROOS^{1,2}, CHRISTIAN SCHMITZ^{1,2}, JENS ULMER^{1,2}, STEFAN GRÄTER^{1,2}, and JOACHIM SPATZ^{1,2} — ¹Max-Planck-Institute for Metals Research, Department New Materials & Biosystems, Heisenbergstr. 3, D-70569 Stuttgart — ²Biophysical Chemistry, University of Heidelberg, INF 253, D-69120 Heidelberg

Arrays of pillars, microfabricated in PDMS, are constructed to serve as a template for mimicking the actin cortex of cells. The three-dimensional template surface prevents confinement effect on the actin filaments hanging between pillars at a height of about 10 microns. A special flow-cell design enables applying flow -an external driving force- around the network of actin. This unique experimental system opens new possibilities, for example to study the mechanics of two-dimensional actin networks as a function of actin-crosslinkers, to observe the active diffusion of molecular motors operating on pending networks and to investigate the alternations in the transport of microscopic particles, coated by different proteins, along these actin cortex models under the drag of flow.

Such transport problems are studies of tracks and external driving forces (motors, flow) on a statistical process under the influence of order and randomness along two-dimensional networks isolated from the complicated and undetermined cellular environment. The filaments are visualized by fluorescent optical microscopy, and their stiffness can be tuned by bundling of actin filaments through various cross-linkers.

CPP 22.5 Thu 15:15 ZEU 160

Dynamic behaviour of quasi spherical vesicles in Stokes flow — ●REIMAR FINKEN and UDO SEIFERT — II. Institut für Theoretische Physik, Pfaffenwaldring 57 / III, 70550 Stuttgart, Germany

The behaviour of soft objects in hydrodynamic flow has received increasing attention in recent years, both theoretically and experimentally. As a paradigmatic model system lipid bilayer vesicles have been investigated extensively. When the viscosity of the fluids inside and outside the vesicle are the same, theories and computer simulations predict a stationary motion with fixed vesicle shape. For increasing viscosity ratio between inner and outer fluid, a dynamical phase transitions towards an unsteady motion is expected. Both behaviours have been observed experimentally very recently for the first time. We present a fully dynamic three dimensional theory that takes advantage of the small deviations from a spherical shape. The tanktreading to tumbling transition is investigated and compared to the recent experiments. This semi-analytical approach has the merit of becoming exact in the limit of small excess area of the vesicle, while allowing more insight into the underlying physics than a purely numerical scheme. We contrast our results with existing simplified analytic theories, which either assume a fixed shape or a two dimensional geometry. The asymptotic exactness of our approach allows a quantitative discussion of these simplifications.

— 15 min. break —

Invited Talk

CPP 22.6 Thu 15:45 ZEU 160

Unconventional Microfluidics — ●RALF SEEMANN¹, JEAN-CHRISTOPHE BARET², K. KHARE¹, CRAIG PRIEST¹, and STEPHAN HERMINGHAUS¹ — ¹MPI for Dynamics and Self-Organisation, Bunsenstr. 10, D-37073 Göttingen, Germany — ²Philips Research Laboratories, NL-5656AA Eindhoven, The Netherlands

Microfluidics usually involves single phase liquids transported through closed microchannel networks. Instead, we explore open systems with freely accessible liquid interfaces as well as compartmented liquids in closed microchannels. In our project we study the wetting morphologies on topographic substrates and explore the possibility to transport liquid by switching in the various liquid morphologies. The morphologies are determined by the contact angle of the liquid and the geometry of the grooves [1]. Electrowetting is used to tune the contact angle, leading to reversible transitions between a drop-like morphology and extended liquid filaments. The transition is capillarity-driven but the behavior of the liquid above the transition is influenced by the electrical properties of the liquid [2]. Furthermore, we employ monodisperse emulsions to compartment liquids for microfluidic processing. If the volume fraction of the continuous phase is small, the dispersed compartments (droplets) assemble into well-defined arrangements, analogous to foam. Hence, the position of a single droplet within an ensemble of droplets is fully determined while being transported through microfluidic channels. We demonstrate an in situ method for the production of such monodisperse emulsions, suitable for microfluidic processing [3] and a variety of channel geometries for positioning, sorting, dividing, and selectively induced coalescing of droplets in 'lab-on-chip' style processing.

[1] R. Seemann, et al. PNAS 102, 1848 (2005)

[2] J.-C. Baret, M. Décré, S. Herminghaus, and R. Seemann, Langmuir (in press)

[3] C. Priest, S. Herminghaus, and R. Seemann, Appl. Phys. Lett. (in press)

CPP 22.7 Thu 16:15 ZEU 160

Dissipative Particle Dynamics as a simulation tool for confined nanofluidic systems. — ●BJÖRN HENRICH^{1,2}, CLAUDIO CUPPELLI³, MICHAEL MOSELER^{2,1}, and MARK SANTER³ — ¹University of Freiburg-FMF, Freiburg Materials Research Center, D-79104 Freiburg, Germany — ²IWM, Fraunhofer Institute for Mechanics of Materials, Wöhlerstraße 11, D-79108 Freiburg, Germany — ³University of Freiburg-IMTEK, Department of Microsystem Engineering, Georges-Köhler-Allee 106, D-79110 Freiburg, Germany

Fluid particle methods such as Dissipative Particle Dynamics are continuum simulation approaches to represent fluids, suspensions or polymers on mesoscopic time and length scales. We report how this simulation technique may be applied to study nano scale ($> 1\text{nm}$ and $< 100\text{nm}$) impregnation and imbibition phenomena. Pursuing the approach of Warren [1] to account for cohesive properties, we show how adequate solid-liquid interfaces based on "live" walls can be constructed to allow for a

variable static contact angle, at the same time avoiding artefacts such as temperature or density oscillations that often occur when rigid walls are used. This model is then utilized to study the impregnation dynamics into a nano slit pore that is filled out of a finite reservoir. We find that the dynamic apparent contact angle within the pore can be determined reliably, and with respect to the capillary number, differs significantly from the one extracted from numerical plug flow experiments.

[1] Phys. Rev. E, 066702 (2003)

CPP 22.8 Thu 16:30 ZEU 160

Ratchet driven microfluidic transport — •KARIN JOHN¹ and UWE THIELE^{1,2} — ¹Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, D-01187 Dresden, Germany — ²Lab. Spectrometrie Physique, Univ. J. Fourier - Grenoble I, 140 Av. Physique, 38402 Saint-Martin d'Herès, France

Transport in spatially extended systems can be induced if nonequilibrium fluctuations and a broken spatial symmetry are present [1]. This can be realized using a global gradient or a globally homogeneous system that displays local time-periodic asymmetries, e.g., a flashing periodic asymmetric potential (ratchet). Examples where a diffusive transport is induced are molecular motors [2] or the particle transport through asymmetric pores [3].

We propose a concept for ratchet driven open microfluidic flow, i.e. involving liquid with a free surface, like droplets and films. After introducing the basic principle, a theoretical model in long-wave approximation [4] is presented. It is used to analyse the ratchet-driven convective transport in detail.

[1] R. D. Astumian, Science **276**, 917–922 (1997).

[2] F. Jülicher, A. Ajdari, A. and J. Prost, Rev. Mod. Phys. **69**, 1269–1281 (1997).

[3] S. Matthias and F. Müller, F., Nature **424**, 53-57 (2003).

[4] A. Oron, S. H. Davis and S. G. Bankoff, Rev. Mod. Phys. **69**, 931-980 (1997).

CPP 22.9 Thu 16:45 ZEU 160

Pearling instability of nanoscale fluid flow confined to a chemical channel — •M. RAUSCHER^{1,2}, J. KOPLIK³, T. S. LO³, and S. DIETRICH^{1,2} — ¹Max-Planck Institut für Metallforschung, Heisenbergstr. 3, 70569 Stuttgart, Germany — ²Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany — ³Benjamin LeVich Institute and Department of Physics, City College of the City University of New York, New York, NY 10031, USA

We investigate the flow of a nano-scale incompressible ridge of low-volatility liquid along a "chemical channel": a long, straight, and completely wetting stripe embedded in a planar substrate, and sandwiched between two extended less wetting solid regions. Molecular dynamics simulations, a simple long-wavelength approximation, and a full stability analysis based on the Stokes equations are used, and give qualitatively consistent results. While thin liquid ridges are stable both statically and during flow, a (linear) pearling instability develops if the thickness of the ridge exceeds half of the width of the channel. In the flowing case periodic bulges propagate along the channel and subsequently merge due to nonlinear effects. However, the ridge does not break up even when the flow is unstable, and the qualitative behavior is unchanged even when the fluid can spill over onto a partially wetting exterior solid region.

CPP 23 POSTER Functional Organic Thin Films

Time: Thursday 17:00–19:00

Room: P2

CPP 23.1 Thu 17:00 P2

Watching organic semiconductors grow: In-situ and real-time spectroscopic ellipsometry — •S. KOWARIK^{1,2}, U. HEINEMEYER¹, G. HUMPHREYS², R. JACOBS², A. GERLACH^{1,2}, and F. SCHREIBER¹ — ¹Institut für Angewandte Physik, Universität Tübingen, Auf der Morgenstelle 10, 72076 Tübingen — ²Physical and Theoretical Chemistry Laboratories, Oxford University, South Parks Road Oxford OX1 3QZ

Thin films of organic semiconductors and dyes are receiving significant attention, and their potential for electronic and optoelectronic device applications is obvious. Optimisation of device performance requires the understanding of the underlying preparation procedures. For this purpose real-time measurements are particularly powerful since they detect possible changes in the functional properties already during growth. We demonstrate the use of spectroscopic ellipsometry as a non-invasive technique for following diindenoperylene and pentacene growth in situ and in real time. It is possible to take spectra in the entire spectral range between 1.25eV and 5 eV sufficiently fast to follow organic molecular beam deposition in detail. We show how this technique can be used to detect spectral changes occurring during growth of these complex materials.

CPP 23.2 Thu 17:00 P2

Growth of Pentacene on clean and modified Gold Surfaces — •DANIEL KAEFER, LARS RUPPEL, GREGOR WITTE, and CHRISTOF WOELL — Physikalische Chemie I, Ruhr Universitaet Bochum, 44780 Bochum

Because of its high charge carrier mobility and the ability to form (poly-)crystalline films pentacene is still one of the most promising organic semiconductor for the fabrication of organic thin film transistors. Of particular interest is the interaction and growth at the gold interface which is commonly used as electrode material. In view of partly controversial results which have been reported so far for growth of pentacene on gold we have carried out a comprehensive study including temperature and rate dependency as well as the influence of substrate roughness. By combining various microscopy techniques (SEM, STM, AFM) with NEXAFS and UPS the growth scenario of pentacene on clean single crystals and polycrystalline gold surfaces has been compared.

On clean gold surfaces the first monolayer forms a chemisorbed seed-layer with planar adsorption geometry while subsequent growth is characterized by a pronounced dewetting and formation of needle-like islands where molecules adopt a bulk-like upright orientation. At very large deposition rates rather disordered films are formed where this molecular

reorientation is quenched. A distinctly different growth scenario was observed for gold surfaces which had been modified before by a SAM. In that case no planar oriented seed-layer is formed and pentacene molecules grow immediately in an upright orientation without any dewetting.

CPP 23.3 Thu 17:00 P2

Quantitative investigation of the dielectric properties in the ab-plane of pentacene single crystals — •MANDY GROBOSCH¹, THOMAS PICHLER¹, HELMUTH BERGER², MARTIN KNUPFER¹, and WIELAND ZAHN³ — ¹IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany — ²Institute of Physics of Complex Matter, EPFL, CH-1015 Lausanne, Switzerland — ³Westsaechsische Hochschule Zwickau (FH), Dr.-Friedrichs-Ring 2a, D-08056 Zwickau, Germany

Polarization dependence of the optical reflectivity spectra of pentacene single crystals grown by sublimation have been investigated over a wide range of frequencies from the middle infrared to the visible range (5meV to 3 eV) at room temperature. Furthermore measurements with electron energy-loss spectroscopy (EELS) in transmission have been performed on pentacene thin films. A series of optical phonon modes and electronic transitions have been observed. The determination of the electronic properties have been carried out in the energy rang from 1.7 eV to 2.3 eV within a Lorentz-model. In addition to previous studies we observed the onset of the optical absorption at 1.87 eV followed by a series of four excitations at 1.97 eV, 2.11 eV, 2.14 eV, and 2.28 eV. The results revealed that the dielectric function of pentacene single crystals shows a strongly anisotropic dependence in the ab-plane on the polarization of the incident light.

CPP 23.4 Thu 17:00 P2

Unit cell and defect densities of pentacene thin films — •STEFAN SCHIEFER, MARTIN HUTH, BERT NICKEL, MATTHIAS FIEBIG, and UDO BEIERLEIN — Department für Physik & CeNS Ludwig Maximilians Universität München

Organic electronic devices generally employ thin films of a semi conducting material as the active region where charge is carried. So far there is no clear understanding of the charge transport mechanisms in the active region. By getting a better understanding of the structure-function relationship of the semi conducting organic thin film layer we hope to further improve the electron charge mobility.

We grew thin films of pentacene on SiO₂ in UHV and performed in situ x-ray diffraction experiments at the synchrotron source at HASY-

Lab, Hamburg. By simulating and analysing the data, we were able to determine the unit-cell dimension and the defect densities of a pentacene thin film on SiO₂ surfaces.

CPP 23.5 Thu 17:00 P2

Optical spectroscopy of vapour deposited rubrene films — ●OLGA KRYLOVA, ANDREAS LANGNER, and MORITZ SOKOLOWSKI — Institut für Physikalische und Theoretische Chemie, Universität Bonn, Wegelerstr. 12, 53115 Bonn, Germany

Thin films of rubrene (150 nm) were fabricated by vapour deposition on glass and the absorption and fluorescence spectra were investigated as a function of temperature. We observe a reversible red-shift of the emission maximum of 500 cm⁻¹ at about 150-200 K. Interestingly, a similar change has been observed in the fluorescence spectra of thin tetracene films earlier and was attributed to a structural phase transition [1]. However, since rubrene films deposited at room temperatures were identified as amorphous [2], the origin of this shift may have a different origin for rubrene, which will be discussed. Supported by the DFG through the research unit 557.

[1] H. Nishimura et al., J. Phys. Soc. Japan 54 (1985) 4.

[2] D. Käfer, G. Witte, Phys. Chem. Chem. Phys. 7(15) (2005) 2850.

CPP 23.6 Thu 17:00 P2

Structure and Crystallinity Study of Conjugated Polymers — ●SIDDHARTH JOSHI¹, ULLRICH PIETSCH¹, SOUREN GRIGORIAN¹, ACHMAD ZEN², and DIETER NEHER² — ¹Festkörperphysik, Universität Siegen, Siegen, Germany — ²Institut für Physik, Universität Potsdam, Potsdam, Germany

The molecular aggregation structure of organic thin films based on semiconducting conjugated polymers has received much attention due to application to polymer electronic devices such as light-emitting diodes, field-effect transistors (FETs) and photovoltaic cells (PVs). One central problem in organic field-effect transistor concerns with the relatively low charge-carrier mobility compared to semiconductor devices. Our current studies are focussed on structure investigations of polymer thin films. Using Ruland's method several fractions of regioregular (RR) polymers (P3HT, P3dHT) with different molecular weight fractions. To have access to thin films of about 10 nm thickness we used the grazing incidence X-ray diffraction (GIXD) and synchrotron radiation. We determined the degree of crystallinity, and average size of crystallites in polymer films. At the same time we have also employed atomic force microscopy AFM (tapping mode) and X-ray reflectivity methods to study the surface morphology and average thickness of organic thin film. As major result we found that polymers with low molecular weight show a higher degree of crystallinity compared to films with high molecular weight. The results of this structure investigations can be used to interpret the charge-carrier mobility for OFETs.

CPP 23.7 Thu 17:00 P2

Effect of the Spacer Chain length on the Molecular Orientation and Packing Density of Terphenylalkanethiols on Au(111): Combined STM and FTIR Characterization: — ●ASIF BASHIR¹, WALEED AZZAM¹, ANDREAS TERFORT², THOMAS STRUNSKUS¹, and CHRISTOF WÖLL¹ — ¹Lehrstuhl für Physikalische Chemie I, Ruhr Universität Bochum — ²Institut für Anorganische und Angewandte Chemie, Universität Hamburg

Recently, the charge transport properties of aromatic thiolate, have received extensive attention because of their relative stability to other potential molecular electronic materials. Here, we report studies on Self-assembled monolayers (SAMs) of 4,4'-terphenyl-substituted alkanethiols C₆H₅(C₆H₄)₂(CH₂)_n-SH (TP_n, n = 1-6) adsorbed on Au (111) substrates using scanning tunneling microscopy (STM) and reflection absorption infrared spectroscopy (RAIRS). At 298 K, the structure and molecular orientation of TP_n films (except TP₂) exhibit a pronounced odd-even effect regarding both, the molecular orientation and packing density. Odd-numbered SAMs adopt a highly ordered (2√3 × √3)R30° structure. SAMs made from even-numbered TP_n thiols, on the other hand exhibit a very different structure with a reduced packing density. At 298 K, a (5√3 × 3) rectangular unit cell was found for TP₄ and TP₆ SAMs. Whereas the structure of the odd numbered TP_n SAMs is retained at a temperature of 333 K, the even-numbered SAMs undergo phase transitions to phases having a lower packing density. We will also report first results obtained for the geometric structures using ab-initio (DFT) electronic structure calculation.

CPP 23.8 Thu 17:00 P2

Spectroscopic Investigation of Thioaromatic Self-Assembled Monolayers on Gold — ●MIHAELA BADIN¹, ANDREAS TERFORT², THOMAS STRUNSKUS¹, and CHRISTOF WÖLL¹ — ¹Lehrstuhl für Physikalische Chemie I, Ruhr-Universität Bochum — ²Institut für Anorganische und Angewandte Chemie, Universität Hamburg

Self-assembled monolayers (SAMs) are the most important model system for investigating the physical and chemical properties of ultrathin molecular layers. Here, we report on several novel tips of SAMs based on synthesized organothiols. SAMs formed from triptyceniethiol (C0T), mercaptomethyltriptyceniethiol (C1T), and mercaptopropyltriptyceniethiol (C3T) on gold are characterized by infrared reflection absorption spectroscopy, X-ray photoelectron spectroscopy and near-edge X-ray absorption fine structure spectroscopy. The aromatic rings and the rigidity of the aromatic system determine the molecular orientation and orientational order of the thioaromatic molecules. In C1T and C3T the insertion of the methylene group creates a conformational flexibility which is important to yield high quality films.[1] Measurement results confirm that these molecules form highly oriented monolayers on the gold surface. C1T and C3T molecules show a tilted orientation with respect to the surface normal. In addition several SAMs formed from different substituted triaryl amines are studied under deprotection conditions.

[1] Cyganik, P.; Buck, M.; Azzam, W.; Wöll, C. J. Phys. Chem B 2004, 108, 4989-4996

CPP 23.9 Thu 17:00 P2

Electronic Properties of DNA Base Layers on H-passivated Si(111)(7x7) — ●STEFAN SEIFERT¹, GIANINA GAVRILA¹, WALTER BRAUN², and DIETRICH R.T. ZAHN¹ — ¹Chemnitz University of Technology, Semiconductor Physics, D-09107 Chemnitz, Germany — ²BESSY GmbH, Albert-Einstein-Straße 15, Berlin, D-12489, Germany

Despite of the increasing interest in the charge transport properties of DNA base stacks and poly DNA strands, reliable data on the electronic properties of DNA bases in the condensed phase is rare if at all available. Therefore, an extensive photoelectron spectroscopy study of layers of adenine, cytosine, and guanine is presented in comparison with density functional theory (DFT) calculations for single molecules. The layers were prepared under ultra high vacuum conditions by organic molecular beam deposition onto H-passivated Si(111)(7x7). The valence band photoemission (VB-PE) spectra of these layers were obtained with 55eV and 150eV excitation energy at the synchrotron facility BESSY. The determined ionization energies for the bio-organic layers are considerably smaller than those of free molecules. The adenine and cytosine layers show formation of an interface dipole with the substrate while the interface between guanine layers and H-Si(111)(7x7) displays nearly vacuum level alignment. The comparison of the VB-PE spectra to DFT/B3LYP calculations for single molecules (with 6-311+G(p,d) basis sets) reveals clear signs of band formation in cytosine and guanine layers.

CPP 23.10 Thu 17:00 P2

Energy Level Alignment at Dihexylsexithiophene-Metal Interfaces — ●STEFFEN DUHM¹, HENDRIK GLOWATZKI¹, ROBERT L. JOHNSON², JÜRGEN P. RABE¹, and NORBERT KOCH¹ — ¹Humboldt-Universität zu Berlin, Institut für Physik, Newtonstr. 15, D-12489 Berlin — ²Universität Hamburg, Institut für Experimentalphysik, Luruper Chaussee 149, D-22761 Hamburg

The energy level alignment at metal-organic interfaces is a key issue for improving the performance of novel organic (opto-) electronic devices. In certain cases, solution-based processing of organic materials is preferred over vacuum sublimation. Frequently, alkyl side-chains are attached to the conjugated moieties for improved solubility. To investigate the influence of alkyl side-chain addition on interface energetics, we studied interfaces formed between the organic molecules sexithiophene (6T) and α,ω-dihexylsexithiophene (DH6T) and the metal surfaces Ag(111) and polycrystalline Au using ultraviolet photoelectron spectroscopy (UPS). Morphology was investigated with Atomic Force Microscopy (AFM) in ultra-high-vacuum. Interestingly, we observed significantly lower hole injection barriers (0.6 eV) for DH6T on the metal surfaces than for 6T. We explain this behavior in terms of the molecular orientation. In addition, we demonstrate that the hole injection barrier at interfaces between DH6T and metals can be further reduced by the insertion of (sub)monolayers of the strong electron acceptor tetrafluoro-tetracyanoquinodimethane (F4-TCNQ).

CPP 23.11 Thu 17:00 P2

Doping and Diffusion Properties of Alkali Metals in PTCDA Thin Films — ●KATHRIN HEIMER, JENS WÜSTEN, STEFFEN BERGER, STEFAN LACH, and CHRISTIANE ZIEGLER — University of Kaiserslautern, Department of Physics, 67663 Kaiserslautern

n-doping of the molecular organic semiconductor perylene-3,4,9,10-tetracarboxylic-dianhydride (PTCDA) is often achieved by evaporation of alkali metals onto the surface of the PTCDA film. It is expected that there are differences in the doping behaviour between the alkali metals [1]. Furthermore it has been believed that the dopant shows a diffusion profile through the layer with most of the dopant accumulated in the first few layers [2].

In this contribution both experimental results concerning chemical composition ((angle resolved) X-ray photoemission spectroscopy ((AR)-XPS), Fouriertransform infrared spectroscopy (FT-IR), electronic structure (ultraviolet photoemission spectroscopy (UPS)), inverse photoemission spectroscopy (IPE)) [3] and theoretical results concerning FT-IR are shown before and after doping with three different alkali metals, sodium, potassium and cesium, respectively.

These results suggest that the three alkali metals diffuse into and react with the PTCDA film in different ways. Models for the dopant distributions are suggested.

[1] K. Heimer, Ch. Ziegler, in preparation

[2] J. Wüsten, Th. Ertl, Ch. Ziegler, Appl. Surf. Sci. 252 (1), 104-107 (2005)

[3] J. Wüsten, S. Berger, K. Heimer, S. Lach, Ch. Ziegler, J. Appl. Phys. 98, 013705 (2005)

CPP 23.12 Thu 17:00 P2

Hot Electron Dynamics in Sodium doped PTCDA thin Films — ●JENS WÜSTEN, STEFFEN BERGER, MARC SALOMON, MICHAEL BAUER, STEFAN LACH, MARTIN AESCHLIMANN, and CHRISTIANE ZIEGLER — University of Kaiserslautern, Department of Physics, Erwin-Schrödinger-Straße 56, 67663 Kaiserslautern

Time resolved 2 photon photoemission (2PPE) measurements of the doping process of PTCDA thin films with sodium give insight into the dynamics of hot electrons in this system. Interaction with sodium results in a charge transfer from sodium to PTCDA ("n-doping") and is accompanied by an increase of the lifetime of electrons excited to unoccupied states 1.4 - 1.8 eV above the Fermi level. Supported by DFT-calculations of molecular orbital energies and excited state energies, this result can be explained from a joint physical viewpoint that combines the one electron picture, treated in "classical" photoemission spectroscopy theory, with many electron excitations as commonly considered in optical spectroscopy. As thin PTCDA layers on a Ag(111) surface show up similar features in UV photoelectron spectroscopy as sodium doped PTCDA, this system has also been investigated by 2PPE. An increase of lifetime can be observed for thin PTCDA coverages, which points at a charge transfer from Ag to PTCDA.

CPP 23.13 Thu 17:00 P2

Development of a high performance OFET on well ordered sapphire — ●SÖNKE SACHS, MATTHIAS PAUL, ACHIM SCHÖLL, and EBERHARD UMBACH — Experimentelle Physik II, Am Hubland, 97074 Würzburg, Germany

The charge carrier mobility in organic field effect transistors strongly depends on the structural quality of the active medium. For thin film transistors the structural order is strongly influenced by the structure, morphology, and interaction potential of the substrate, which in case of a bottom gate geometry is an insulator.

For such a geometry we try to optimize the film growth by using a highly-ordered, clean, and well-characterized single-crystalline (11 $\bar{2}$ 0) sapphire (α -Al₂O₃) substrate. With the organic semiconductor diindenoperylene (DIP) we demonstrate that the organic film grows polycrystalline with large single crystalline domains. An AFM analysis indicates that under optimized preparation conditions the size of these crystallites is only limited by the dimensions of the substrate terraces. Moreover, XPS and NEXAFS results show only weak interaction at the interface and a preferential upright orientation of the DIP molecules within the crystallites, thus exhibiting very favorable conditions for a high performance OFET. A design for an optimized model OFET is discussed.

CPP 23.14 Thu 17:00 P2

Charge carrier transport in P3HT diodes and transistors — ●SILVIU GRECU, ANDREAS OPITZ, and WOLFGANG BRÜTTING — Experimental Physics IV, University of Augsburg, 86135 Augsburg, Germany

It has been demonstrated recently that the hopping mobility in semiconducting polymers depends on the charge carrier concentration. Owing to differences in the densities of injected carriers of several orders of magnitude between organic field-effect transistors (FETs) and diodes, significant differences in the charge carrier mobilities of these devices have been observed.

We have investigated the temperature dependence of the mobility for three different kinds of organic devices: hole-only diodes, metal-insulator-semiconductor (MIS) diodes and FETs fabricated from regular poly(3-hexylthiophene) (rr-P3HT). Surface treatment of the substrate and different solvents for the polymer are used to change the degree of ordering of the polymer and study its influence on charge carrier transport. The charge carrier mobilities as extracted from space-charge limited currents of diodes, from relaxation frequencies in MIS diodes and from the transfer characteristics of FETs show different magnitude and temperature dependence. Applying an analytical model [1] for the hopping mobility in amorphous films a distinction between the effects of charge carrier density on the one hand and of structural anisotropy on the other hand is possible.

[1] W.F. Pasveer et al., *Phys. Rev. Lett.* **94** (2005) 206601.

CPP 23.15 Thu 17:00 P2

Field-Effect Mobility in n-doped C₆₀ Thin Films: Dependency on Gate Bias and Temperature — ●KENTARO HARADA¹, FENGHONG LI¹, MARTIN PFEIFFER¹, ANSGAR G. WERNER², and KARL LEO¹ — ¹Institut für Angewandte Photophysik, Technische Universität Dresden, 01062 Dresden, Germany — ²Novald GmbH, Tatzberg 49, 01307 Dresden, Germany

We study the gate bias and temperature dependence of field-effect mobility in n-doped C₆₀ thin films with different doping concentrations of Acridine Orange Base (AOB, C₁₇H₁₉N₃). The n-doping of AOB enhances the bulk conductivity of C₆₀, whereas the application of a gate bias leads to an increase of transverse conductance between source and drain. For a heavily doped C₆₀ sample, the field-effect mobility has already reached its maximum without gate bias, and an increase of the gate bias does not give a contribution to the mobility at all. Yet, an elevation of temperature from 180 K to 340 K does give rise to the activation of the field-effect mobility until a clear transition to the saturation regime appears around 270 K; thereafter the mobility stays nearly constant at 0.13 cm²/Vs. On the other hand, for a lightly doped sample, the field-effect mobility is gate bias dependent within the measured bias and temperature range, indicating that both the field induced and the thermally activated carrier density play a role in mobility enhancement. We discuss these phenomena in accordance with the trap-filling models that have been proposed to explain the charge transport mechanism in organic materials.

CPP 23.16 Thu 17:00 P2

Organic Field-Effect Transistors Utilising Highly Soluble Oligothiophene Based Swivel Cruciform — ●ACHMAD ZEN¹, PATRICK PINGEL¹, DIETER NEHER¹, JOERG GRENZER², ASKIN BILGE³, TONY FARRELL³, ULLRICH SCHERF³, FERDINAND GROZEMA⁴, and LAURENS SIEBBELES⁴ — ¹Institute of Physics, University of Potsdam, Am Neuen Palais 10, 14469 Potsdam, Germany — ²Institute of Ion Beam Physics and Materials Research, Bautzner Landstrasse 128, 01328 Dresden, Germany — ³Macromolecular Chemistry, University of Wuppertal, Gauss Str.20, 42097 Wuppertal, Germany — ⁴Interfaculty Reactor Institute, Delft University of Technology, Mekelweg 15, 2629 JB Delft, The Netherlands

Two types of highly soluble oligothiophene based swivel cruciforms are presented as semiconducting materials in OFETs. Transistors made from these oligomers exhibited mobilities of more than 0.01 cm²/Vs and current on/off ratio of >10⁵. This is among the highest values reported to date for wet processed OFETs utilising oligothiophenes. In fact, the OFET-mobilities are comparable to values extracted from pulse-radiolysis time resolved microwave conductivity (PR-TRMC) experiments, indicating that carrier trapping is insignificant. In depth examination of the morphological, optical characteristics and thermal stability of the materials were carried to obtain information on the packing of the oligomers in the layer. Finally, the correlation between the

transistor performance and the crystallinity of the layers is addressed.

CPP 23.17 Thu 17:00 P2

Growth and Characterisation of Substituted Phthalocyanines for Applications in Organic Field Effect Transistors — ●HARRY BRINKMANN, CHRISTIAN KELTING, and DERCK SCHLETTWEIN — Justus-Liebig-Universität Gießen, Institut für Angewandte Physik, Heinrich-Buff-Ring 16, D-35392 Gießen

Partially fluorinated phthalocyanines were examined aiming at their electric properties. According to the position of their electronic energy levels, located just intermediate between unsubstituted and perfluorinated phthalocyanines, interesting properties as molecular semiconductors can be expected. Thin films of these partially fluorinated phthalocyanines were deposited either on glass or polyimide, the latter serving as an insulator substrate to study possibilities in realization of an all organic field-effect-transistor. The organic layers were grown by PVD. Optical absorbance and electrical conduction were studied dependent on the film thickness, substrate and contact material. Applicability of such layers in technical devices will be discussed.

CPP 23.18 Thu 17:00 P2

60nm to 40µm channel lengths poly(3-hexyl-thiophene) field effect transistors - Identifying the inner transistor — ●J. SEEKAMP, A. HOPPE, T. BALSTER, T. MUCK, and V. WAGNER — School of Engineering and Science, International University Bremen, 28759 Bremen, Germany

Polymer based nanoscale field effect transistors with poly(3-hexylthiophene)(P3HT) as the organic semiconductor were characterised and compared to longer channel devices. Meaningful mobility values are essential for this comparison. Recent publications agree on applied models either not fitting sufficiently or demanding for physical insight hardly obtainable [1,2]. A slightly different approach to analyse bottom contact field effect transistors with interdigitated Ti/Au (3nm/20nm) gold electrodes, 50nm silicon oxide as the gate insulator, P3HT and channel lengths between 60nm and 40µm is proposed here. Firstly, results were analysed using the "classical" gradual channel approximation[2]. Apparent mobilities[1] achieved this way varied between $0.2\text{cm}^2/(Vs)$ for 40µm channel length and $10^{-3}\text{cm}^2/(Vs)$ for 60nm channel length in linear regime for high V_{gs} . These mobilities vary with V_{ds} and V_{gs} . To achieve more consistent values the measured data were corrected for a gate source and a bulk current modelled as voltage controlled current sources. Analysis of such corrected data resulted in mobilities of around $10^{-3}\text{cm}^2/(Vs)$ for channel lengths between 20µm and 125nm. Apparent short channel effects were only observed for shorter channel lengths which are comparable to the oxide thickness.[1]G.Wang,et al.,J.Appl.Phys.93(10)(2003)6137;[2]M.L.Chabinye,et al.,J.Appl.Phys.96(4)(2004)2063

CPP 23.19 Thu 17:00 P2

Electrical investigations on nanoscale oligothiophene transistors — ●ARNE HOPPE, JÖRG SEEKAMP, TOBIAS MUCK, TORSTEN BALSTER, and VEIT WAGNER — International University Bremen, Bremen, Germany

High transfer frequencies demand for nanoscale channel lengths combined with relatively high mobilities. Since contact properties seem to play an important role when downscaling the channel lengths of the device, materials have to be found, which show acceptable mobilities and good contact properties in short channels. Potential candidates are alkyl-substituted oligothiophenes. We showed already for micrometer-sized organic field-effect transistors (OFETs) that with growing number of thiophene rings the mobility increases. Channel lengths of interdigitated electrodes in the range from 40µm to below 50 nm, produced by e-beam lithography, were investigated. We used Dihexyl-n-thiophenes (DHnT) with n, the number of thiophene rings, ranging from four to seven as organic semiconductor. Organic molecular beam deposition (OMBD) in ultra-high vacuum was used to deposit the semiconductor onto the substrate at temperatures between 100 °C and 190 °C. The 40µm devices serve as a long channel reference point. Mobility values evaluated within the gradual channel approximation are as high as $0.11\text{cm}^2/(Vs)$ for the 40µm reference transistor. Lower mobilities were observed for smaller channel lengths. We found an increase in mobility with a higher number of thiophene rings for nanoscale channels. A model is presented to explain the correlation between mobility values, the length of the π -system and the channel length.

CPP 23.20 Thu 17:00 P2

Patterning of Thin Films for Organic Electronics by Microcontact Printing of Self Assembled Monolayers — ●AMARE BENOR, KAH-YOONG CHAN, and DIETMAR KNIPP — International University Bremen, School of Engineering and Science, 28759 Bremen, Germany

Micro Contact Printing (μ CP) has become widely used technique in patterning thin film structures on the micron and nanoscale. Printing self-assembled monolayers (SAMs) in combination with selective surface wetting was used to realize radio frequency micro coils and electrodes of pentacene thin film transistors for radio frequency information tags (RFID tags). In this study we used the self-assembled monolayers (Octadecyltrichlorosilane, OTS), $\text{CH}_3(\text{CH}_2)_{17}\text{SiCl}_3$, which was printed on cleaned silicon or glass substrate by a poly(dimethylsiloxane), PDMS. The printed monolayer leads to the formation of hydrophobic regions, and the unprinted region remained hydrophilic which facilitates the selective deposition of polymers or resists like Poly(methyl methacrylate), PMMA on the hydrophilic region. In the next step, a standard lift-off process was used to pattern gold, titanium metal thin films. This technique was applied to realize radio frequency (RF) coils and electrodes for pentacene thin film transistors. The influence of processing parameters like: the geometry of the structures, the chemistry of the heterogeneous substrate and the polymer will be discussed. Moreover, fundamental printing limits of the method will be seen based on simple model to describe the limiting factors. Finally, the pentacene transistors will be compared with transistors prepared by optical lithography.

CPP 23.21 Thu 17:00 P2

Improvement of the ambience stability of field effect transistors based on poly(3-hexylthiophene) by molecular design modification — ●DESSLAVA SAINOVA¹, SILVIA JANIEZ¹, UDOM ASAWAPIROM¹, LORENZ ROMANER², NORBERT KOCH², and AN-TJE VOLLMER³ — ¹Fraunhofer Institute for Applied Polymer Research, Geiselbergstr. 69, 14476 Golm — ²Humboldt-Universität zu Berlin, Institut f. Physik, 12489 Berlin — ³BESSY GmbH, 12489 Berlin

Regioregular poly(3-hexylthiophene) (P3HT) belongs to the most attractive soluble polymers for applications in organic field effect transistors (OFETs). The key feature of P3HT is the self-alignment ability that facilitates the formation of crystalline thin films with well-ordered lamellae of co-facially stacked main chains. This assembly ensures fast charge transport in the layer of the ordered backbones and consequently high field effect mobilities. Nevertheless the successful performance of P3HT in OFETs is hindered by the limited operation under air. Both high field effect mobility and ambience stability are essential for practical application purposes. To achieve this attractive combination of properties we have modified the molecular structure of P3HT by introducing tetrafluorobenzene (TFB) units linked in the main chain. The TFB amount is varied to find an optimum between the processability, the ionization potential (IP) and the transistor performance of the synthesized polymers. As a result have been achieved field effect mobilities of 10-2cm²/Vs and ON/OFF ratios of 104. In addition, the OFET performance is retained after several days of air exposure due to the IP-shift up to 0.3 eV as determined by photoemission investigations.

CPP 23.22 Thu 17:00 P2

Encapsulated organic thin film transistors at elevated temperatures — ●S. MEYER¹, J. PFLAUM¹, S. SELNER², G. ULBRICHT², F. SCHREIBER³, H. DOSCH², M. FISCHER⁴, and B. GOMPE⁴ — ¹III. Physikalisches Institut, Universität Stuttgart — ²Max-Planck-Institut für Metallforschung, Stuttgart — ³Institut für Angewandte Physik, Universität Tübingen — ⁴I. Physikalisches Institut, Universität Stuttgart

To address the problem of thermal stability of organic semiconducting layers under realistic device conditions we have performed studies on pentacene thin film transistors with and without encapsulation. The capping is realized by a 2 µm polymer layer of poly-*para*-xylylene (PPX) or, alternatively, by a 100 nm thick sputtering layer of aluminum oxide (AlOx). On capped pentacene TFTs a field-effect can be demonstrated for both encapsulations up to temperatures of 140°C which is about 40°C above the desorption point of uncapped pentacene films on SiO₂. From the TFT characteristics a complex behavior of the temperature dependent hole mobility can be deduced, indicating that the device operation at these elevated temperatures is predominantly limited by the transistor structure and not by the organic material itself.

This is confirmed by thermal desorption spectroscopy and X-ray diffraction studies on pentacene thin films, showing that the organic layer remains crystalline for both capping materials far above the breakdown

temperature of the TFTs. As was previously demonstrated for AlO_x-capped diindenoperylene thin films [1], the structural breakdown is a function of heating rate and thickness of the capping layer.

[1] Sellner et al., *Adv. Mat.* **16**, 1750 (2004)

CPP 23.23 Thu 17:00 P2

Influence of source/drain contact metal on organic field-effect transistors and MIS-capacitors — ●ANDREI HERASIMOVICH, INGO HOERSELMANN, and SUSANNE SCHEINERT — TU Ilmenau, PF, 98684 Ilmenau, Germany

We have investigated the influence of the contact material on the current characteristics of organic field-effect transistors (OFETs) and on the frequency response of MIS-capacitors, based on spin coated poly(3-hexylthiophene) (P3HT). Aluminium contacts were evaporated on one half of the substrate and gold contacts on the other one. The measured frequency response of the capacitance shows clearly a smaller cut-off frequency in the case of the Al contact. The measured output characteristics of the transistor with gold source/drain contacts show a linear dependence at small drain voltages whereas the increase of the current for Al contacts is non-linear. Such non-linearity was attributed in [1] to the field dependence of the mobility due to the Poole-Frenkel effect, whereas in [2] series resistances are described as the reason. Using different materials for the contacts, we can investigate these effects separately. We discuss the temperature influence on the non-linearities in the characteristics of the OFETs and on the impedance of the MOS-capacitors and compare the obtained results with these ones obtained from 2D simulations to clarify the reasons for the measured peculiarities.

[1] P. Stallinga et al., *Appl. Phys. Lett.* **96**, 5277 (2004)

[2] G. Horowitz et al., *J. Appl. Phys.* **87**, 4456 (2000)

CPP 23.24 Thu 17:00 P2

Analysis of pentacene-OFET characteristics by a modified a-Si-model — ●SUSANNE SCHEINERT¹ and GERNOT PAASCH² — ¹TU Ilmenau — ²IFW Dresden

Measured current characteristics of pentacene OFETs depend strongly on the silanisation process [1]. Traps can be the reason for such peculiarities in organic field-effect transistors (OFET) and often the so-called a-Si-model is the appropriate one. We have investigated whether it is possible to describe the measurements with this model. Numerical two-dimensional simulations have been carried out with a systematic variation of interface and bulk trap parameters. Comparison with the measured curves shows, that both donor-like and acceptor-like traps near the valence band have to be supposed to describe the measurements. However, with a high trap concentration in a narrow distribution one obtains the same current characteristics, including the temperature dependence, as with a lower concentration and a broader distribution. Moreover, in addition also distributed interface traps have to be taken into account to obtain a satisfactory description of the experimental current characteristics. Even though the characteristics can be described well, a unique extraction of trap parameters solely from transistor current characteristics is not possible.

[1] I K.P. Pernstich, S. Haas, D. Oberhoff, C. Goldmann, D.J. Gundlach, B. Batlogg, A.N. Rashid, G. Schitter, *J. Appl. Phys.* **96** (2004) 6431.

CPP 23.25 Thu 17:00 P2

Analysis of OTFT Device Parameters based on Measurement and Simulation of IV and CV Characteristics — ●CHRISTOPH ERLÉN and PAOLO LUGLI — Munich University of Technology

Advances in fabrication techniques have led to organic TFTs (OTFTs), which are increasingly interesting for electronic applications. We have used different methods including finite element device simulations in a commercial environment (ISETCAD)[1] in order to extract relevant material and transistor parameters from experimental data. Dynamic CV measurements have been analyzed to crosscheck results for e.g. interface charges and trap densities obtained by simulation. These measurements are additionally employed to address dynamic OTFT characteristics. It is shown that next to material properties, device layout plays an important role in determining the transient transistor behavior. The research is conducted in close cooperation with M. Fiebig, S. Schiefer, M. Huth, U. Beierlein and B. Nickel, Department fuer Physik, Ludwig-Maximilians Universitaet, Munich, who provided the experimental data for bottom contact Pentacene TFTs.

[1] Bolognesi et al. *IEEE Trans. Elect. Dev.*, 51(12):1997, 2004.

CPP 23.26 Thu 17:00 P2

Charge mobility in Pentacene TFTs: a comparison of I-V and capacitance measurements — ●MATTHIAS FIEBIG, STEFAN SCHIEFER, MARTIN HUTH, UDO BEIERLEIN, and BERT NICKEL — Department für Physik and CeNS, Ludwig-Maximilians-Universität, München

Pentacene is one of the most promising materials for organic thin film transistors (OTFTs). We have prepared bottom contact Pentacene TFTs on SiO₂ by deposition in UHV. The high structural quality of the devices has been characterized by AFM and synchrotron x-ray diffraction. Transistor behavior has been tested by IV-measurements and mobilities of the order of 1 cm²/Vs have been achieved. Complementary capacitance measurements have been performed to address dynamic properties of the charge transport. The experimental results are simulated and analysed in collaboration with C. Erlen and P. Lugli, Institute for Nanoelectronics, TU München.

CPP 23.27 Thu 17:00 P2

The influence of SiO₂ dielectric interface modification on ambipolar transport in Pentacene TFTs — ●NIELS BENSON¹, MARCUS AHLES¹, THOMAS MAYER¹, ERIC MANKEL¹, ANDREA GASSMANN¹, ROLAND SCHMECHEL², and HEINZ V. SEGGERN¹ — ¹TU Darmstadt, Institute of Materials Science, Petersenstraße 23, D-64287 Darmstadt, Germany — ²Forschungszentrum Karlsruhe (FZK) Institut für Nanotechnologie, PF 3640, 76021 Karlsruhe, Germany

Recently an n-type Pentacene OFET, using traces of Calcium between SiO₂ and Pentacene has been demonstrated. This OFET exhibits electron transport properties similar to those of holes observed in a corresponding p-type OFET. Results on XPS measurements unveiling the influence of Ca on the SiO₂ surface are presented. According to these measurements, the first deposited Ca performs a chemical reaction with the SiO₂ interface. Metallic Ca is found only at higher nominal thickness. Moreover, characteristics of OFETs are presented, where thin intermediate polymer dielectrics selected with respect to functional end groups and their polarity have been employed between SiO₂ and Pentacene. A clear correlation between the occurrence of ambipolar transport and the molecular polarity has been revealed. From the present results, interface modifications with different polymer dielectrics as well as traces of Ca result in different interfacial electron trap densities, allowing a modification of the OFET threshold. This is a step toward to a better control of the device properties for organic integrated circuits and ambipolar OFETs.

CPP 23.28 Thu 17:00 P2

P(VDF/TrFE) as ferroelectric insulation layer for organic field effect transistors — ●KLAUS MÜLLER, KARSTEN HENKEL, IOANNA PALOUMPA, and DIETER SCHMEISSER — Brandenburgische Technische Universität Cottbus, Angewandte Physik-Sensorik, Konrad-Wachsmann-Allee 1, 03046 Cottbus

The ferroelectric polymer poly(vinylidene fluoride trifluoroethylene) (P(VDF-TrFE)) is used as insulating material for organic field effect transistors (OFET) and metal-insulator-semiconductor (MIS)-structures. For the MIS-structures, we find the typical hysteresis in the CV characteristic upon increasing the voltage scan window. Based on these results, we fabricate OFET with regioregular poly(3-hexylthiophene) (P3HT) as organic semiconductor. The transistors are constructed in bottom gate architecture with thin layers of spincoated P(VDF-TrFE) as gate insulation (100nm). The drain-source current of the OFET is reversibly affected by the polarized gate, which gives opportunities for organic nonvolatile memory elements. We present characteristic features like the hysteretic drain current response or the data retention. Furthermore, we present measurements with Kelvin probe force microscopy, a method which gives informations on the lateral distributions of the surface potential.

CPP 23.29 Thu 17:00 P2

Toward the fabrication of a monomolecular insulator film — ●MICHAEL ZHARNIKOV, YIAN TAI, HIROYUKI NODA, ANDREY SHAPORENKO, and MICHAEL GRUNZE — Angewandte Physikalische Chemie, Universität Heidelberg, Im Neuenheimer Feld 253, Heidelberg

Progress in fabricating smaller and more efficient structures in electronic and spintronic devices depends on better dielectric materials for nanofabrication. A perspective nanoinsulator is a molecular thin organic film - self-assembled monolayer (SAM), which provide an alternative to commonly used oxide dielectrics. A so far unresolved technological problem for insulator applications of SAMs is the difficulty of fabricating

stable metal layers on their surfaces, i.e. at the SAM-ambient interface. Such a film is generally leaky for metal adsorbates, which makes it impossible to integrate it into a multilayer assembly (e.g. in a tunnel junction magnetic memory cell) or to fabricate metal electrodes on its surface (e.g. in an organic thin film transistor). Using nickel as a test metal adsorbate and several different substituted and non-substituted SAMs as test substrates, we show that this difficulty can be overcome by the combination of a special design of the SAM constituents and their extensive cross-linking by low-energy electron irradiation. The properties of the SAM insulator and the metal overlayer were monitored by several complementary experimental techniques, including X-ray absorption spectroscopy and electrochemical measurements. The approach represents an important step toward the technological applications of monomolecular dielectric layers.

CPP 23.30 Thu 17:00 P2

Top emitting organic light emitting diodes with improved out-coupling efficiency by organic capping layer — •QIANG HUANG¹, KARSTEN WALZER¹, MARTIN PFEIFFER¹, GUFENG HE¹, KARL LEO¹, MICHAEL HOFMANN², and THOMAS STÜBINGER² — ¹Institut für Angewandte Photophysik, TU Dresden, D-01062 Dresden, Germany — ²Novald GmbH, Tatzberg 49, D-01307 Dresden, Germany

The improvement of light outcoupling from organic LEDs is a significant way for increasing the device efficiency. One way to reach this is the use of organic outcoupling layers. We study the emission properties of top emitting OLEDs with different organic capping layer thickness to understand the effect of the capping layer. The distribution pattern of the emitted light from a top emitting OLED depends strongly on the capping layer thickness, with a maximum enhancement of current efficiency by 38%, and quantum efficiency by 35%. This enhancement is not due to the redistribution of emitted light but mainly due to the improvement of outcoupling efficiency by changing the overall optical device structure. At 90 nm capping layer thickness, the device has optimum performance, showing 78 cd/A at 1000 cd/m² in forward direction as well as a quantum efficiency of 17.8 % and power efficiency of 69 lm/W.

[1]V. Bulovic, G. Gu, P. E. Burrows, V. Khalfin, V. G. Kozlov, and S. R. Forrest, *Nature (London)* 380, 29 (1996). [2]H. Riel, S. Karg, T. Beierlein, B. Ruhstaller, and W. Rieß, *Appl. Phys. Lett.* 82, 466 (2002). [3]G. F. He, M. Pfeiffer, K. Leo, M. Hofmann, J. Birnstock, R. Pudzych, and J. Salbeck, *Appl. Phys. Lett.* 85, 3911 (2004).

CPP 23.31 Thu 17:00 P2

Efficient polymer electrophosphorescent devices with interfacial layers — •XIAOHUI YANG¹, FRANK JAISER¹, BURKHARD STILLER¹, DIETER NEHER¹, FRANK GALBRECHT², and ULLI SCHERF² — ¹Universität Potsdam, Am Neuen Palais 10, 14469 Potsdam — ²Bergische Universität Wuppertal, Fachbereich Chemie, Makromolekulare Chemie, Gaußstr. 20, 42097 Wuppertal

We show that several large band-gap hole-transporting polymers can form insoluble interfacial layers on PEDOT:PSS. The thickness of the interlayer is dependent of the characteristics of underlying PEDOT:PSS and the molecular weight of the polymers. It is further shown that the electronic structures of the interlayer polymers have a significant effect on the properties of red-emitting polymer-based electrophosphorescent devices. Upon increasing the HOMO and LUMO level positions, a significant increase in current density and in device efficiency was observed. This is attributed to the efficient blocking of electrons in combination with the direct injection of holes from the interlayer to the triplet dye. Upon proper choice of the interlayer polymer, efficient polymer deep-red electrophosphorescent devices with a peak luminance efficiency of 5.5 cd/A (external quantum efficiency = 6 %) and a maximum power conversion efficiency of 5 lm/W could be realized.

CPP 23.32 Thu 17:00 P2

High efficiency white organic light emitting devices combining fluorescent and phosphorescent emitter systems — •GREGOR SCHWARTZ, KARSTEN WALZER, MARTIN PFEIFFER, and KARL LEO — Institut für Angewandte Photophysik, Technische Universität Dresden, D-01062 Dresden

Light sources suitable for lighting applications need to combine high power efficiency at high brightness, good color rendering as well as color coordinates matching those of the standard reference illuminants. We demonstrate white organic light emitting devices (WOLED) combining a blue fluorescent dye with red and green Iridium based phosphorescent dopants in separate host materials. The devices are competitive

with the best reported ones based on three phosphorescent emitters. In our WOLEDs, we could simultaneously achieve a power efficiency of 13.7lm/W at a brightness of 1000cd/m², a color rendering index of 85 and color coordinates of (0.47/0.42), which is a color very close to the standard warm white illuminant A. Crucial features of the devices are the use of electrically doped transport layers (p-i-n concept) which leads to low driving voltages, and a thin additional layer separating the fluorescent dye from the two phosphorescent emitter systems to prevent Dexter type quenching of the phosphorescent emission. We studied the influence of thickness and doping ratio of the different layers on the electroluminescence spectrum and on the current-voltage characteristics to understand the charge carrier balance and mechanisms of exciton generation inside the devices.

CPP 23.33 Thu 17:00 P2

Highly efficient and long-living red p-i-n bottom emission OLEDs based on triplet emitter systems — •RICO MEERHEIM, KARSTEN WALZER, MARTIN PFEIFFER, and KARL LEO — Institut für Angewandte Photophysik (IAPP), Technische Universität Dresden, George-Bähr-Str. 1, D-01062 Dresden, Germany

A way to reach highly efficient red bottom emission OLEDs is the use of doped transport layers and phosphorescent emitter materials for high quantum yield. We will show how the efficiency of such devices can be further increased. The p-i-n devices consist of doped transport layers, charge and exciton blockers, and a dilute emitter substance within an appropriate emitter matrix. Most advantageous for high efficiency is a nearly ambipolar emission system to create a broad light generation zone. Therefore, the favoured charge carrier type of different emission layers was studied. By combining preferably electron and hole conducting hosts, doped with the same triplet emitter dye, we reach a well-balanced emission layer (leading to a double emission layer structure) where the charge recombination occurs mainly close to the interface of both emission layer. This approach enables us to increase the 100 cd/m² efficiency from 9,3 cd/A to 11,2 cd/A with a high device stability of more than 50.000 hours lifetime. Both can be explained by reduced number of charge carriers leaking to the opposite blocking layers and less exciton-exciton quenching due to a reduced charge and exciton accumulation.

CPP 23.34 Thu 17:00 P2

Investigation of triplet exciton quenching in red phosphorescent OLEDs — •SEBASTIAN REINEKE, MARTIN PFEIFFER, KARSTEN WALZER, and KARL LEO — Institut für Angewandte Photophysik, Technische Universität Dresden, George-Bähr-Str. 1, D-01062 Dresden, Germany

We studied the quenching processes which contribute to the roll-off in quantum efficiency of phosphorescent OLEDs at high brightness. Possible processes are triplet-triplet annihilation (TTA), energy transfer to charged molecules (polarons) and the dissociation of excitons into free charges. The investigated OLED comprises a host-guest system as emission layer (EML) within a five layer structure including blocking and p- and n-doped transport layers. Here, N,N'-di(naphthalen-2-yl)-N,N'-diphenyl-benzidine is used as matrix and tris(1-phenylisoquinoline) iridium as phosphorescent emitter material. We found that the decrease of efficiency can be appointed to both TTA and energy transfer to charged molecules. Field-induced dissociation of excitons was not observed. Time-resolved measurements for the investigation of TTA as well as cw measurements for triplet-polaron quenching were performed. They are analyzed and combined to understand the efficiency drop in OLEDs. This work shows that both processes occur in the range of current density which is typical for OLED operation. An analytical discussion of both processes will be used to point out the magnitude of the different mechanisms.

CPP 23.35 Thu 17:00 P2

Enhancement of light out-coupling for OLEDs — •DIRK BUCHHAUSER^{1,2}, CHRISTOPH GAERDITZ^{1,3}, RALPH PAETZOLD¹, OLIVER WEISS^{1,4}, JOACHIM WECKER¹, and JUERGEN RUEDIGER NIKLAS² — ¹Siemens AG, Corporate Technology, Günther Scharowsky Str. 1, 91058 Erlangen, Germany — ²Department of Experimental Physics, University of Freiberg, Silbermannstrasse 1, 09599 Freiberg, Germany — ³Department of Material Science VI, University Erlangen-Nuremberg, Germany — ⁴Department of Materials Science, Technical University of Darmstadt, Petersenstraße 23, 64287 Darmstadt, Germany

OLED technology is attracting more and more attention for lighting

applications, because they provide striking advantages over competing technologies and can cover completely new application fields by offering a new freedom in design and shape for next generation lighting. Large area OLEDs might hence be used as 2-dimensional light sources which are thin and lightweight while providing diffuse illumination. OLEDs for illumination require brightness levels of 1000 cd/m² or more and an active area in the order of tens of cm². The efficiency of the lighting tiles can be significantly enhanced by using scattering structures on top of the substrate in order to improve the out-coupling behavior. Furthermore, such scattering layers can provide improved color stability over the entire viewing angle. Scattering layers are realized by films containing a certain concentration of particles or by physically structured surfaces. We present results on OLEDs based on white light-emitting polymers. The impact of scattering foils for light extraction and angular color stability are analyzed compared with simulations.

CPP 23.36 Thu 17:00 P2

Distributed Feedback Structures in active OLED-Layers by Photolithography — ●MATTHIAS DE LA ROSA, KLAUS MEERHOLZ, and JONAS KREMER — Physical Chemistry Department II, Luxemburgerstr. 116, 50939 Köln

Waveguide losses often result in poor external efficiencies with thin-film organic light emitting diodes (OLEDs). Among other approaches distributed feedback (DFB) structures have been used to overcome this problem by applying additional structured layers underneath the emissive layers in the device. Correct choice of the DFB structure properties like amplitude and period of the grating can lead to enhanced directed emission. Furthermore, such periodic modulations are of great importance in amplified spontaneous emission (ASE) applications like organic polymer lasers. We introduced a lithographic pathway of direct structuring to the OLED fabrication process using cross-linkable emitter and hole-transport materials, respectively. The impact of the DFB gratings onto the performance and spectral emission of the OLEDs was examined and an increase in the efficiency [Cd/A] by a factor of 1.5 could be observed whilst the emission spectra of the corrugated devices hardly changed. Other experiments with DFB structures in ASE materials are in progress to achieve better understanding for further organic polymer laser applications.

CPP 23.37 Thu 17:00 P2

Optical Studies on the Leaky Mode Emission of Organic Light Emitting Devices — ●NILS A. REINKE, MICHAEL HUTZEL, JOHANNES HÖCHTL, CLAUDIA ACKERMANN, and WOLFGANG BRÜTTING — Experimental Physics IV, Institute of Physics, University of Augsburg, Germany

In bottom emitting OLEDs, usually a large fraction of light generated in the organic multilayer stack is wave-guided inside the substrate and is either reabsorbed by the organic layers or edge emitted. Thus light propagating at angles larger than the critical angle for total internal reflection ($\approx 42^\circ$) is not accessible. These losses can be decreased by coupling the substrate to an optical element. This allows observation of light emission over all angles and increases the emission intensity of ITO-based OLEDs in forward direction by 50% with respect to the freestanding device.

In order to enhance the coupling of the guided leaky modes to the adjacent optical element and therefore to external modes, we utilized a microcavity structure by replacing the ITO anode by a thin metal film. In this configuration, the metal film enhances the gain of guided leaky modes whereas the contribution of non-guided modes is suppressed. These devices show highly polarised emission (TE mode) and tuneable emission wavelength over a wide angular range. The observed behaviour can be predicted quantitatively by simulations which are based on the transfer matrix formalism.

CPP 23.38 Thu 17:00 P2

Lasing from Optically Structured Organic Microcavities — ●PHILIPP SCHNEEWEISS, MARKO SWOBODA, ROBERT GEHLHAAR, VADIM G. LYSSENKO, MICHAEL HOFFMANN, and KARL LEO — Institut für Angewandte Photophysik, Technische Universität Dresden, 01062 Dresden, Germany, www.iapp.de

The emissive properties of an organic microcavity laser filled with the guest:host system of tris-(8-hydroxy quinoline)aluminium (AlQ₃) and 4-(dicyanomethylene)-2-methyl-6-(p-dimethylaminostyryl)-4H-pyran (DCM) are studied. Simultaneous excitation with two pump-pulses leads to the formation of an interference grating-structure in the active layer. Besides to the expected vertical cavity-surface emitting

laser behaviour, this results in two additional outer modes appearing under an angle defined by the distance of the interference fringes. The outer modes show a blueshift varying around 0.2 nm that can be tuned with the interference pattern. Optical anisotropy in the dielectric layers of the microcavity mirrors leads to polarization splitting and emission at two perpendicularly polarized lines.

CPP 23.39 Thu 17:00 P2

Pump-probe spectroscopy of organic semiconductor-hetero-systems — ●R. NÜSKE, E. ENGEL, K. LEO, and M. HOFFMANN — Institut für Angewandte Photophysik, TU Dresden, 01062 Dresden, Germany, www.iapp.de

The transport properties of photo-generated excitons in organic semiconductors are important parameters for the development of optoelectronic devices. We investigate double-layer systems with thin films of PTCDA (perylene-3,4,9,10-tetracarboxylic-dianhydride) and TiOPc (titanyl-phthalocyanine). Excitons generated in PTCDA are transferred by diffusion or Förster transfer to TiOPc. A femtosecond white-light continuum is used to record transient absorption spectra in the range between 1.2 eV and 2.6 eV. From the dynamics of the transient spectra, we infer the transfer rates of excitons from PTCDA to TiOPc. These rates are in accordance with luminescence quenching experiments reported recently [1].

[1] R.Schüppel et al., J.Lumin. **110**, 309 (2004).

CPP 23.40 Thu 17:00 P2

The different effect of anode/organic-interlayers on electrical fatigue and photodegradation of organic light emitting diodes — ●ARNE FLEISSNER, CHRISTIAN MELZER, ROLAND SCHMECHEL, and HEINZ VON SEGGERN — Electronic Materials Department, Institute of Materials Science, Darmstadt University of Technology, Petersenstr. 23, 64287 Darmstadt, Germany

Recently, the photodegradation of organic light emitting diodes (OLEDs) due to the exposure to visible and near-ultraviolet light through the Indium Tin Oxide (ITO) anode has been investigated [J. Appl. Phys. **97**, 124501 (2005)]. The ITO/organic-interface and the occurrence of excited organic molecules has been identified as crucial. Introducing appropriate interlayers between ITO and organic, e.g. a thin film of pentacene, suppressed the photodegradation. However, a PEDOT:PSS interlayer did not. In this work, the influence of such anode/organic-interlayers on electrical fatigue is studied. For that purpose, OLEDs with different interlayers between ITO and organic are operated in constant current mode while the time dependent driving voltage, electroluminescence intensity, and photoluminescence intensity are measured. The PEDOT:PSS interlayer shows a remarkable difference in the two degradation modes: It decreases electrical fatigue, however, it does not suppress photodegradation. The different role of PEDOT:PSS in photodegradation and electrical fatigue and the underlying mechanisms are discussed.

CPP 23.41 Thu 17:00 P2

Comparison of the SIMS and XPS depth profile of new and aged OLED structures — ●SEBASTIAN SCHOLZ¹, KARSTEN WALZER¹, STEFFEN OSWALD², and KARL LEO¹ — ¹Institut für Angewandte Photophysik, TU Dresden, George-Bähr-Straße 1, 01069 Dresden — ²Leibniz-Institut für Festkörper- und Werkstofforschung Dresden, Helmholtzstraße 20, 01069 Dresden

An important issue of current organic light emitting diodes (OLED) research is the understanding of degradation mechanisms and the improvement of device lifetime. In this work we study the migration and/or diffusion of several metals (in neutral or ionic state) through the OLED during lifetime measurements. We take a closer look to the contact materials Ag, Al, Au, Sn and In, and the behaviour of Cs, the doping material in the electron transport layer. Since these metals are expected to quench the radiative recombination in the emitting layers of OLEDs, they should not enter the emission zone at any time. For the analysis of the metal diffusion we performed depth profiling on new and aged OLEDs and test devices by secondary ion mass spectroscopy (SIMS) and X-ray photoemission spectroscopy (XPS) for the characterization of the organic and metallic layers.

CPP 23.42 Thu 17:00 P2

Temperature Stability of Organic Light Emitting Diodes — ●PHILIPP WELLMANN, MICHAEL HOFMANN, ANSGAR WERNER, ANDRÉ GRÜSSING, MICHAEL LIMMERT, ANDREA LUX, and JAN BIRNSTOCK — Novald GmbH, Tatzberg 49, 01307 Dresden, Germany

Organic Light Emitting Diodes (OLED) have received much attention during the last years and are now approaching mass production. Using the so-called PIN-Technology (p- and n-doped transport layers) we have demonstrated a combination of very low driving voltage, high efficiency and long lifetime. However, for applications (especially for automotive) a high temperature stability is an important issue. A well know material combination for n-doping is BPhen (4,7-diphenyl-1,10-phenanthroline) doped with pure Cs in a co-evaporation process. However, this system is known to have a low temperature stability. BPhen has a Tg of approx. 65°C and the conductivity of n-doped BPhen quickly decreases at temperatures about 70°C. Using improved host materials and newly developed organic dopands, we have been able to increase Tg and the thermal stability of our n-doped transport layers significantly. A storage test at 110°C leads to a significant increase in driving voltage and strongly decreased efficiency for BPhen:Cs, whereas the OLEDs using a molecular dopand stay essentially unchanged. The operational lifetime of PIN-OLEDs has strongly increased in the last year reaching values of more than 20.000h for red /green and 5.000h for a deep blue at 500 cd/m² and room temperature. Using our molecular doping we have now been able to demonstrate a lifetime of more than 6.000h at 500 cd/m² at 80°C.

CPP 23.43 Thu 17:00 P2

Numerical Simulation of Multilayer Organic Light Emitting Diodes — ●OLIVER WEISS^{1,2}, CARSTEN TSCHAMBER^{3,2}, CHRISTOPH GÄRDITZ^{3,2}, DIRK BUCHHAUSER^{4,2}, ARVID HUNZE², JOACHIM WECKER², and HEINZ VON SEGGERN¹ — ¹Dept. Materials Science, Technical University of Darmstadt, Germany — ²Siemens AG, CT MM 1, Günther-Scharowsky-Str. 1, 91058 Erlangen, Germany — ³Dept. Materials Science VI, University of Erlangen-Nuremberg, Germany — ⁴Dept. Experimental Physics, University of Freiberg, Germany

Modelling of OLED devices helps understanding the corresponding physics and accelerates the development of stable and efficient organic stacks. A one-dimensional numerical model for the quantitative simulation of multilayer OLEDs was introduced by Staudigel. It includes amongst others charge carrier drift and diffusion, trapping, recombination, singlet exciton diffusion and quenching. The simulation program being developed at Siemens CT MM 1 is based on Staudigels work. The model is extended to handle an arbitrary number of organic layers and was further improved in numerous points. For low injection barriers, ohmic contacts are assumed and charge carriers drift from the electrodes to the organic monolayers driven by the electric field. For barriers higher than 0.3 eV a thermionic injection mechanism was implemented. Analytical solutions of a simple monolayer device including one discrete trap level are reproduced over several orders of magnitude by numerical simulation using the same set of input parameters. The presented results of modelling an efficient organic stack demonstrate the simulation tool's ability of characterising up-to-date multilayer OLEDs.

CPP 23.44 Thu 17:00 P2

Kinetic Monte Carlo Model of Space Charge Limited Currents in Organic Semiconductors — ●MICHAEL MÜLLER, KARSTEN ALBE, YURI GENENKO, FREDERIK NEUMANN, ROLAND SCHMECHEL, and HEINZ VON SEGGERN — Institut für Materialwissenschaft, Technische Universität Darmstadt, D-64287 Darmstadt

Kinetic Monte Carlo (KMC) simulations have proven to be a valuable tool for investigating the characteristics of hopping charge transport in disordered organic semiconductors [1]. However, owing to their long range nature, electrostatic interactions between the individual charge carriers commonly had to be neglected. In consequence, the applicability of the KMC method has been restricted to hopping transport at low charge carrier densities where interactions are regarded negligible, as it is the case for the injection limited regime.

Here, we present a KMC model that fully includes the electrostatic interactions between the charge carriers. Using this model, we investigate the current-voltage characteristic and the field dependence of the charge carrier mobility in the space charge limited regime for hopping systems with various degrees of disorder. In doing so, different models for the microscopic hopping rates (Miller-Abrahams hopping in the exact and the commonly used approximated formulation as well as the small polaron model) are applied. A significant dependence of the obtained characteristics on the choice of model is found and discussed.

[1] H. Bässler, *phys. stat. sol. (b)* **175**, 15 (1993)

CPP 23.45 Thu 17:00 P2

Electronic Transport in Thin Layers of Nano-Composites — ●VOLKER KUNTERMANN^{1,2}, CAROLA KRYSCHI¹, and DIETRICH HAARER² — ¹Department of Physical Chemistry I, Friedrich-Alexander-Universität Erlangen — ²Experimentalphysik/BIMF, Universität Bayreuth

We are reporting dynamic TOF (time-of-flight) experiments on single and double layers of organic and inorganic photoconductors. These experiments yield mobilities of the involved organic materials and of the inorganic/organic composite materials. As inorganic particles we focus on nano silicon particles, these we characterize in conjunction with typical organic hole transport materials, such as various TPDs (triphenyl-diamines). Parallel experiments are performed with the standard xerographic technique. The comparison of both experimental techniques allows us to cover an extremely wide range of materials mobilities.

CPP 23.46 Thu 17:00 P2

High Temperature Stable Solar Cells — ●RUDOLF LESSMANN, MARTIN PFEIFFER, and KARL LEO — Institut für Angewandte Photo-physik - Technische Universität Dresden

We present an efficient MIP solar cell with p-doped layer using organic dopants that shows only low degradation upon 100 hours irradiation with a full sun at 80 °C and even withstands heating to 105 °C for some hours. The active layer is formed by a blend of buckminsterfullerene (C₆₀) and zinc-phthalocyanine (ZnPc); for the hole transport layer, a large triarylamine-based amorphous wide gap material with high glass transition temperature (NPD2) is used. The device structure is ITO / C₆₀ (5 nm) / C₆₀ : ZnPc [2:1] (30 nm) / NPD2 (5 nm) / p : NPD2 (40 nm) / p : ZnPc (10 nm) / Au (30 nm). The organic p-dopant was provided by NOVALED GmbH. It is used instead of the widely used F₄TCNQ because of its better thermal stability. Devices with good performance and high fillfactors up to 53% are obtained when grown with substrate temperature of 110 °C for the active layer and 40 °C for the p-doped layer. The power efficiency of these cells, working at ambient temperature, is around 1.5%.

CPP 23.47 Thu 17:00 P2

Investigation of excited states in P3HT and P3HT/PCBM composites — ●MORITZ LIEDTKE, JOHANNES SIEGER, CARSTEN DEIBEL, and VLADIMIR DYAKONOV — Experimental Physics VI, Physical Institute, University of Würzburg, 97074 Würzburg, Germany

Polymere-Fullerene composites exhibit efficient charge carrier generation due to ultrafast electron transfer which can be exploited for photovoltaic applications. Power efficiencies up to 5% have been achieved with bulk heterojunction solar cells fabricated from Poly(3-hexylthiophene) (P3HT) / [6,6] phenyl-C61-butyric acid methyl ester (PCBM) (1). In our work we studied excited states in regio-regular and regio-random P3HT by optical spectroscopy techniques like photoluminescence and photoinduced absorption (PIA) measurements. We discuss our results with respect to the morphology of the P3HT and P3HT / PCBM blend films. (1) *Appl Phys Lett* **87**, 083506, 2005, Marisol Reyes-Reyes, Kyungkon Kim, and David L. Carroll

CPP 23.48 Thu 17:00 P2

Photoinduced Charge Transfer versus Triplet Exciton Formation in Polymer-Fullerene Composites: Consequences for Photovoltaic Performance — ●JOHANNES SIEGER¹, CARSTEN DEIBEL¹, VLADIMIR DYAKONOV¹, INGO RIEDEL², and MICHAEL PIENKA³ — ¹Experimental Physics VI, Physical Institute, University of Würzburg, 97074 Würzburg, Germany — ²Bavarian Centre for Applied Energy Research (ZAE Bayern), Am Hubland, 97074 Würzburg, Germany — ³Energy and Semiconductor Research, Department of Physics, University of Oldenburg, 26129 Oldenburg, Germany

The conjugated polymer OC1C10-PPV blended with the electron accepting fullerene derivative PCBM is a material system which had a strong impact on the development of organic photovoltaics. Searching for alternative acceptor materials, the attention has recently been drawn to a class of dimethanofullerenes, which are fullerene derivatives with a higher solubility and a well established chemistry enabling structural modification of the side groups in a desired way. By replacing the PCBM with 1,1-bis(4,4-dodecyloxyphenyl)-(5,6)C61 (DPM-12), a high open-circuit voltage (close to 1 V) combined with a rather low photocurrent was obtained in DPM-12 based devices. In order to explain the phenomena observed, i.e., the formation of triplet excitons in the solar cell absorber containing DPM-12, systematic studies using light induced

electron spin resonance and photoluminescence detected magnetic resonance were applied. For proving the triplet nature of the new photoinduced absorption band, a spin sensitive technique called photoinduced absorption detected magnetic resonance was used.

CPP 23.49 Thu 17:00 P2

Enhanced intersystem crossing in oligothiophene:fullerene blends — ●R. SCHÜPPEL¹, T. MÜLLER¹, C. UHRICH¹, A. PETRICH¹, M. PFEIFFER¹, K. LEO¹, P. KILICKIRAN², E. BRIER², and P. BÄUERLE² — ¹Institut für Angewandte Photophysik, Technische Universität Dresden, Germany, www.iapp.de — ²Abteilung Organische Chemie II, Universität Ulm, Germany, www.uni-ulm.de/oc2

Photoinduced and transient absorption spectroscopy is used to study the excited state properties in thin films of Dicyanovinyl-terthiophene (DCV3T) and blends of DCV3T with fullerene C₆₀. We find an enhanced triplet exciton generation in the blend layer, which is explained as an excitonic “ping-pong”-effect: Singlet energy transfer from DCV3T to C₆₀, evidenced by sensitized emission of C₆₀, followed by immediate intersystem crossing on C₆₀ and triplet exciton back transfer. The rate constants involved into the certain energy transfer mechanisms are discussed in detail. Furthermore, we discuss the triplet exciton densities achieved by the pump laser irradiation including annihilation processes in the precursor singlet state to obtain the triplet diffusion length. Based on long-ranged triplet exciton diffusion in combination with efficient intersystem crossing, a promising new concept of solar cells with an enlarged active layer thickness is introduced.

CPP 23.50 Thu 17:00 P2

Self assembled nanostructured photovoltaic devices made of functionalized block copolymers — ●SVEN HÜTTNER¹, STEFAN LINDNER², ARNAUD CHICHE¹, GEORG KRAUSCH¹, and MUKUNDAN THELAKKAT² — ¹Physikalische Chemie II, Universität Bayreuth, D-95440 Bayreuth, Germany — ²Makromolekulare Chemie I, Universität Bayreuth, D-95440 Bayreuth, Germany

We investigate the concept of photovoltaic devices based on block copolymers. The use of a functionalized block copolymer made of electron donor (D) and acceptor (A) polymers lead to a self assembled microstructure that insures the photon to be absorbed within a very short distance (tens nm) to the D-A interface. A block copolymer made of a poly(vinyltriphenylamine) (D) and poly perylene bisimide acrylate (A) has been synthesized [1]. Photovoltaic devices made of such a copolymer film have shown significantly better efficiencies than similar devices made from a blend of the corresponding homopolymers. The reason for that clearly lies in the different morphologies. The blend-based device exhibits a phase separation resulting in micron sized domains and resulting in an important loss of post-absorption excited states that cannot reach the interface.

[1] S. Lindner, M. Thelakkat: *Macromolecules* 37, (2004) 8832-8835

CPP 23.51 Thu 17:00 P2

Optimization of organic thin-film photovoltaic cells based on the low gap oligothiophene derivative DCV3T — ●CHRISTIAN UHRICH¹, RICO SCHÜPPEL¹, KERSTIN SCHULZE¹, KARL LEO¹, MARTIN PFEIFFER¹, and PETER BÄUERLE² — ¹Institut für Angewandte Photophysik, TU Dresden — ²Abteilung Organische Chemie II, Universität Ulm

We have recently reported about a new oligothiophene derivate featuring dicyanovinylene end groups that can be used as acceptor material in organic thin-film photovoltaic cells. The material DCV3T has a high absorption coefficient ($\alpha = 2.5 \times 10^5 \text{ 1/cm}^2 @ 540\text{nm}$) absorbing light in a wide range. We prepared cells based on a flat heterojunction between DCV3T and 4P-TPD, a weekly donor-type amorphous material, embedded between ITO and a p-doped hole-transport layer. These cells reach an open-circuit-voltage of up to 1.04 V. Supported by optical simulations, we optimized the individual film thicknesses and improved the efficiency to 2.3 % at 100 mW/cm² simulated sunlight. The simulations also allow us to estimate the exciton-diffusion length in DCV3T. Moreover, we investigated the heterointerfaces comprised in the solar-cell structure by UPS and XPS measurements. These measurements give information about the HOMO-levels and possible interface dipoles.

CPP 23.52 Thu 17:00 P2

Efficient heterojunction organic solar cells with high photovoltages based on a new low-band-gap oligothiophene — ●KERSTIN SCHULZE¹, CHRISTIAN UHRICH¹, KARL LEO¹, MARTIN PFEIFFER¹, EDUARD BRIER², and PETER BÄUERLE² — ¹Institut für Angewandte Photophysik, Technische Universität Dresden, George-Bähr-Str. 1, 01069 Dresden — ²Abteilung Organische Chemie II, Universität Ulm, Albert Einstein Allee 11, 89081 Ulm

We report on efficient vacuum deposited heterojunction organic solar cells containing a new oligothiophene derivative with absorption onset at around 700nm as a donor and fullerene C₆₀ as an acceptor. At the heterointerface between the low-band-gap oligothiophene and C₆₀, photogenerated excitons from both materials are efficiently separated into electrons on C₆₀ and holes on the low lying HOMO of the oligothiophene. With these materials we can reach high open circuit photovoltages of up to 1.0V. The most efficient solar cells (3.1% power efficiency at 133mW/cm² simulated sunlight) are obtained when the photoactive heterojunction is embedded between a p-doped hole transport layer on the anode side and a thin exciton blocking layer and aluminium on the cathode side. However, due to the high ionization energy of the oligothiophene (around 5.6+/-0.1eV as determined from UPS), hole injection from any anode or hole transport layer is difficult and the IV-curves thus show a characteristic s-shape which reduces the fill factor FF. It is found that the actual FF sensitively depends on the workfunction of the p-doped hole transport layer and the thickness of the oligothiophene layer.

CPP 23.53 Thu 17:00 P2

Exciplex dynamics in a M3EH-PPV:CN-Ether-PPV blend film and a D-A block copolymer film — ●CHUNHONG YIN¹, TH. KIETZKE^{1,2}, H.H. HÖRHOLD³, and D. NEHER¹ — ¹Am Neuen Palais 10, 14469 Potsdam — ²Institute of Materials Research and Engineering (IMRE), Research Link 3, Singapore — ³University of Jena, Institute of Organic Chemistry and Macromolecular Chemistry, Humboldtstr.10, 07743 Jena

Solar cells based on semiconducting polymers have attracted a lot of interest. However, currently the efficiencies of polymer-based solar cells are still lower than the values obtained from their inorganic counterparts. Here, we demonstrate efficient charge carrier recombination via exciplex emission in blends of M3EH-PPV and CN-Ether-PPV. We also show that the intensity of exciplex emission is significantly reduced upon annealing. At the same time, the corresponding solar cell efficiency increases largely. We attribute the improvement of solar cell efficiency to partial de-mixing of the polymer components. Apparently, charge carrier recombination via exciplex formation constitutes one of the loss channels which limits the efficiency of solar cells based on these polymers. In addition, a statistical D-A block copolymer, which can be considered as a model system of an ultra fine blend, was studied. In this case, the intensity of exciplex emission and the solar cell efficiency was only weakly altered upon annealing, indicating that the significant changes observed for the blends are due to morphological effects.

Reference: Th. Kietzke, H.-H. Hörhold, D. Neher, *Chem. Matter*, in press

CPP 23.54 Thu 17:00 P2

Nanoporous TiO₂ / polyelectrolyte films — ●ROLF KNIPRATH and STEFAN KIRSTEIN — Humboldt University of Berlin

Porous TiO₂ films are a prerequisite for the fabrication of efficient dye-sensitized solar cells (DSSCs). They are used as an electrode and for sufficient absorption of light a very rough and highly porous TiO₂ surface is desired. In this work we report on the preparation and characterization of thin porous films of TiO₂ by alternate adsorption of TiO₂ nanoparticles and various polyelectrolytes from aqueous solutions. It is found that the structure of the films depends on the polyelectrolyte used and the preparation method. Besides surface roughness the porosity is determined by adsorption / desorption of dye molecules. The current transport through the films is investigated by measuring the current voltage characteristics of ITO/TiO₂/Au structures. The samples behave like Schottky diodes and it will be shown that the energy barriers at the Au / TiO₂ interface depends on the film structure.

CPP 24 POSTER Microfluidics

Time: Thursday 17:00–19:00

Room: P2

CPP 24.1 Thu 17:00 P2

Semiflexible polymer brushes in shear flow — ●LUKAS HOLZER and WALTER ZIMMERMANN — Theoretische Physik Ia, Universität Bayreuth, D-95440 Bayreuth

We investigate semiflexible polymers with a persistence length of the order of the polymer length such as for actin-filaments. Anchored at a flat surface they are exposed to a linear shear flow. Results concerning their stationary and dynamical deformation with respect to their mean distance or with respect to the shear rate etc. are presented.

CPP 24.2 Thu 17:00 P2

Free-Surface shapes of strongly deformed driven micro-droplets — ●MICHAEL SCHINDLER¹, PETER TALKNER¹, PETER HÄNGGI¹, and UWE THIELE² — ¹Institut für Physik, Universität Augsburg — ²MPI Physik Komplexer Systeme, Dresden

We propose a Finite-Element algorithm to compute free surface shapes that are significantly deformed by an applied static (gravitation) or dynamic (surface-acoustic waves) driving. In the micro-fluidic regime, where the surface tension forces become important the central difficulty resides in the approximation of the discretized curvature. We present a method how the discretization of the free surface can automatically be kept regular using a smooth transition to the behaviour of a rubber band.

By employing a variational approach we can show that the surface position must be discretized with the same order of accuracy as the velocity components. Otherwise, the free-surface boundary problem will be inconsistently formulated and give rise to approximation errors, as numerical observations confirm.

As examples we show pending pinned droplets on a flat substrate under the sole influence of gravity and capillarity and also droplets driven by surface-acoustic waves. In the limit of droplets with small equilibrium contact angles the results of our Finite-Element technique are compared to results of a lubrication approximation model.

CPP 24.3 Thu 17:00 P2

Hydrodynamic interactions in Brownian ratchets — ●ANDREJ GRIMM and HOLGER STARK — Universität Konstanz, Fachbereich Physik, 78457 Konstanz

Brownian ratchets are often used as model systems for molecular motors such as kinesin and myosin [1]. These proteins always work in an aqueous environment. It has recently been shown that hydrodynamic interactions play an important role and lead to a novel type of dynamics of colloidal particles driven by a tilted sawtooth potential [2]. Using Brownian dynamics simulations, we study the influence of hydrodynamic interactions on Brownian ratchets. We consider particles in toroidal traps moving under the influence of an on-off sawtooth potential. Our objective is to investigate how the velocity of the particles depends on the relevant parameters of the potential and on the particle density.

[1] F. Jülicher, A. Ajdari, J. Prost, Rev. of Mod. Phys. **69**, 1269 (1997)

[2] C. Lutz, M. Reichert, H. Stark, C. Bechinger, cond-mat/0510135 (2005)

CPP 24.4 Thu 17:00 P2

Wettability-control of droplet deposition and detachment — ●JEAN-CHRISTOPHE BARET¹ and MARTIN BRINKMANN² — ¹Institut Charles Sadron, 6, rue Boussingault, F-67083 Strasbourg, France — ²Max-Planck-Institut für Dynamics and Self-Organization, Bunsenstr. 10 D-37073 Goettingen, Germany

The conditions for droplet deposition on a plane surface are studied using the electrowetting effect to continuously modulate the substrate wettability. Droplets of various volumes attached to the tip of a pipette are brought into contact with the surface. When pulled up the droplets are deposited at sufficiently small contact angles and large volumes or completely detach from the substrate at small volumes and large contact angles. We demonstrate that electrowetting on dielectric (EWOD) provides an ideal tool to systematically study capillary instabilities involving a free contact line. The experimental limit between deposition and detachment in the contact angle/volume plane is in good agreement with analytical and numerical predictions obtained within the capillary model. In the case of zero buoyancy, the droplet contour can be expressed in terms of elliptic integrals which allows to derive an approximate expression for the droplet volume at the transition between the two modes

of instability. This criterion can be applied in technological processes which involve the production and placement of small droplets, e.g., in spotting arrays of biomolecules or in microcontact printing.

CPP 24.5 Thu 17:00 P2

Wetting random assemblies of cylindrical rods — ●MARTIN BRINKMANN — Max-Planck-Institut für Dynamics and Self-Organization, Bunsenstr.10, D-37073 Goettingen, Germany

The mechanical properties of loose random assemblies of rigid rods undergo a significant change when a liquid phase is dispersed in between the bodies. In experiments a strong tendency to form bundles of rods is observed. The anisotropic capillary interaction between cylindrical rods can be obtained from numerical minimizations of the interfacial energy and, for elongated liquid states, computed in an analytical model. As the relative tilt angle α of the cylinders tends to zero the liquid spreads between the two cylinders. If the surfaces are in contact the wetted length L and the capillary torque T diverge as $L \propto \alpha^{-\xi}$ and $T \propto \alpha^{-(\xi+1)}$, respectively, for hydrophilic contact angles $\theta < \pi/2$. As predicted from the analytical model and confirmed by numerical minimizations one has $\xi = 1$ if the Laplace pressure of the bridge is prescribed while $\xi = 3/4$ if the volume of the liquid of bridge is fixed. In the latter case, one finds a discontinuous transition between droplets localized at the contact point for $\alpha \approx 1$ and elongated liquid filaments for small tilt angles $\alpha \ll 1$. The capillary force F between the cylinders is studied for a variety of fixed tilt angles including the particular cases $\alpha = \pi/2$ and $\alpha \ll 1$.

CPP 24.6 Thu 17:00 P2

Wetting Morphologies in Triangular Grooves — ●KRISHNACHARYA KAREH¹, MARTIN BRINKMANN¹, EVGENY GUREVICH¹, BRUCE LAW², STEPHAN HERMINGHAUS¹, and RALF SEEMANN¹ — ¹MPI for Dynamics and Self-Organization, Bunsenstr. 10, D-37073 Göttingen, Germany — ²Kansas State University, Department of Physics, 327 Cardwell Hall, Manhattan, KS 66506, USA

We studied the wetting behavior of liquids in triangular grooves with chemically homogeneous walls. The length scale has been chosen to be small compared to the capillary length in order to avoid gravitational effects, but large enough for long range wetting forces (such as the van der Waals force) to be irrelevant. Droplets form elongated morphologies with negative mean curvature for contact angles smaller than 90deg minus half the opening angle of the groove. For larger contact angles, the liquid either forms elongated filaments of finite length and positive mean curvature or drop-like morphologies. For in situ manipulation of small amounts of liquid on this substrate topography (open microfluidics), we used electrowetting. We could vary the contact angle of the liquid on the substrate as a function of the applied Voltage. The filling and drainage behavior of these grooves were studied as a function of time and contact angle. In contrast to grooves with rectangular cross section, the liquid filaments in triangular grooves undergo a dynamic instability when being quenched from a filling to a non-filling situation. The liquid filament breaks up into isolated droplets with a preferred distance which compares favorably with a straightforward theoretical

CPP 24.7 Thu 17:00 P2

Digital Microfluidics with Monodisperse Gel Emulsions — ●RALF SEEMANN, CRAIG PRIEST, and STEPHAN HERMINGHAUS — MPI for Dynamics and Self-Organization, Bunsenstr. 10, D-37073 Göttingen, Germany

Microfluidics usually involves single phase liquids transported through microchannel networks. Instead of single phase flow, we have employed monodisperse emulsions to compartment liquids for microfluidic processing. If the volume fraction of the continuous phase is very low, the dispersed compartments (droplets) assemble into well-defined arrangements, analogous to foam. Hence, the position of a single droplet with a certain chemical content within an ensemble of droplets is fully determined while being transported through microfluidic channels. We demonstrate a one-step, in situ method for the production of monodisperse gel emulsions, suitable for microfluidic processing [1]. A variety of channel geometries is employed for positioning, sorting, dividing and exchanging droplets in 'lab-on-chip' style processing. Furthermore, we have selectively induced coalescence to initiate chemical reactions between adjacent compartments. Our method is well-suited for applications in combinatorial

chemistry, DNA sequencing, drug screening, and protein crystallization.

[1] C. Priest, S. Herminghaus, and R. Seemann, *Appl. Phys. Lett.* (in press)

CPP 24.8 Thu 17:00 P2

Monodisperse Emulsions Confined in Channels — ●ENKHTUUL SURENJAV, MAGDALENA ULMEANU, CRAIG PRIEST, DMYTRO MELENEVSKY, STEPHAN HERMINGHAUS, and RALF SEEMANN — MPI for Dynamics and Self-Organization, Bunsenstr. 10, D-37073 Göttingen, Germany

Emulsion droplets with diameter in between 2 and 20 microns provide suitable compartments for very small quantities of solvents or reagents. We present a comparative study of several techniques for the preparation of monodisperse emulsions. For some preparation techniques, the continuous phase of the emulsion has to be reduced subsequent to the preparation. It exhibits a variety of transitions in its topology upon interaction with an externally provided geometric constraint or applied field. This is demonstrated, e.g., using an organic ferrofluid as continuous phase and an inhomogeneous applied magnetic field. Furthermore, we study the formation of 2D and 3D emulsion crystals by mixing droplets with two distinct diameters with a certain size ratio, which may lead to a novel type of chemical reaction setup and new materials.

CPP 24.9 Thu 17:00 P2

Wetting properties of nanostructured composite surfaces and patterning of monolayer and polymer surfaces — ●OLIVER BÄUMCHEN, RENATE FETZER, and KARIN JACOBS — Experimental Physics, Saarland University, D-66123 Saarbrücken, Germany

Two main factors influence the wettability of a surface: On the one hand there is chemical heterogeneity (e.g. coatings or silane layers), on the other hand topographical roughness (surface structure) on the micro- and nanometer scale. Very rough surfaces can suspend small liquid drops and produce very large contact angles. Our goal is to fabricate and to characterize physically and chemically nanostructured surfaces. Moreover, we aim at characterizing the impact of microscopic local wetting properties to the macroscopic wetting behavior. By AFM, we study wetting at the nanoscale, whereas on the macroscale, we utilize optical microscopy. That way, we investigate a new nanocomposite material based on aluminum and its oxide [1], that exhibits complex topographical structures. In addition, we are interested in chemically structured surfaces and their wetting behavior. Therefore we utilize TEM masks to turn hydrophobic PDMS (poly(dimethylsiloxane)) films by plasma etching partially into hydrophilic silicone oxide-like layers. Furthermore we apply the microcontact-printing technique to pattern self-assembled thiol and silane monolayers on gold and silicon surfaces.

[1] M. Veith et al., *Eur. J. Anorg. Chem.* 24, 4387 (2003)

CPP 24.10 Thu 17:00 P2

Structured Micro- and Nanotubes for Microfluidic and Nanoprinting applications. — ●VALERIJ LUCHNIKOV and MANFRED STAMM — Institut für Polymersforschung e.V. Dresden, Hohe Str. 6, 01069 Dresden

Tubes and pores of micro- and nanoscale dimensions find numerous applications in separation science, biotechnology, microfluidics, sensors. However possibilities of engineering tube-based devices are strongly limited by hard access to inner walls of the mesotubes. We surmount this problem by formation of tubes via rolling-up of strained bilayers released in controllable manner from a solid substrate [1]. In our fabrication scheme bending moment arises in the bilayer film, composed of two chemically distinct polymers due to swelling of the bottom component of the bilayer upon immersion in a selective solvent [2]. (For example, poly(4-vinyl pyridine)/polystyrene bilayer rolls up in acidic water due to swelling of P4VP). Before rolling, the bilayer can be exposed to variety of planar methods of surface modification, such as micro-contact printing, photolithography, plasma activation, magnetron metal sputtering, and others. Geometrically complex patterns (e.g. intermittent hydrophilic/hydrophobic regions) can be created atop of bilayer lithographically and then form patterned interior of the tubes upon rolling. This opens new broad opportunities for design of mesotube-based devices and basic research.

[1] V.Ya. Prinz et al. *Physica E* 2000, 6, 828

[2] V.A. Luchnikov, O. Sydorenko, M. Stamm, *Adv. Mater.* 2005, 17, 1177

CPP 24.11 Thu 17:00 P2

Polymer Droplets on Soft, Brush-Coated Substrates — ●TORSTEN KREER¹, CLAUDIO PASTORINO², KURT BINDER², and MARCUS MUELLER³ — ¹Institut Charles Sadron, 6 rue Baussingault, 67083 Strasbourg Cedex, France — ²Institut fuer Physik, WA331, Johannes-Gutenberg-Universitaet, 55099 Mainz, Germany — ³Institut fuer theoretische Physik, Georg-August-Universitaet, 37077 Goettingen, Germany

Brushes are soft, elastically deformable substrates exhibiting a rich wetting behavior and additional dissipation mechanisms for the motion of droplets. We study thin polymer films and droplets on brushes by NEMD simulation using a DPD thermostat. The brushes consist of chemically identical polymers as the droplets.

The properties of the interface between the brush and the melt of identical molecules in equilibrium and under shear are dominated by universal entropic effects. Upon increasing the grafting density the free polymers are expelled from the brush and a brush-melt interface gradually builds up. Molecular conformations and the overlap between brush and melt are studied for different grafting densities. The slip length of the melt on the brush substrate is extracted from the velocity profiles and adopts large positive values for low grafting densities, but decreases and becomes negative for dense, autophobic brushes.

At high grafting density the polymer melt forms droplets (autophobic dewetting). Nanoscopic polymer droplets driven by volume forces (e.g. inclined plane or centrifugal forces) are investigated. The steady state at which the droplet moves at constant velocity is discussed.

CPP 24.12 Thu 17:00 P2

Nanoscale Flow-Cells and their Application — ●TILMANN ROGGE¹, KRISTIN MANDISLOH¹, TIMO MAPPE¹, MARTINA SCHÜRSMANN², AXEL ROSENHAHN², AHMED ABDELMONEM², and MICHAEL HIMMELHAUS² — ¹Institut für Mikrostrukturtechnik, Forschungszentrum Karlsruhe, 76021 Karlsruhe — ²Angewandte Physikalische Chemie, Universität Heidelberg, 69120 Heidelberg

Our goal is to study aqueous, organic, and biological liquid flows in micro- and nanochannels. Although liquid flows in micro- and nanocapillaries usually still can be treated within the framework of conventional continuum mechanics, the situation differs from that in macrosystems due to the smaller characteristic length scales, such as channel length and width, and the significantly increased surface-to-volume ratio of the fluid and its surrounding. Therefore, the balance between the various forces contributing to the overall behavior of the fluidic system is changed. Since the flow velocities are small, interface forces are an important contribution to the overall performance of microfluidic devices. We use pressure tight flow cells with optically transparent windows allowing for optical investigations with UV-, VIS- and IR radiation. The micro- and nanostructures are fabricated by X-ray lithography and other lithographic methods yielding channel widths of some hundreds of nanometers and channel heights below 10 micrometers. An appropriate periphery allows the use of flow volumes in the nanoliter range. Applications of these flow cells are adsorption studies with non-linear optical techniques. Furthermore, digital in-line holography is used to track tracer particles carried by the flow. The results are compared to those obtained by conventional microscopy.

CPP 24.13 Thu 17:00 P2

Thin-film field-effect-transistors for liquid movement detection in microfluidic systems — ●PAGRA TRUMAN, PETRA UHLMANN, and MANFRED STAMM — Leibniz-Institut für Polymerforschung Dresden e.V., Hohe Str. 6, 01069 Dresden, Germany

In microfluidic Lab-on-Chip systems and for applications in fundamental research there is a high demand for cost efficient minimal invasive massive parallel highly sensitive liquid movement detection with high spatial resolution. Currently available techniques like optical observation, scattering techniques or scanning techniques do not fulfill all requirements. Therefore we develop a new thin-film Field-Effect-Transistor based detection scheme where single transistor devices measure flow speed and filling level of capillaries besides being capable to analyze liquid properties like ionic strength. We present electrical transport measurements on large-scale transistor structures based on Silicon-on-Insulator (SOI) technology in aqueous solutions. Planar thin-film Silicon source-drain layers with lateral dimensions of few mm times few centimeters were laterally patterned out of the 55 nm thick top Silicon layer by standard circuit board lithography and wet chemical etching. The devices were electrically connected via metal contacts evaporated on such layers. Af-

ter integration into a microfluidic cell the latter was utilized to perform the previously described sensing operations.

CPP 24.14 Thu 17:00 P2

An experimental setup to handle liquids in a nanofluidic device — ●EVELYN MEYER and HANS-GEORG BRAUN — Leibniz Institute of Polymer Research, Max-Bergmann Center of Biomaterials, D-01069 Dresden, Hohe Strasse 6

The manipulation of fluids of femto- to picoliter volume in micro or nanosized channels is realized by a piezodriven manipulation unit adapted to an inverse fluorescence microscope. A truncated PDMS pyramid with a basal plane of 20 to 400 micrometer is mounted to a piezomotor system and can be controlled in x,y,z direction and enables filling and sealing of an underlying micro- and nanochannel structure. This assembly allows the encapsulation of DNA molecules for dynamic studies in confined geometries. The success of the filling process depends on the wettability of the microstructured surface according to the Wenzel regime for wetting of rough surfaces. Using an adjustable slit geometry between pyramid and substrate fluids entrapped in the slit can be transported along a substrate with controllable velocity to study the behaviour of propagating fluids on chemical and topographical heterogeneous surfaces.

CPP 24.15 Thu 17:00 P2

Integrated peristaltic pumps tailored for new migration phenomena — ●STEFAN GERKENS, DARIO ANSELMETTI, and ALEXANDRA ROS — Experimental Biophysics & Applied Nanosciences, Bielefeld University, Department of Physics, Universitaetsstrasse 25, 33615 Bielefeld, Germany

Peristaltic pumps based on PDMS can be used as fluidic driving-mechanism for a fully-integrated lab-on-a-chip evading difficulties involved with electrokinetic approaches. The characteristics of such a device are well suited for a large variety of microfluidic applications, for example the transport of biological compounds or colloidal particles. The fabrication is possible by soft lithography requiring only two PDMS moulds. External control is performed by an array of digitally assessable microvalves providing the necessary pressure for actuation. Both the lithography process (e.g. channel geometry) and the parameters controlling the external microvalves (e.g. actuation pressure and valve sequence) yield a large possibility to optimize the micropump for different problems. In this contribution, the application of a fully PDMS based peristaltic pump for the driving of colloidal particles in microfluidic networks is presented. Characterisation of this setup will be carried out in terms of flow rates, periodic driving amplitudes and single pumping-cycle analysis. This microfluidic pump will be used for the development of new migration phenomena in tailored microfluidic devices.

CPP 24.16 Thu 17:00 P2

Simple Method for the Stretching and Alignment of Single Adsorbed Synthetic Polycations — ●VERA BOCHAROVA¹, ANTON KIRIY¹, MANFRED STAMM¹, FRANCOIS STOFFELBACH², ROBERT JÉRÔME², and CHRISTOPHE DETREMBLEUR² — ¹Leibniz Institute of Polymer Research Dresden, D-01069 Dresden (Germany) — ²Center for Education and Research on Macromolecules (CERM), University of Liege, Sart-Tilman, B6, 4000 Liege, Belgium

It was found that positively charged macromolecules co-deposited with octylamine (OA) onto mica appear in a considerably more stretched conformation compared to adsorption onto untreated mica. Furthermore, the molecular thickness is considerably larger whenever the macromolecules are co-deposited with OA, which indicates a change in the local conformations of the chains and the orientation of their side-groups with respect to the substrate. These observations can be explained by the formation of an ultra-thin liquid-like film of OA onto mica that decreases the surface energy, weakens the interactions of the macromolecules with the surface and allows them to be stretched. The contour length and molar mass for the stretched macromolecules can be directly measured. The increase in the molecular height in case of co-deposition with OA drastically improves the molecular resolution, makes even ultra-thin polycations detectable and thus extends significantly the range of objects, which can be involved in single-molecule experiments.

CPP 24.17 Thu 17:00 P2

Adsorption and desorption of solvents by periodic mesoporous organosilica of different pore sizes — ●M.A. SCHREIBER¹, M. GÜNGERICH¹, P.J. KLAR¹, W. HEIMBRODT¹, J. MORELL², V. REBBIN², M. FRÖBA², T. HENNING³, L. EICHHORN³, J.J. BRANDNER³, and K. SCHUBERT³ — ¹Dept. Physics and WZMW, Philipps-University of Marburg, Germany — ²Institute of Inorganic and Analytical Chemistry, Justus-Liebig-University, Gießen, Germany — ³Forschungszentrum Karlsruhe, IMVT, Eggenstein-Leopoldshafen, Germany

Periodic mesoporous silica (PMOs) are organic-inorganic hybrid materials with regular pore systems and well defined pore sizes in the range of 3 to 15 nm yielding inner surfaces of about 1000 m²/g. The organic units in the pore walls are two-point attached within the silica matrix through covalent bonds and therefore are homogeneously distributed and a genuine part of the 3D pore wall framework. The choice of the organic functionalisation is very versatile making these hybrids interesting for applications in catalysis and micro-reactor technology. Here we study the adsorption and desorption behaviour of the solvents ethanol and benzene by benzene-functionalized and ethane-functionalized PMOS with different pore sizes in the temperature range between 20 and 140 °C by Raman spectroscopy. We find significant differences in the adsorption-desorption behaviour for different solvents as well as for different pore sizes suggesting that PMOs make a selective separation of solvent vapours possible.

CPP 25 POSTER Electronic Structure and Spectroscopy

Time: Thursday 17:00–19:00

Room: P2

CPP 25.1 Thu 17:00 P2

Theoretical investigation of the excited states of tungstate molecular groups in zinc tungstate crystals — ●TATIANA NIKOLAENKO, SERGIY NEDILKO, and YURIY HIZHNYI — Faculty of Physics, Kyiv National Taras Shevchenko University, 2, block 1, Hlushkova av., 03680, Kyiv, Ukraine

The crystals of zinc $ZnWO_4$ tungstate are well known scintillation and laser materials, which are used in different applications. The composition and structure of the luminescence centers in zinc tungstate are still the subjects of discussion. Nevertheless, it is commonly believed that the optical and luminescence properties of $ZnWO_4$ are determined largely by their anionic structural components, the tungstate groups. In order to study the luminescence processes in zinc tungstate theoretically, we perform quantum-chemical calculations of the electronic structure of

WO_6^{6-} molecular groups in $ZnWO_4$.

Molecular cluster of $ZnWO_4$ consisted of WO_6^{6-} group and the nearest Zn^{2+} cation was taken into consideration. Multiconfigurational self-consistent field wavefunctions of the cluster are calculated using GAMESS quantum chemistry package [1]. Dependencies of energies of the ground and excited electronic states of the cluster on several normal coordinates are obtained. The schemes of luminescence processes in $ZnWO_4$ are constructed using the obtained results. The origin of several bands in absorption and reflection spectra of the crystals is discussed on the base of the calculations.

[1] Schmidt M.W., et al., J. Comput. Chem., 14, 1347, (1993)

CPP 25.2 Thu 17:00 P2

Electronic Properties of Metals Embedded into Porous Polymeric Nanotemplates — ●RADIM KRENEK¹, VERA CIMROVA², OLAF SEIFARTH³, VERA BOCHAROVA¹, GANNA GORODYSKA¹, ALEXANDER SIDORENKO⁴, DIETER SCHMEISSER³, and MANFRED STAMM¹ — ¹Leibniz-Institut für Polymerforschung e.V., Dresden, Germany — ²Institute of Macromolecular Chemistry, Academy of Sciences of Czech Rep., Prague, Czech Rep. — ³Brandenburgische Technische Universität, Cottbus, Germany — ⁴Bell Labs, Lucent Technologies, Murray Hill, USA

We report on electrical measurements (current-voltage characteristics (CVC)) of metals which are templated via porous polymeric nanotemplates. The nanotemplates are based on self-organization of poly(styrene-block-4-vinylpyridine) (PS-PVP). The cylindrical pores of 8 nm in the diameter are ordered in a hexagonal lattice (24 nm in the period). Chromium and gold were embedded in the nanotemplates by magnetron sputtering, nickel was electrodeposited. These thin films were characterized by AFM, ellipsometry, x-ray reflectivity, XAS, XPS and NEXAFS.

CVC were acquired by a connection common for light emitting diodes discussing a further use of nanotemplated metals in these devices. To make the connection, the nanotemplate was deposited on glass with ITO electrodes, then metal was embedded into it and finally Al electrodes were evaporated on the device. Behaviour of space charge limited currents (SCLC) was observed. Also, we deal with the electrical mode of AFM as well. Finally electronic behaviour of the metallic nanorods embedded in polymeric nanotemplates is discussed in respective to the structure and chemical composition obtained by AFM and x-ray techniques.

CPP 25.3 Thu 17:00 P2

⁷Li NMR as a tool for the characterization of functional materials for lithium secondary batteries — ●NIKOLAUS NESTLE¹, SINA GUMANN¹, VERENA LIEBAU², ROBERT KOLB², CLAUDIA FASEL², HANS-GERHARD BREMES², RALF RIEDEL², NATALIA BRAMNIK², and HELMUT EHRENBERG² — ¹Institute of condensed matter physics, TU Darmstadt, Hochschulstr. 6, D-64289 Darmstadt, Germany — ²Department of materials science, TU Darmstadt, D-64289 Darmstadt, Germany

Rechargeable lithium batteries have found wide-spread use in mobile electronic appliances during the last few years. Improving the performance of the electrode materials and the electrolyte with respect to electrical cycling stability, safety, energy density and cost is a major challenge for the further improvement of lithium batteries. To achieve these goals, a microscopic understanding of the chemical structure of the materials and the processes taking place during charging and discharging is needed. A significant part of the research efforts in the SFB 595 "Electric fatigue in functional materials" is devoted to this topic. One of the experimental tools in this project is solid state NMR which is used to characterize the chemical environment of the Li ions in the materials and also their dynamic and transport properties. Results on various types of materials such as lithiated SiCN ceramics and LiCoO₂ are presented and discussed in the context of findings from other techniques such as electrochemical measurements, ESR, X-ray and Raman spectroscopy. Furthermore, approaches to improving the sensitivity of NMR for studies on materials extracted from tiny battery models are discussed.

CPP 25.4 Thu 17:00 P2

Irradiation defects in Fluoranthene radical cation salts - an Overhausershift analysis — ●DOMINIK STÖFFLER, MALTE DRESCHER, and ELMAR DORMANN — Physikalisches Institut, Universität Karlsruhe (TH), D-76128 Karlsruhe, Germany

After the exposure of Fluoranthene radical cation salts with high-energy protons, we encountered various interesting changes in their physical properties, e.g. a lowered Peierls transition temperature and an increased strength of a narrow line low temperature ESR signal. Analysing the caused defects, which can be detected at low temperatures by their Curie-paramagnetism, we hope to obtain details of the electronic and crystallographic structure. We deduce from the narrow ESR-linewidth that the electron spin is delocalised over several molecules, but it is a priori unclear if this arises from either the exchange interaction of several localized spins or the delocalisation of a single electron over multiple molecules. Method of choice is the ESR and the Overhausershift technique to gather additional information about the wave function of the unpaired electrons at low temperature.

CPP 25.5 Thu 17:00 P2

Hierarchical and approximate quantum master equations based on a decomposition of the spectral density applied to electron injection into a DNA base pair — ●G.-Q. LI, M. SCHRÖDER, M. SCHREIBER, and U. KLEINEKATHÖFER — Institut für Physik, Technische Universität Chemnitz, 09107 Chemnitz

The relaxation process of a system of one and of two interacting harmonic oscillators coupled to a thermal heat bath is studied. On short time scales memory effects play an important role for the relaxation behavior of the systems density matrix. For the description of such dynamical effects Meier and Tannor proposed a time-nonlocal scheme [1] based on second-order perturbation theory. In their scheme a set of auxiliary density matrices enters the quantum master equation and gives rise to the memory effects [2]. In our work we will use a modified and numerically less expensive version of recently proposed hierarchical methods [3,4] for exactly solving the quantum master equation of the reduced systems density matrix. This method can be shown to be identical with the scheme of Meier and Tannor to second order in the system-bath coupling but can be easily extended to higher orders. The different levels of theories are tested for a damped harmonic oscillator and for two coupled oscillators mimicking the electron injection from a donor into a DNA base pair.

[1] C. Meier, D. Tannor, *J. Chem. Phys.* **111** 3365, (1999).

[2] U. Kleinekathöfer, *J. Chem. Phys.* **121**, 2505 (2004).

[3] Y. Yan, F. Yang, Y. Liu, J. Shao, *Chem. Phys. Lett.* **395** 216 (2004).

[4] R.-X. Xu et al, *J. Chem. Phys.* **122** 041103 (2005).

CPP 25.6 Thu 17:00 P2

CIDNP and ¹⁹F-¹H Spin Polarization Transfer in 3-Fluorotyrosine — ●SERGEY KORCHAK¹, VITOR NASCIMENTO DE CARVALHO PINTO¹, KONSTANTIN IVANOV², and HANS-MARTIN VIETH¹ — ¹Department of Physics, Free University of Berlin, Arnimallee 14, D-14195 Berlin, Germany — ²International Tomography Center of SB RAS, 630090, Institutskaya 3a, Novosibirsk, Russia

The transfer of dynamic spin polarization between different nuclei in biological molecules can be used for labeling specific nuclear positions and applied to NMR spectroscopy in biology and medicine or for sensitivity enhancement in magnetic resonance imaging. Here, we report on strong Chemically Induced Dynamic Nuclear Polarization (CIDNP) created in reversible photoreactions between biological molecules and triplet excited dyes involving transient radical pairs. In particular, the ¹⁹F-¹H polarization transfer in CIDNP experiments with 3-fluoro-DL-tyrosine is examined by means of ¹⁹F-CIDNP and ¹H-CIDNP. For the first time, the magnetic field dependence of ¹⁹F-CIDNP at 0-7 T is obtained. The mechanism of polarization transfer is revealed and optimum conditions for getting high spin polarization transfer are discussed. By comparing the experimental results with model calculations the g-factor of the 3-fluorotyrosine radical is obtained. The fluorinated amino acids incorporated in proteins may be used for the investigation of protein folding with the advantage that fluorine exhibits a higher CIDNP effect than proton and that the background ¹H polarization is absent.

CPP 25.7 Thu 17:00 P2

Comparison of the Layered Semiconductors GaSe, GaS, and GaSe_{1-x}S_x by Raman and Photoluminescence Spectroscopy — ●LOTHAR KADOR¹, CARMEN PÉREZ LEÓN¹, KERIM R. ALLAKHVERDIEV², TARIK BAYKARA², and ALI A. KAYA² — ¹University of Bayreuth, Institute of Physics and Bayreuther Institut für Makromolekülforschung (BIMF), D-95440 Bayreuth, Germany — ²Marmara Research Centre of TÜBİTAK, Materials Institute, P. K. 21, TR-41470 Gebze/Koçaeli, Turkey

The room-temperature Raman spectra of single crystals of GaSe, GaS, and mixed compounds GaSe_{1-x}S_x with 0.02 ≤ x ≤ 0.8 were measured with a HeNe laser in confocal configuration. The changes in the spectra indicate changes of the crystal structure. The spectra of pure GaSe and of the mixed compound with x = 0.02 show, in addition, pronounced photoluminescence signals blue-shifted from the laser line. Their origin is interpreted as second-harmonic generation in the laser focus causing the formation and radiative decay of Wannier excitons. Two-photon absorption is ruled out, since the effect is absent in the centrosymmetric crystals with x > 0.02. With a green laser whose photon energy is larger than the band gap, strong photoluminescence is also observed in crystals with higher sulfur content.

CPP 25.8 Thu 17:00 P2

Imaging and Spectrally Discriminated Time-Resolved Photoluminescence of Single Aggregates of Semiconductor Nanocrystals — •THOMAS BLAUDECK and FRANK CICHOS — Photonics and Optical Materials, TU Chemnitz, 09107 Chemnitz

In our contribution, we present results of single-particle spectroscopy and time-resolved photoluminescence measurements on single NP aggregates. We make use of a home-built confocal microscope and time-resolved single-photon counting equipment with a precision in the ps regime. Using a photon-by-photon correlation technique, our idea is to determine fluorescence lifetime fluctuations on timescales shorter than accessible via conventional techniques. The results are correlated with typical processes of charge diffusion in the nanocrystals. The optical detection allows spectral discrimination in two channels.

CPP 25.9 Thu 17:00 P2

Photothermal Microscopy on Single Quantum Objects — •ROMY RADUENZ, ACHIM GRUBER, and FRANK CICHOS — Photonics and Optical Materials, Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz

Single chromophore detection is typically restricted to highly fluorescent entities such as dye molecules or quantum dots. But it fails to access non-fluorescent species. An extension of single chromophore detection to the spectroscopy of non-fluorescent species would thus open a completely new field of studies and analytical possibilities. A technique, which can provide this extension is photothermal detection. Within this technique the conversion of the absorbed photon energy into heat and finally a refractive index change of the local environment is employed to detect single chromophores. This refractive index change is directly proportional to the absorption cross section of the chromophore and therefore allows in principle the measurement of the absorption spectrum. Within our study we present experimental and theoretical results of photothermal confocal microscopy. Our detection scheme is based on the creation of a photothermal lens in the local surrounding of the absorbing species, that is excited by a laser beam. The thermal lens is used to modulate a probe laser beam. The sensitivity of this method is evaluated based on measurements on single gold nanoparticles.

CPP 25.10 Thu 17:00 P2

Defocused Wide Field Imaging of Single Quantum Dots — •ROMAN SCHUSTER¹, MICHAEL BARTH², REBECCA WAGNER³, ACHIM GRUBER³, THOMAS BLAUDECK³, and FRANK CICHOS³ — ¹Leibniz Institute for Solid State and Materials Research Dresden, 01171 Dresden — ²Nano-Optics group, Institute of Physics, Humboldt University Berlin, Hausvogteiplatz 5-7, 10117 Berlin — ³Photonics and Optical Materials, Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz

We have applied fluorescence wide-field imaging to study the details of the transition moment of single CdSe/ZnS core/shell quantum dots. [1] Introducing a slight defocusing into the imaging creates a well resolved pattern from the light emitted by a single quantum dot. This pattern is a consequence of the diffraction of the light on the aperture of the microscope objective and contains information on the angular anisotropy of the light emitted by the quantum dot. By comparing these images to numerical calculations of the diffraction patterns we find, that the transition moment of CdSe quantum dots is not circular at room temperature. All images can be either fitted with an elliptical transition moment or even a 3-dimensional transition moment. The results suggest that the transition moment at room temperature is more complex than so far suggested and determined by the mixing of different valence band states, which form finally a 3-dimensional transition moment. A combination of different polarization projection methods with defocused imaging are evaluated to unravel the details of the 3-dimensional transition moment. [1] R. Schuster et al., Chem. Phys. Lett., 2005, 413, 280.

CPP 25.11 Thu 17:00 P2

Electronic excitation energy transfer in individual donor-acceptor dyads — •REMI METIVIER¹, FLORIAN FEIST¹, FABIAN NOLDE², KLAUS MÜLLEN², and THOMAS BASCHÉ¹ — ¹Institut für Physikalische Chemie, Johannes Gutenberg-Universität Mainz — ²Max Planck-Institut für Polymerforschung, Mainz

We have studied a new class of structurally well-defined donor-acceptor dyads which exhibit efficient unidirectional energy transfer. The dyads are formed by connecting a variable number of donor chromophores (peryleneimide/peryleneediimide) to an acceptor chromophore

(terrylenediimide) through a rigid poly(phenylene) linker. In a first set of experiments a linear dyad was investigated, where the donor and the acceptor are linked by a p-terphenyl spacer. Fluorescence emission spectra showed acceptor emission only indicating highly efficient energy transfer. Single molecule spectroscopy at low temperature (1.4K) offers the possibility to directly extract the energy transfer rates from the line widths of the donor fluorescence excitation spectra. The distribution of energy transfer times was centered around 5 picoseconds. Comparison to a distribution calculated by assuming a Förster mechanism showed that an additional through-bond interaction might play a role in this bichromophoric dyad. The second multichromophoric system studied is a polyphenylene dendrimer in which four peripheral donor chromophores are build around a central acceptor core. Besides measuring energy transfer rates for individual donor chromophores within an isolated aggregate, we will also show that the orientation of the donor chromophores can be estimated from the distribution of transfer times.

CPP 25.12 Thu 17:00 P2

Setup for flowcytometric based fluorescence measurements of red fluorescent dyes — •BABETTE HINKELDEY, ALEXANDER SCHMITT, and GREGOR JUNG — Biophysical Chemistry, Saarland University, Building B2.2, D-66123 Saarbrücken, Germany

In the last decades, Single Molecule Detection (SMD) has become an important scientific field in biophysical and biomedical applications. By coupling individual molecules with fluorescent dyes, observation of the movements of these individual molecules even in living cells is possible. Due to reduced autofluorescence in living cells, red dyes are favoured. Thus, the understanding of the photophysical properties of fluorescent dyes is one of the relevant domains. Especially the photostability is of great interest, as a precise prediction of the average number of excitation cycles before dye degradation is highly recommended for quantitative and comparable results. In addition, the correlation between chemical structure and physical properties could result in improved strategies of synthesis of application matched dyes. Therefore it is necessary to develop a method which fulfills the conditions to obtain quantitative results in order to being able to compare different fluorescent dyes. In our contribution we show the setup for flowcytometric based fluorescence measurements. Finally, performance data and first results with a red fluorescent dye are presented.

CPP 25.13 Thu 17:00 P2

Single-Molecule Spectroscopy of Individual Perylene Bisimide Derivatives — •HANNA ENGELKE¹, ERWIN LANG¹, PETER OSSWALD², FRANK WÜRTHNER², and JÜRGEN KÖHLER¹ — ¹Experimental Physics IV, University of Bayreuth — ²Institute for Organic Chemistry, University of Würzburg

We present a detailed characterisation of the photophysical properties of three different perylene bisimide derivatives. The probe molecules have been immobilized in a Shpol'skii matrix of hexadecane and were investigated by single-molecule spectroscopy at cryogenic temperatures. Exploiting single-molecule techniques, we compare the three derivatives as regards their saturation behaviour, triplet substate kinetics and fluorescence quantum yield.

CPP 25.14 Thu 17:00 P2

Photobleaching on the Single Molecule and Ensemble Level — •JÖRG BRABANDT, JÖRG SCHUSTER, and CHRISTIAN VON BORCZYKOWSKI — Institute of Physics, TU Chemnitz, 09107 Chemnitz

We study the photobleaching of dye molecules on the single molecule and ensemble level. Ensemble photobleaching is characterized by a reversible and an irreversible part, the latter one being the well established photodestruction of the dye. The reversible part of the photobleaching is due to the existence of dark periods where the molecule reversibly switches between on- and off-states, so called photoblinking [1] [2]. The discrimination between the two mechanisms is a difficult task, since the decision whether a given dye molecule is in a long dark state or already irreversibly photochemically destroyed requires extremely long observation times. We show, how both aspects of photobleaching can be inferred from single molecule observations. Furthermore, we present a detailed analysis of the reversible part of photobleaching by a number of ensemble experiments.

[1] Orrit et al., J. Phys. Chem. A 107 (2003), 6770

[2] Schuster et al., Appl. Phys. Lett. 87 (2005), 051915

CPP 25.15 Thu 17:00 P2

Optical Switching and Dielectric Response of Nematic Liquid Crystals Dispersed in a Ferroelectric Poly(Vinylidene Fluoride/Trifluoroethylene) Matrix — ●LAKSHMI MEENA GANESAN, AXEL MELLINGER, MICHAEL WEGENER, WERNER WIRGES, and REIMUND GERHARD-MULTHAUPT — Department of Physics, University of Potsdam, Am Neuen Palais 10, 14469 Potsdam

Liquid-crystal (LC) droplets embedded in a polymer matrix induce switching behaviour in the composite film through the alignment of the director along an external electric field. When a ferroelectric material is used as host polymer, hysteretic effects in the electric-field dependence of the optical transmission occur, making these materials interesting candidates for electro-optical switches (light valves) and fundamental studies of the internal electric field in the LC cavities. Polymer-dispersed liquid-crystal (PDLC) films were prepared by dispersing a nematic liquid crystal in a ferroelectric copolymer of vinylidene fluoride and trifluoroethylene [P(VDF-TrFE)] using a solvent-induced phase-separation method. Along with the field-dependent optical transmission of the PDLC, the hysteresis between electric displacement and electric field was measured and compared with that of the pure copolymer. As the liquid-crystal content was increased in the composite film, the coercive field was reduced, whereas the difference in transmission between the "on" and "off" state increased. In addition, the dielectric behaviour of the pure liquid crystal, of the PDLC and of the pure copolymer was measured and compared with each other.

CPP 25.16 Thu 17:00 P2

Non-linear optical properties of fluorescein — ●CHRISTIAN MEFFERT, SVEN VERPOORT, and HILMAR FRANKE — Fachbereich Physik / Angewandte Physik, Universität Duisburg-Essen, Lotharstr. 1, D-47048 Duisburg, Germany

During the irradiation of an optical cuvette filled with fluorescein by laser-light a self-focusing effect has been detected. At first this effect has been measured quantitatively before the light-induced change of the refractive index has been characterized. The refractive index change of guest-host films was measured as a function of light exposure using ATR leaky mode spectroscopy. Fluorescein has been indiffused into the polymer Nafion. The non-linear optical feedback of the ATR-layer stack with the incoupling light has been investigated. Finally the non-linear influence on the fluorescence coupling in optical fibers is being discussed.

CPP 25.17 Thu 17:00 P2

Holographic Information Storage in Azobenzene-Containing Diblock Copolymers — ●MICHAEL HÄCKEL¹, LOTHAR KADOR¹, DANIELA KROPP², CARSTEN FRENZ², ROLAND WALKER², ANJA GRESS², KLAUS KREGER², and HANS-WERNER SCHMIDT² — ¹Institute of Physics and BIMF, University of Bayreuth, 95440 Bayreuth, Germany — ²Macromolecular Chemistry I and BIMF, University of Bayreuth, 95440 Bayreuth, Germany

The optically induced birefringence in different azobenzene- and mesogen-containing block copolymers has been studied with holographic methods. In the block copolymers, the light-sensitive blocks containing the azobenzene moieties are embedded in a matrix of polystyrene. Angular multiplexing of holographic plane-wave gratings as well as of two-dimensional images has been performed in samples with thicknesses up to 1.1 mm. The achievable refractive-index modulation, the photosensitivity, and the stability of the inscribed gratings were compared for different materials. In contrast to photopolymers, our materials do not exhibit shrinkage upon illumination. Instead a weak light-induced volume expansion was detected and studied in detail.

CPP 25.18 Thu 17:00 P2

Luminescent characterization of perovskite-like layered strontium lanthanum titanate compounds — ●VOLODYMYR CHUMAK¹, YU. TITOV¹, M. SLOBODYANIK¹, S. NEDILKO², O. CHUKOVA², and P. SMOLYAR² — ¹Chemistry faculty of Kyiv National Taras Shevchenko University, 64, Volodymyrska str., 01033, Kyiv, Ukraine — ²Physics faculty of Kyiv National Taras Shevchenko University

First the peculiarities of the luminescent emission of the five-slab perovskite-like $SrLa_{4-x}Ln_xTi_5O_{17}$ ($Ln = Pr, Yb$) compounds belonged to the $A_nB_nO_{3n+2}$ - family are found and described.

Photoluminescence and excitation spectra were obtained at 4.2, 77 and 300 K. Luminescence was excited by radiation from the the N_2 -laser, the Ar-laser, powerful xenon lamp DKsL-1000. The luminescence was reg-

istered using MDR-2 and DFS-12 diffraction spectrometers which cover wide spectral region. Reflection, excitation and luminescence spectra were also investigated using synchrotron radiation in the energy region 3.5-20 eV. Experiments with synchrotron radiation were carried on at SUPERLUMI station at HASYLAB (DESY), Hamburg, Germany.

Results of experimental studies allowed us to conclude that mentioned above the sets of compound could be regarded as perspective phosphors, i. e. the transformers of the UV or IR emission into visible light, or the white-light-emitting and storage phosphors, perspective laser materials. When doped with the rare earth ions Pr^{3+} or Yb^{3+} they are considered as perspective fast-scintillation materials.

CPP 25.19 Thu 17:00 P2

Holographic recording of more-dimensional periodic refractive index patterns — ●RAFAEL MEINHARDT — University Duisburg-Essen, Applied Physics, 47057 Duisburg, Germany

Based on multiple-beam interference, 1-D, 2-D or 3-D optical lattices were created to generate refractive index patterns with crystalline and quasi-crystalline structure inside two different photosensitive material systems by applying the method of holographic lithography.

For the relationships between the recording parameters and the desired optical lattice numerical simulations calculate the spatial intensity profile formed by N coherent plane waves. The resulting optical lattice can be visualized in the form of an animation or several plots and its lattice constants can be described by using standard crystallographic formalisms.

Considering the simulation parameters, different holographic setups in vertical and horizontal geometry are realized, with which we are able to perform either consecutive or simultaneous structuring of the material. These optical lattices were transferred both in solid plates of photosensitive PMMA and in evaporated films of the azo dye Disperse Red 1.

The recorded structures were characterized by evaluating the resulting diffraction patterns and AFM images. In PMMA a pure refractive index pattern was observed whereas in DR1 a dual grating was formed which is made up of a refractive and a surface relief. In both cases the simulated structures have been confirmed.

CPP 25.20 Thu 17:00 P2

Holographic recording of more-dimensional periodic refractive index patterns — ●RAFAEL MEINHARDT¹, ANSGAR DRAUDE¹, HILMAR FRANKE¹, and ROGER A. LESSARD² — ¹department of applied physics, university of Duisburg-Essen, Lotharstr.1, 47057 Duisburg, Germany — ²COPL, departement de physique, university of Laval, G1K7P4, Quebec, Canada

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For the relationships between the recording parameters and the desired optical lattice numerical simulations calculate the spatial intensity profile formed by N coherent plane waves. The resulting optical lattice can be visualized in the form of an animation or several plots and its lattice constants can be described by using standard crystallographic formalisms.

Considering the simulation parameters, different holographic setups in vertical and horizontal geometry are realized, with which we are able to perform either consecutive or simultaneous structuring of the material.

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The recorded structures were characterized by evaluating the resulting diffraction patterns and AFM images. In PMMA a pure refractive index pattern was observed whereas in DR1 a dual grating was formed which is made up of a refractive and a surface relief part. In both cases the simulated structures have been confirmed.

CPP 25.21 Thu 17:00 P2

Investigation of gratings formed in the interface pDR1m / PMMA — ●KNUT MORAWETZ¹, ULRICH PIETSCH², BURKHARD SCHULZ¹, PERTSH MIRZOYAN¹, MARINA SAPHIANNIKOVA¹, OLIVER HENNEBERG¹, and BIRGIT DIETZEL³ — ¹University of Potsdam, Institute of Physics, Am Neuen Palais 10, D-14469, Germany — ²University of Siegen, Solid state physics, 57068 Siegen, Germany — ³IDM-Teltow, Kantstraße 55, D-14513 Teltow, Germany

Surface relief gratings (SRGs) can be inscribed onto azobenzene polymer films by holographic illumination with the actinic light (488 nm). By exposing the initially flat surface of a polymer film to an interference pattern of two counter-circularly polarized beams one can create a SRG with amplitudes of several nanometer height within a few minutes of ex-

posure. The lateral spacing D can be tuned between $D=500$ and 5000 nm by changing the angle between the two parts of split up laser beam. To get a multiplayer system it was covered a pDR1m film by a second transparent polymer layer (PMMA) that is not affected by the actinic light. After holographic illumination of these layer system it was found a diffraction pattern of light. The PMMA layer was removed by washing the sample with a solvent. The free surface of the azobenzene polymer layer was inspected by AFM. In the washed region the grating height was found to be inverse proportional to the PMMA height. Theoretical simulations conform the experimental results.

CPP 25.22 Thu 17:00 P2

Photo induced aging of polymers — ●KNUT MORAWETZ¹, BURKHARD STILLER¹, JAROSLAV ILNYTSKIY¹, DIETER NEHER¹, STEFAN KATHOLY¹, RONALD RIES², and ASTA RICHTER² — ¹University of Potsdam, Institute of Physics, Am Neuen Palais 10, D-14469, Germany — ²University of Applied Sciences, Engineering Physics Section, Bahnhofstraße ,15745 Wildau, Germany

The photo induced aging of freshly prepared azobenzene films is studied. It was found that under illumination the film undergoes essential changes in both its mechanical and optical properties. In the first illumination cycle, an abnormal response was observed. At first, the layer stiffness increased, afterwards the film becomes softer. However, a long time (24h) illumination leads to a strong increase of both hardness and stiffness as well as to the change of the film colour. The experiments were performed using different techniques. The method of nano indentation was used to obtain the absolute values for the E modulus and for a hardness of films, these data were compared with the measurements for the stiffness and thickness made by AFM with high lateral resolution. Optical properties, in particular the absorption and refractive index were measured by UV-VIS spectroscopy and ellipsometry.

CPP 26 POSTER Dynamics and Diffusion

Time: Thursday 17:00–19:00

Room: P2

CPP 26.1 Thu 17:00 P2

Influence of isotopic substitution of cyclohexane on transport coefficients of binary liquid mixtures — ●GERHARD WITTKO and WERNER KÖHLER — Physikalisches Institut, Universität Bayreuth

In a binary system, a temperature gradient does not only lead to a heat flux but also to a mass flux. The latter effect is known as thermal diffusion, or Ludwig-Soret-effect. The Soret coefficient S_T is a measure for the concentration gradient in the stationary state, where the mass flux due to thermal diffusion is compensated by the mass flux due to Fickian diffusion. Until now there is no microscopic theory on neither thermal diffusion nor diffusion that allows to predict values of S_T or the diffusion coefficient D in liquids from molecular properties. We present experimental results on the influence of the isotopic substitution of protonated cyclohexane by perdeuterated cyclohexane in binary liquid mixtures on D , S_T and the thermal diffusion coefficient D_T . For D we find almost the same value in both the mixture containing protonated and perdeuterated cyclohexane. In contrast to this, S_T of the mixture containing the heavier isotope is lower than S_T of the mixture containing the lighter isotope by about $\Delta S_T = 1 \times 10^{-3} \text{K}^{-1}$ at all mole fractions.

CPP 26.2 Thu 17:00 P2

Overlap Concentration of Polymers in a Good Solvent determined by Fluorescence Correlation Spectroscopy (FCS) — ●UTE LIPPERT¹, HEIKO ZETTL¹, ALEXANDER BÖKER¹, JÖRG ENDERLEIN², and GEORG KRAUSCH¹ — ¹Physikalische Chemie II, Universität Bayreuth — ²Institute for Biological Information Processing IBI 1, Forschungszentrum Jülich

For polymer solutions the dilute and concentrated regime is well investigated by light scattering, rheology, and fluorescence recovery after photo bleaching. The crossover concentration between the dilute and semi-dilute regime and the properties of solutions in the semi-dilute regime are less investigated. This concentration range is difficult to assess with the above mentioned methods. We have prepared monodisperse batches of polystyrenes labeled with a single dye molecule per chain. We use fluorescence correlation spectroscopy (FCS) to determine the diffusion behavior of these chains in solutions containing varying amounts of unlabelled chains. We are able to assign the crossover between dilute and semi-dilute for molecular weights in the range of 4 kg/mol to 1500 kg/mol. We find a scaling law for the dependence of the overlap concentration on molecular weight in agreement with theoretical predictions.

CPP 26.3 Thu 17:00 P2

N-Alkanes confined in Nanoporous Silicon: An Infrared Spectroscopy and X-ray Diffraction Study — ●ANKE HENSCHEL, RENÉ BERWANGER, KLAUS KNORR, and PATRICK HUBER — Technische Physik, Universität des Saarlandes, 66123 Saarbrücken

The conformation and arrangement of linear hydrocarbons ($C_{16}H_{34}$ - $C_{21}H_{44}$) confined in tubular pores of porous silicon (mean pore diameter 10nm) is investigated by combined infrared spectroscopy and x-ray diffraction measurements. We find distinct changes in the vibration char-

acteristics, in the structure factor as well as the phase transition temperatures of confined n-alkanes as compared to the bulk phases.

CPP 26.4 Thu 17:00 P2

Neutron Spectroscopy on Polymers Confined to Nanoporous Glasses — ●ANDREAS SCHÖNHALS¹, HARALD GOERING¹, BERNHARD FRICK², and REINER ZORN³ — ¹Bundesanstalt für Materialforschung und prüfung, Unter den Eichen 87, D-12205 Berlin — ²Institut Max von Laue - Paul Langevin (ILL) 6, rue Jules Horowitz, B.P. 156, F-38042 Grenoble Cedex 9 — ³Forschungszentrum Jülich, Institut für Festkörperforschung, D-52425 Jülich

The behavior polymers confined to geometries of a nanometer scale has become an interesting field. Neutron scattering (NS) is valuable tool to investigate such systems because of the high penetration depth of neutrons. Incoherent NS was carried out on poly(dimethyl siloxane) and poly(methyl phenyl siloxane) confined to Sol/Gel-glasses (7.5, 5.0, 2.5 nm). To cover a broad dynamical range of the scattering function $S(Q,E)$ time-of-flight and backscattering are combined. For the frequency range of the Boson peak the vibrations at lowest frequencies are depressed by the confinement. Elastic scans were carried out and the mean square displacement msd was calculated. Above T_g the characteristic increase of the msd found for the bulk is strongly influenced by the confinement but for both materials in a different manner. The main influence of the confinement on $S(Q,t)=FT(S(Q,E))$ is an broadening of $S(Q,t)$ with increasing confinement. These results are discussed together with dielectric measurements.

CPP 26.5 Thu 17:00 P2

Semiflexibility accelerates barrier crossing of hinged polymers — ●WOLFRAM MÖBIUS, RICHARD. A. NEHER, and ULRICH GERLAND — Arnold Sommerfeld Center for Theoretical Physics (ASC) and Center for Nanoscience (CeNS), LMU München

We study the planar rotational diffusion of a semiflexible polymer with one free and one hinged end. The hinged end is subject to a periodic potential that acts on the angle of the attachment. We find that the rate for the crossing of the potential barriers is considerably larger for a semiflexible polymer than for a stiff rod. This enhancement of the rate occurs even at persistence lengths which are much larger than the contour length, so that the average end-to-end distance of the polymer is close to its limiting value. To understand this behavior we consider a system where the polymer is replaced by two elastically jointed segments. This toy model is amenable to analytic treatment and we derive expressions for the diffusion and barrier crossing rates for large bending rigidities. Both models may help to understand the thermally activated wrapping and unwrapping of DNA in nucleosomes.

CPP 26.6 Thu 17:00 P2

Molecular dynamics in semifluorinated side-chain Polyesters as studied by Broadband Dielectric Spectroscopy — ●J TSUWI¹, F KREMER¹, L HARTMANN¹, D POSPIECH², L HÄUSSLER², and D JEHNICHEN² — ¹Institute for Experimental Physics I, University of Leipzig, Linné Straße 5, 04103 Leipzig, Germany — ²Leibniz-Institute of Polymer Research Dresden, Hohe Straße 6, 01069 Dresden, Germany

The molecular dynamics in fluorinated side-chain polyesters was studied using Broadband Dielectric Spectroscopy in the frequency range from 0.1 Hz to 10 MHz and temperatures between 120 K and 500 K. The chemical structure of the main chain was selectively varied in order to elucidate the effect of backbone flexibility on the molecular motion. It is observed that the fluorinated side-chain exhibits two relaxation processes γ and δ -like. The γ process is assigned to librational fluctuations at the terminal position of the side chain while the δ -like process reflects a cooperative motion of the side chain as a whole. Two more processes (α and β) are observed, which are associated with motion of the main chain. With respect to the flexibility of the main chain, an interesting behavior is seen in the dynamics of the backbone when compared to side chain motion. Based on the analysis of the activation plot, it is concluded that a flexible main chain exhibits faster mobility in direct contrast to its side chain motion. The dielectric results are discussed in the context of micro-phase separated layered structures, supported by recent data from DSC and t-SAXS. References [1] Tsuwi, J et al.; Coll. Polym. Sci. 2005, 283:1321 [2] Tsuwi, J et al.; Macrom. 2004, 37:6050 [3] Tsuwi, J et al.; J. Polym. Sci. B: (submitted)

CPP 26.7 Thu 17:00 P2

Examination of iterative phenomena during the final stages of the pinching processes of polymeric solutions — ●RAINER SÄTTLER¹, CHRISTIAN WAGNER¹, and JENS EGGERS² — ¹Universität des Saarlandes, Experimentalphysik — ²University of Bristol, School of Mathematics, J

We examine the stretching dynamics of dilute and semidilute solutions of Polyethylene Oxide in both droplet-pinch and capillary-breakup using microscope objectives and high speed video cameras. We investigate the nature and prerequisites for the supposedly iterative formation of beads on the thinning filament, which form as the extension of the polymers saturates. We varied molecular weight, concentration, viscosity of the solvent using different mixtures of glycerol and water and initial diameter, by using different sets of plates and nozzles. Evaluation of the rich behaviour and the present phenomena has yet to prove under which circumstances and for which number of generations the behaviour really shows iterative character and whether or not the size ratios obey deterministic rules. Furthermore the causes for the growth of these instabilities are not yet fully understood and there is not in all cases good agreement between experiments and existing descriptions.

CPP 26.8 Thu 17:00 P2

The retraction process captured by SANS : segmental fluctuations — ●EKKEHARD STRAUBE¹, ARIANE BLANCHARD², WIM PYCKHOUT-HINTZEN², and DIETER RICHTER² — ¹Uni Halle-Saale — ²Forschungszentrum Jülich

The retraction process of linear chains after a fast non-linear stretch was re-investigated in long polyisoprene chains, characterized by approximately 58 entanglements. For the first time, the non-linear process of retraction, along with measurable amounts of constraint-release events could be detected from time-resolved but quenched small angle neutron scattering experiments. This contrasts numerous attempts to proof already decades ago. The results are in fair agreement with a recent curvilinear description, which heavily relied on linear rheology concepts concerning path length fluctuations and constraint release mechanisms. In this work quantitative evaluations of the segmental fluctuation range are now enabled on the basis of a modified single chain approach to which dynamic parameters had been added in a defined way. Also extensive use is made in the experimental carry-through of the parameters of linear rheology. This experimental study covers various strains from linear to non-linear regime and is discussed within the framework of the original Doi-Edwards work. Inadequately described features of the scattering curves in the previous communication, mainly due to the straight comparison of theory with data without optimizing could be relieved. We conclude that segmental fluctuations are anisotropic and comparison to rheology is critical.

CPP 26.9 Thu 17:00 P2

The flow resistance of single DNA-grafted colloids as measured by optical tweezers — ●C. GUTSCHE¹, M. SALOMO², Y.W. KIM³, R. NETZ³, and F. KREMER¹ — ¹Institut für Experimentelle Physik I der Universität Leipzig — ²Institut für Biochemie der Universität Leipzig — ³Physik Department TU München

Optical tweezers are microscopic tools with extraordinary precision in the determination of the position (± 2 nm) of a colloid (diameter: 2.2 μm) in 3D-space and in the measurement of small forces acting on it in the range between 0.1 pN - 100 pN ($\text{pN} = 10^{-12}$ N). In rheological experiments the flow resistance of single blank or DNA-grafted colloids is determined and compared. The length of the double-stranded (ds)-DNA varies between 1000 base pairs (bp), 4000 bp and 6000 bp corresponding to contour lengths between 340 nm and 2040 nm at a grafting density of $0.03 \pm 0.01 \mu\text{m}^2/\text{chain}$. The degree of swelling of the grafted DNA is adjusted by exchanging the ion concentration of the surrounding medium. For all examined flow velocities ranging between 100 $\mu\text{m}/\text{s}$ to 1200 $\mu\text{m}/\text{s}$ one observes an interesting deviation from Stokes law which can be traced back to a shear-dependent conformational change of the brush layer. The ratio of the effective hydrodynamic radii of DNA-grafted and blank colloids shows a pronounced dependence on the flow velocity, but as well on the length of the grafted DNA and the ionic strength of the solvent. The experimental findings are in qualitative agreement with hydrodynamic simulations based on an elastically-jointed chain model.

CPP 26.10 Thu 17:00 P2

The interaction between single colloids grafted with DNA of varying molecular weight as measured by optical tweezers — ●K. KEGLER¹, C. GUTSCHE¹, M. SALOMO², J. REIMUTH¹, V. SKOKOV¹, and F. KREMER¹ — ¹Institute for Experimental Physics I, University of Leipzig, Linnéstr. 5, 04103 Leipzig — ²ceLectra, Deutscher Platz 5, 04103 Leipzig

Optical tweezers are used to measure the interaction forces between single blank and DNA-grafted colloids (length of DNA: 1000 base-pairs (bp), 2000 bp, 3000 bp, 4000 bp). The forces are measured in two directions, parallel and perpendicular to the axis between the two colloids under study. For blank colloids on approach repulsive forces are observed which depend in their force and range on the ionic strength of the surrounding medium. At a certain separation the colloids jump into contact. This is not the case in deionised water. DNA-grafted colloids behave in principle similarly but with a softer interaction potential. Moving DNA-grafted colloids which are in contact perpendicularly to their central axis results in stick-slip phenomena. Their intensity and dynamics are studied for different molecular weights of the DNA and in media of varying ionic concentration.

CPP 26.11 Thu 17:00 P2

Spacer effects in branched polymer dynamics — ●CRISTIAN SATMAREL¹, CHRISTIAN VON FERBER^{1,2}, and ALEXANDER BLUMEN¹ — ¹Theoretische Polymerphysik, Universität Freiburg, Hermann-Herder Str. 3, 79104-Freiburg, Deutschland — ²Jagellonian University, Reymonta 4, 30-059 Krakow, Poland

We investigate the relation between structure and viscoelastic behavior of branched copolymeric structures, highlighting the important effects of linear spacer segments between branching points [1,2]. In the framework of generalized Gaussian models we succeed in determining the eigenvalue spectra of such networks, by developing an analytical procedure which involves an exact real-space renormalization. This allows us to relate the spectrum of the extended structure (in which the branching points are linked to each other through spacer segments) to that of a simpler, "reduced" structure without spacers. In so doing, we find that the dynamic spectra are related through a global transformation. To exemplify our procedure, we apply the method to typical hyperbranched polymers [1], as well as to randomly linked star polymers [2].

[1] C. Satmarel, C. von Ferber and A. Blumen, in preparation.

[2] C. Satmarel, C. von Ferber and A. Blumen, J. Chem. Phys. 123, 034907, 2005.

CPP 26.12 Thu 17:00 P2

Dynamic properties of strongly confined dipolar liquids — ●VLADIMIR FROLTISOV¹ and SABINE KLAPP² — ¹Stranski-Laboratorium fuer Physikalische und Theoretische Chemie, Sekr. C7, TU Berlin, Strasse des 17. Juni 135, 10623 Berlin — ²Institut fuer Theoretische Physik, Sekr. PN 7-1, TU Berlin, Hardenbergstrasse 36, 10623 Berlin

We report molecular dynamics simulation results for a Stockmayer fluid confined to a narrow (5.0 or less particle diameters) slit pore with structureless, non-conducting walls. Translational and rotational dynamics of the dipolar particles are investigated by calculating autocorrelation functions, diffusion coefficients and relaxation times for various pore widths and directions parallel and perpendicular to the walls. The dynamical properties of the confined systems are compared to corresponding bulk properties under the condition of all compared systems having the same chemical potential. We find that the dynamic behavior inside the pore depends on the distance from the walls and can be strongly anisotropic even in globally isotropic system. Relaxation of dipole orientations and angular velocities is slower in directions parallel to the walls, especially close to the walls, and faster in perpendicular direction as compared to the bulk.

CPP 26.13 Thu 17:00 P2

Length scales and mechanisms of motion in entangled polymer melts — ●EKKEHARD STRAUBE¹ and RALF EVERAERS² — ¹Martin-Luther-Universität Halle-Wittenberg, Fachbereich Physik, Germany — ²Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, Dresden, Germany

Using a lattice-free dynamical Monte-Carlo method for rod-bead chains up to 512 segments as models of entangled polymer melts the monitoring of the behavior of copies of the system subjected to identical en-

tanglement conditions but different time evolutions created by different sequences of random numbers allows the investigation of the structure of the topological constraints. The investigation of systems with different segment densities supports that the packing length governs the local motion in entangled melts. The analysis of the fluctuation structure of the copies allows the construction of the corresponding tube axis, the tube radius, the step length of the primitive path and the Rouse-like dynamics of the tube axis due to constraint release processes.

CPP 26.14 Thu 17:00 P2

Structure and IR frequencies of small water clusters on Ni surfaces from DFT calculations — ●TATIANA MURAKHTINA, LUIGI DELLE SITE, and DANIEL SEBASTIANI — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz

We present adsorption energies, geometries and harmonic frequencies of a series of water oligomers (molecule, dimer, trimer) on nickel surfaces, paying special attention to the effect of a step defect on the adsorption. These frequencies and the change in the electron density distribution upon adsorption are used to characterize the nature of the molecule-surface bonds. We use the "free energy functional" module of Car-Parinello Molecular Dynamics (CPMD) package which allows for fractional occupation numbers of all bands and compare to a standard Density Functional Theory (DFT) calculation where $n=2$ is imposed for all electronic states.

CPP 27 POSTER Polymer Physics and Materials

Time: Thursday 17:00–19:00

Room: P2

CPP 27.1 Thu 17:00 P2

Microfocus-Infrared Synchrotron Ellipsometry for analysis of laterally patterned organic thin films — ●MICHAEL GENSCH¹, ERNST HEINER KORTE², NORBERT ESSER¹, ULLRICH SCHADE³, and KARSTEN HINRICHS¹ — ¹ISAS - Institute for Analytical Sciences, Department Berlin, Albert-Einstein-Str. 9, 12489 Berlin, Germany — ²ISAS - Institute for Analytical Sciences, Bunsen-Kirchhoff-Str. 11, 44131 Dortmund, Germany — ³Berliner Elektronenspeicherring-Gesellschaft für Synchrotronstrahlung mbH, Albert-Einstein-Str. 15, 12489 Berlin, Germany

A purpose-built infrared spectroscopic ellipsometer is presented that enables to investigate sample areas of less than 1 mm² with monolayer sensitivity. This sensitivity is achieved for films on metallic as well as on semiconducting substrates by utilizing radiation from an infrared synchrotron beamline at BESSY II. Measurement principle and performance of the instrument are discussed on selected examples and an outline of the recently performed upgrade of the set-up is given. It is shown how thickness, structure and composition of patterned nanofilms can be characterized by evaluation of the infrared ellipsometric parameters [2]. This is of technological relevance to investigate the functionality of e.g. stimuli responsive 1D polymer brush gradient films, biodiagnostic arrays or monomolecular films for solar cell applications. [1] M. Gensch, K. Roodenko, K. Hinrichs, R. Hunger, A. Merson, U. Schade, Y. Shapira, Th. Dittrich, J. Rappich, N. Esser, J. Vac. Sci. Technol. B 23, 1838 (2005). [2] K. Hinrichs, M. Gensch, N. Esser, Appl. Spectrosc. 59, 272A (2005).

CPP 27.2 Thu 17:00 P2

IR-VIS Ellipsometry for characterization of ultra-thin polymer films — ●K. HINRICHS¹, M. GENSCH¹, N. ESSER¹, L. IONOV², M. STAMM², S. MINKO³, and K.-J. EICHHORN² — ¹ISAS - Institute for Analytical Sciences, Department Berlin, — ²Leibniz Institute for Polymer Research Dresden, Hohe Str. 6, D-01069 Dresden — ³Chemistry Department, Clarkson University, Potsdam, New York 13699, USA

Mid infrared (MIR) spectroscopic ellipsometry [1] and Visible (VIS) ellipsometry have been jointly used for the study of mixed polystyrene-poly(2-vinylpyridine) and polystyrene-poly(ter-butyl acrylate) polymer grafted films (mixed brushes) with gradually changing composition (1D gradient mixed brushes). In the first step from ellipsometric measurements the optical constants of the single polymers in thin films (PS, P2VP, PBA) have been evaluated. In a second step the thickness and composition of mixed polymer brush films ($d < 10$ nm) of these compounds were determined. It is evident that infrared optical properties of polymer thin films are correlated to the chemical structure of the thin film and can be used for lateral compositional analysis, whereas conventional

VIS ellipsometry is limited by the similarity of refractive indices of different polymers. Present limitations of IRSE are due to the signal to noise ratio and restricted lateral resolution. This can be improved at the synchrotron ellipsometer at BESSY/Berlin, which is presently upgraded for mapping experiments.

[1] K. Hinrichs, M. Gensch, N. Esser, Appl. Spectrosc. 59 (2005) 272(A)-282(A). [2] L. Ionov, A. Sidorenko, K.-J. Eichhorn, M. Stamm, S. Minko, K. Hinrichs, Langmuir 21 (2005) 8711.

CPP 27.3 Thu 17:00 P2

Optical and mechanical anisotropy of oriented PET films studied by reflectance difference spectroscopy — ●KLAUS SCHMIDEGG¹, LI DONG SUN¹, GÜNTHER MAIER², JOZEF KECKES², and PETER ZEPPENFELD¹ — ¹Institut für Experimentalphysik, Johannes Kepler Universität Linz, Altenbergerstr. 69, A-4040 Linz — ²Erich Schmid Institut für Materialwissenschaften, Jahnstr. 12, A-8700 Leoben

A new method for the characterization of molecular orientation in polymers is presented, which is based on the determination of the optical anisotropy by reflectance difference spectroscopy (RDS). Its advantages are the sensitivity to birefringence, spectroscopic information, high time resolution and superior measurement precision as compared to refractive index measurements. The capabilities of RDS are presented for the special case of biaxially oriented poly(ethylene terephthalate) (PET) films, for which both magnitude and direction of the optical anisotropy can be determined. The data are consistent with refractive index measurements using spectroscopic ellipsometry and wide-angle X-ray scattering. The high time resolution and the simple setup enabled us to perform in-situ measurements during tensile testing of thin PET films. A clear correspondence of the initial optical and mechanical anisotropy directions can be seen. The RDS signal depends linearly on the applied strain and the gradient shows the same angular behavior. A closer look reveals that not only the size of the optical anisotropy changes, but also the position of the axes is rotated towards the drawing direction, which is a consequence of the reorientation of the molecules in the polymer.

CPP 27.4 Thu 17:00 P2

Surface roughness and adsorption isotherms of molecularly thin liquid films — ●MICHAEL PAULUS¹, CRISTIAN GUTT², and METIN TOLAN¹ — ¹Institute of Physics, University of Dortmund, D-44221 Dortmund, Germany — ²Deutsches Elektronen Synchrotron (HASYLAB), Notkestraße 85, D-22607 Hamburg, Germany

We present an x-ray reflectivity study of molecularly thin adsorbed isobutane films on liquid glycerol. The interaction between the isobutane and the liquid glycerol is usually dominated by long-range van der

Waals interaction which gives rise to the formation of thin films of gas molecules on the glycerols surface. Surfaces of liquids are modulated by thermally excited capillary wave fluctuations. Concerning thin films, this capillary wave fluctuations are strongly suppressed by the substrate-film interaction. This leads to a layer thickness dependent roughness of thin adsorbed films. The x-ray reflectivity measurements provide both, the adsorption isotherms and the rms roughness of the adsorbed film. The measured surface roughness of the isobutane film is smaller than expected from a calculation based on a harmonic approximation of the interaction potential. It turned out that the calculation of surface roughness of molecularly thin adsorbed films leads to good agreement with experiment, only when higher order terms of the interaction potential are considered. This is causally connected by the strong coupling between the glycerol and layer surface at low layer thickness.

CPP 27.5 Thu 17:00 P2

Phase properties of confined dipolar fluids — ●MATTHIAS GRAMZOW¹ and PD DR. SABINE H. L. KLAPP^{1,2} — ¹Stranski Laboratorium für Physikalische und Theoretische Chemie, Technische Universität Berlin, Strasse des 17. Juni 135, 10623 Berlin — ²TU Berlin, Institut für Theoretische Physik, Hardenbergstrasse 36, 10623 Berlin

The phase behavior and structural properties of various dipolar model fluids confined to a slit pore are investigated using density functional theory in meanfield (MF) and truncated modified meanfield (MMF) approximation. As a first step we approximate the inhomogeneous number density in the pore as a constant and consider only the orientational structure. Our focus lies on the description of isotropic and anisotropic fluid phases.

In the MF calculations we find first- and second-order isotropic-to-ferroelectric as well as isotropic liquid-to-gas phase transitions. For both types of phase transitions the confinement shifts the critical points towards lower temperatures. It also shifts the chemical potential, where the direction of the shift depends on the model considered. Moreover, in very narrow pores the isotropic liquid-to-gas phase transition is entirely suppressed.

Finally, we compare our MF results for the phase behavior to those from the more sophisticated MMF approach. The latter also provides information on the local orientational structure which turns out to be anisotropic even in globally isotropic phases.

CPP 27.6 Thu 17:00 P2

Gradient nanotubes by wetting — ●MARC MILBRADT¹, PAUL MICLEA¹, ANDREAS GREINER², and RALF WEHRSPHORN¹ — ¹Physics Department, University of Paderborn — ²Philipps University Marburg

Using the wetting-assisted templating (WASTE) process for the preparation of single homogeneous nanotubes we produced gradient nanotubes. The WASTE process is based on the spontaneous wetting of high-energy surfaces (macroporous silicon or porous alumina) by low-surface energy materials (organic compounds, here: polymeres). The wetting can be done in solution or in melt state. With modifications on the WASTE-process it is possible to prepare nanotubes with a longitudinal gradient. The so-called "face-to-face"-wetting allows wetting of two different materials placed on the opposite ends of the template pores.

We prepared gradient nanotubes by the use of PMMA and a fluorescent PMMA/9-Vinylanthracene copolymer. The gradient is formed at the point of contact of the two polymers. Another way to prepare gradient nanotubes is to use a mixture of polystyrene and a fluorescent dye (here: DANS) on the one side and polystyrene on the other side of the template pores. In this case the gradient is formed by diffusion of the dye into the polymer. The gradient nanotubes were investigated by fluorescence microscopy.

The gradient nanotubes can be used for graded-index optical fibers or waveguides and gradients in the surface-energy can be used to direct fluids on a given path.

CPP 27.7 Thu 17:00 P2

Unexpected preparative effects on the properties of thin polymer films — ●ANATOLI SERGHEI¹, HEIKO HUTH², CHRISTOPH SCHICK², and FRIEDRICH KREMER¹ — ¹University of Leipzig, Institute for experimental physics I, 04103 Leipzig, Germany — ²University of Rostock, Physics Department, , 18051 Rostock, Germany

Thin supported PS films dewet a solid substrate when kept above T_g in vacuum (~ 3 mbar), while in high vacuum (10⁻⁶ mbar), under identical experimental conditions, i.e. same thickness, temperature and annealing time, no dewetting takes place. When sandwiched between two thin

metal electrodes a characteristic pattern is developed in ambient air above T_g, whereas no changes are observed in high vacuum or in a pure nitrogen atmosphere. These two seemingly unrelated phenomena are suggested to have a common physical origin: due to the presence of remanent oxygen in the immediate vicinity of the polymer films, chain scissions are induced, which result in a pronounced decrease of the average molecular weight. This causes an enhancement of the molecular mobility and a reduction of the corresponding glass transition temperature T_g, as proven by Broadband Dielectric Spectroscopy, AC-calorimetry and capacitive dilatometry. No shifts of the glass transition in thin PS films down to a thickness of 20 nm are detected when the samples are annealed in high vacuum and measured in a pure nitrogen atmosphere.

A. Serghei et al., Phys. Rev. E 71, 061801 (2005).

CPP 27.8 Thu 17:00 P2

Spin-Echo Neutron Reflectivity on Diblock-Copolymer Films — ●MAX NÜLLE¹, ADRIAN RÜHM², JANOS MAJOR¹, ULRICH WILDGRUBER², and HELMUT DOSCH¹ — ¹Max-Planck-Institut für Metallforschung, Heisenbergstr. 3, 70569 Stuttgart — ²Max-Planck-Institut für Metallforschung, ZWE Neue Forschungsneutronenquelle Garching, Lichtenbergstr. 1, 85747 Garching bei München

SERGIS (Spin-Echo Resolved Grazing Incidence neutron Scattering) is a recently developed novel neutron scattering technique which will be routinely employed at the new X-ray/neutron reflectometer N-REX+ at FRM-II. In contrast to conventional scattering methods, SERGIS measures the lateral structure and morphology of surfaces and thin film systems in real space. The spatial resolution is achieved by measuring the total polarization of the scattered beam, without the usual need to collimate the beam in the direction of interest. Therefore SERGIS combines a high neutron flux with the ability to characterize structures from the nanometer scale up into the micron range, and can thus yield novel information about both equilibrium and time-dependent phenomena on these length scales. One typical example is morphologies produced by dewetting phenomena. First results of experiments on diblock-copolymer films will be presented.

CPP 27.9 Thu 17:00 P2

Bottom-Up Lithography: Growing Layout-Defined 3-dimensional Micro- and Nano-Structures by Molecular Self-Assembly — ●MATTHIAS BARCZEWSKI^{1,2}, ALFRED BLASZCZYK¹, MARCEL MAYOR^{1,3}, THOMAS SCHIMMEL^{1,2}, and STEFAN WALHEIM¹ — ¹Institute for Nanotechnology, Forschungszentrum Karlsruhe, 76021 Karlsruhe (Germany) — ²Institute of Applied Physics, University of Karlsruhe, 76131 Karlsruhe (Germany) — ³Chemistry Department, University of Basel, 4056 Basel (Switzerland)

We present a novel soft-lithographic approach for the formation of metal-organic micro- and nanostructures on surfaces. The structures are grown from bottom up, instead of removing material from a resist layer [1]. This can be achieved by making use of an anisotropic molecular self-assembly process which leads to the formation of a metal-organic film which we call Substrate-Consuming Metal-Organic Layer (SCMOL). This growth can be laterally controlled by the pre-deposition of a monomolecular two dimensional pattern, by Micro-Contact Printing. This patterned self-assembled monolayer (SAM) acts as a lateral stencil mask for the growth process of the SCMOL film. This process yields structures with perpendicular walls and a lateral resolution of about 20 nm. The height of the structures reaches up to 600 nm - hundred times the height of the constituent molecules.

[1] S. Walheim, M. Barczewski, A. Blaszczyk, M. Mayor, Th. Schimmel Patent application: DE 102005025693.7 (2005)

CPP 27.10 Thu 17:00 P2

Mixed monolayers of phospholipids and amphiphilic block copolymers at the air/water interface — ●S. RALEVA¹, H. HUSSAIN², J. KRESSLER², V. SCHÖN³, P. HUBER³, and B. STÜHN¹ — ¹TU Darmstadt, D-64289 Darmstadt — ²MLU Halle-Wittenberg, D-06099 Halle — ³University of Saarland, D-66041 Saarbrücken

We have investigated the behaviour of mixed monolayers of phospholipids and amphiphilic block copolymers at the air/water interface by measuring the surface pressure/area isotherms in conjunction with x-ray reflectivity measurements. The samples are the synthetic phospholipid diphtanoylphosphatidilcholine (DPhPC) and amphiphilic di- and triblock copolymers of poly(ethylene oxide) and poly(perfluorohexylethyl methacrylate). From the isotherms we obtain information about the monolayer conformation as a function of the degree of compression. From

the x-ray reflectivity measurements we obtain information about the surface roughness, film thickness and electron density variation along the surface normal. We discuss the results as a function of the film composition and the surface pressure. DPhPC isotherms show that the phospholipid exists in the liquid-expanded phase at all surface pressures. The results of monolayer thickness at the air/water interface are in agreement with the results for monolayer of DPhPC on solid substrate. Analysis of the surface pressure/area isotherms shows that the addition of polymer results in homogeneously mixed as well as of non mixed films, depending on the concentration of the added polymer, its composition and surface pressure. X-ray reflectivity measurements results show clear change in the thickness of the film after addition of the polymer.

CPP 27.11 Thu 17:00 P2

Polarized Fourier Transform Infrared Spectroscopy on Thin Chiral Liquid Crystal Elastomer Films — ●MICHAEL TAMMER¹, PATRICK KÖLSCH¹, BIN CHEN², HEINO FINKELMANN², and FRIEDRICH KREMER¹ — ¹Universität Leipzig, Institut für Experimentelle Physik I, Linnéstr. 5, 04103 Leipzig — ²Albert-Ludwigs-Universität Freiburg, Institut für Makromolekulare Chemie, Stefan Meier Str. 31, 79104 Freiburg

Liquid crystalline elastomers (LCE) are consisting of crosslinked polymers with mesogenic units connected to the polymer network. Embedding an anisotropic liquid crystals in an elastic polymer network results in a variety of remarkable features. Their macroscopic form changes strongly with temperature, they are birefringent due to the alignment of the mesogens or they change volume in electric fields, just to name a few of the sophisticated features of this relatively new class of material. The potential applications range from soft contact lenses, artificial muscles, multicolor laser devices to electro-mechanical devices. Polarized Fourier Transform Infrared Spectroscopy (FTIR) is applied to investigate the molecular response of thin liquid crystal elastomer (LCE) films with a cholesteric mesogen structure to an external mechanical stress. The analysis of the absorbance bands for molecular vibrations of the main chain, the spacer groups and bands of the mesogens yields the mean orientations and the order parameters of these molecular units. The influence of the applied strain on the orientation and order is determined.

CPP 27.12 Thu 17:00 P2

Structural and mechanical properties of thin PMMA films prepared by pulsed laser deposition — ●ANDREAS MESCHÉDE, ERIK SÜSKE, THORSTEN SCHARF, and HANS-ULRICH KREBS — Institut für Materialphysik, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

Thin polymer films were grown by pulsed laser deposition (PLD) at 248 nm in ultra high vacuum (UHV). In the case of poly(methyl methacrylate) (PMMA), the observed films consist of two components which differ in chemical and mechanical properties as molecular mass or amount of crosslinking. These properties can be controlled by deposition parameters like substrate temperature and laser fluence or by using absorption optimized target material. In this contribution the deposition mechanism with respect to the film characteristics, as for example microstructure and mechanical properties, which have been examined by scanning electron microscopy, mechanical spectroscopy and nano-indentation measurements, will be discussed.

CPP 27.13 Thu 17:00 P2

Faster dynamics in thin polymer films? — ●ANATOLI SERGHEI¹, LUTZ HARTMANN¹, YULIA MIKHAILOVA², KLAUS-JOCHEN EICHHORN², BRIGITTE VOIT², and FRIEDRICH KREMER¹ — ¹Leipzig University, Institute for Experimental Physics I, Leipzig, Germany — ²Leibniz Institute of Polymer Research, Dresden, Germany

The molecular dynamics in thin films of polymers with different macromolecular architectures (linear and hyperbranched structures) are investigated by Broadband Dielectric Spectroscopy. Pronounced confinement-effects are detected: the average relaxation rate of the dynamic glass transition increases with decreasing film thickness, indicating a faster dynamics in thin films. The molecular mechanism of these effects is revealed by the quantitative determination of the relaxation time distribution in dependence on the confinement size. It turns out that: a) the increase in the average relaxation rate is caused by a gradual suppression (freezing-out) of the slower relaxation modes in confinement; b) at a molecular level no polymer segments are found to relax faster in thin films than in the bulk.

L. Hartmann et al., Eur. Phys. J. E 8, 145 (2002). A. Serghei et al.,

Eur. Phys. J. E 17, 199 (2005).

CPP 27.14 Thu 17:00 P2

Mechanical Properties of Free Standing Liquid Filaments — ●ALEXANDRU NEMES, ALEXEY EREMIN, and RALF STANNARIUS — Institute of Experimental Physics, University of Magdeburg, Universitätsplatz 2, D-39106 Magdeburg, Germany

Stable free standing filaments with slenderness ratios (length to diameter ratio) of more than 1000 can be prepared in some mesophases of liquid crystals. In our work, the mechanical properties of such structures are described. With a special excitation technique, we pluck the filaments and excite damped oscillations. Experimental relaxation times and oscillation frequencies of such liquid chords are discussed within a model that describes the damped vibrations of a liquid string under the influences of surface tension, inertial, viscous, and elastic forces. Reference: R. Stannarius, A. Nemeş and A. Eremin, Phys. Rev. E, 72 020702(R) (2005)

CPP 27.15 Thu 17:00 P2

AFM-Nanolithography on self-assembled monolayers — ●HARALD GRAAF¹, MAIK VIELUF¹, MASATO ARA², and HIROKAZU TADA² — ¹Optische Spektroskopie und Molekülphysik, Institut für Physik, Technische Universität Chemnitz, 09107 Chemnitz — ²Division of Materials Physics, Graduate School of Engineering Science, Osaka University, Osaka 560-8531 JAPAN

We report on the anodic oxidation of self-assembled monolayers (SAM) on silicon surfaces by Atomic Force Microscopy (AFM). These SAM are prepared by heat-induced chemical reaction of an alkene with a hydrogen terminated silicon surface. They are characterized by a high order of the molecules and a strong physical as well as chemical stability. By varying the headgroup of the alkenes the properties of the surface can be easily tuned, e.g. from hydrophobic to hydrophilic. By anodic oxidation the SAM can be locally degraded and the below silicon oxidized leading to silicon oxide nanostructures. These silicon oxide structures can either be modified by attaching different Silane molecules or can be selectively removed by chemical etching followed by chemical modification of the formed ditch.

CPP 27.16 Thu 17:00 P2

Molecular Editing of Polymer Brushes with the Tip of an AFM — ●ROLAND GROEGER¹, INGO SAMERSKI¹, THOMAS SCHIMMEL^{1,2}, and STEFAN WALHEIM¹ — ¹Institute for Nanotechnology, Forschungszentrum Karlsruhe, 76021 Karlsruhe (Germany) — ²Institute of Applied Physics, University of Karlsruhe, 76131 Karlsruhe (Germany)

Polymer brushes prepared from low molecular-weight carboxyl-functionalized polystyrene and polybutadiene were prepared on silicon oxide surfaces. Their topography and their adhesion properties are investigated by Atomic Force Microscopy (AFM). We describe how these ultra-thin polymer films can be mechano-chemically removed by the tip of an AFM at pre-defined locations and subsequently replaced by another polymer species. In this way it was possible to generate polymeric surfaces with a pre-defined chemical pattern. This opens perspectives for generating specifically functionalized nano-scale patterns, e.g. for nano-biology.

CPP 27.17 Thu 17:00 P2

Thin Films of Crystalline Diblock Copolymers — ●CHARLES DARKO¹, I. BOTIZ², G. REITER², and C. PAPADAKIS¹ — ¹Physik Department E13, Technische Universität München, James-Frank Str. 1, 85748 Garching — ²Institut de Chimie des Surfaces et Interfaces, CNRS, Mulhouse, France

In thin films of diblock copolymers having one crystallizing block, a number of surface structures have been observed, e.g. edge-on or flat-on lamellae with high persistence lengths, spirals and dendrites, allowing the structuring of organic surfaces on a large range of length scales. The crystallization growth process in thin films of lamellar poly(styrene-*b*-ethyleneoxide) diblock copolymer was followed by in-situ optical microscopy. Using grazing-incidence small-angle X-ray scattering (GISAXS) and grazing-incidence X-ray diffraction (GIXD), we investigate the orientation of the mesoscopic structures with respect to the substrate as well as the orientation of the crystalline chains with respect to lamellar interfaces. This information on the structure inside the film is compared to the surface texture obtained by atomic force microscopy with the focus on the effect of crystallization temperature.

CPP 27.18 Thu 17:00 P2

Electrostatic field induced patterning: a method for controlling the anisotropy of films of polar organic molecules — ●SVEN VERPOORT¹, ANSGAR DRAUDE¹, RAFAEL MEINHARDT¹, HILMAR FRANKE¹, and ROGER A. LESSARD² — ¹Fachbereich Physik / Angewandte Physik, Universität Duisburg-Essen, Lotharstr. 1, D-47048 Duisburg, Germany — ²COPL, department de physique, génie physique et optique, Université Laval, Québec, Canada G1K7P4

The presence of electrostatic charges on the surface of electrically isolating substrates like glass or polymers is able to control the orientation of vapor deposited polar organic molecules.

Different methods for the fabrication of charge patterns have been used with inorganic glass: friction, Corona, contact charging, e-beam charging...

Optically anisotropic layers of the azo dye DR1 have been prepared. The anisotropy is detectable by a change in the optical transparency and the pattern reflects the previously recorded charge distribution.

CPP 27.19 Thu 17:00 P2

AFM as a Tool for Observation and Nanomanipulation — ●ALEXANDER SCHMATULLA¹, DIETER MEINHARDT², BERNHARD RIEGER², and OTHMAR MARTI¹ — ¹Department of Experimental Physics, University of Ulm, 89069 Ulm, Germany — ²Department of Anorganic Chemistry II, University of Ulm, 89069 Ulm, Germany

We show the possibility of a custom built Atomic Force Microscope (AFM) as an useful tool for observation and nanomanipulation in material science. In particular we have analysed spin coated polymer networks. First we demonstrate an appropriate preparation of the polymer sample. Using the AFM, particular polymer strains have been pulled over several well defined distances. Further we will compare our results with SEM images, GPC results and other methods. Finally the corresponding changes on the sample will be discussed.

CPP 27.20 Thu 17:00 P2

Solvent Effect in NMR Spectra of Nucleic Bases from Hybrid QM-MM Simulations — ●SITTIPONG KOMIN and DANIEL SEBASTIANI — Max Planck Institute for Polymer Research, Ackermannweg 10, D-55128 Mainz, Germany

We present a study of structural properties and ¹H NMR chemical shifts of nucleic bases in aqueous solution using hybrid quantum mechanics/molecular mechanics (QM/MM) molecular dynamics simulations. The purpose of this work is to study the solvent effect in NMR shifts. We benchmark our computational setup by applying it to water dimer, methanol dimer and ethanol-water dimer, which is particularly relevant to the development and validation of model in QM scheme comparing with QMMM scheme. The method is used to compute the ¹H NMR chemical shifts of Adenine, Guanine, Adenine-9methyl, Guanine-9Methyl in aqueous solution.

CPP 27.21 Thu 17:00 P2

Investigation of spatially confined polyelectrolytes using fluorescence microscopy — ●DANIEL RAPOPORT¹, DAN ANGHEL², HELMUTH MÖHWALD¹, and REGINE V. KLITZING³ — ¹MPI für Kolloid- und Grenzflächenforschung, D-14224 Potsdam — ²Institute of Physical Chemistry, Spl. Independentei 202, RO-77208 Bucharest — ³Institut für Physikalische Chemie, CAU Kiel, Ludewig-Meyn-Strasse 8, D-24118 Kiel

Confinement phenomena are common to a vast number of natural and technical processes, such as the transfer of proteins or DNA through a narrow pore, filtration or nanoencapsulation. The effect can be intermolecular like an increased ordering of the molecules or it can be intramolecular like conformational changes. In the case of aqueous solutions of polyelectrolytes it is largely unknown, how these respond to the restrictions of geometrical confinement. Although numerous investigations of integral thermodynamic values have been carried out, a detailed molecular picture is still missing. Here we report on fluorescence measurements with pyrene labeled poly(acrylic acid) inside thin free standing liquid films, which were formed using sodium dodecylsulfate (SDS) as a surfactant. Upon film formation we found an increase of the excimer/monomer fluorescence intensity ratio. Moreover, at high pH stratification of the film leads to an additional rise of the excimer/monomer ratio, thereby directly proving the confinement effect on a molecular level.

CPP 27.22 Thu 17:00 P2

Manipulation of the smectic layer spacing in liquid crystal elastomer films by mechanical stress — ●VICTOR AKSENOV¹, JÜRGEN BLÄSING¹, RALF STANNARIUS¹, MARTIN RÖSSLE², and RUDOLF ZENTEL² — ¹Otto-von-Guericke-Universität Magdeburg, Inst. für Experimentalphysik — ²Johannes-Gutenberg-Universität Mainz, Inst. für Organische Chemie

Liquid crystal elastomers (LCEs) are rubbers with anisotropic elastic moduli. For deformations in the plane of smectic layers, they behave like two-dimensional isotropic rubbers, with elastic moduli close to those of conventional rubber materials. For deformations perpendicular to the layers, the elastic moduli can be two orders of magnitude higher than for conventional rubbers, comparable to the smectic layer compression modulus. It was observed earlier that deformations of SmA LCE parallel to the smectic layers do not change the sample thickness, this corresponds to a Poisson ratio close to 1 parallel to smectic layers, and zero perpendicular to it [1]. In our material, the measured Poisson ratio is close to 1/2. Simultaneous optical reflectometry and small angle X-ray scattering reveal that in-plane deformations of the LCE sample cause changes of the smectic layer spacing [2]. SmA and SmC* phases show similar elastic behaviour, comparable to isotropic rubber. A layer compression up to 30 % was achieved mechanically. Such an effect has been observed for the first time in smectic LCE.

[1] E. Nishikawa and H. Finkelmann, *Macromol. Chem. Phys.* 200, 312 (1999). [2] V. Aksenov et al., *Liq. Cryst.* 32, 805 (2005).

CPP 27.23 Thu 17:00 P2

Freestanding polyelectrolyte multilayer membranes as pressure sensors and separation membranes — ●INGO DÖNCH, MARC NOLTE, BJÖRN SCHÖLER, and ANDREAS FERY — Max-Planck-Institut für Kolloid- und Grenzflächenforschung, 14424 Potsdam

Polyelectrolyte multilayer membranes can be prepared with thicknesses on the nanoscale and they are semipermeable. This makes them interesting candidates for miniaturized osmotic pressure sensors or separation membranes. We demonstrate first steps towards such devices and applications.

A method has been developed that allows the transfer of membranes onto topographically structured PDMS substrates, so that parts of the membrane are freestanding. In the case of cylindrical cavities, the deformation of the resulting circular freestanding membrane patches can be readily described by continuum mechanical approaches. Experimentally, we probe the deformation using AFM (for small deformations) and osmotic pressure differences (for large deformations). In the latter case, we can quantitatively describe our findings which show an extraordinarily high sensitivity of these membranes towards pressure differences. Similarly, we show that large molecular weight molecules can be entrapped in the cavities and discuss possible uses of such systems in combinatorial chemistry.

CPP 27.24 Thu 17:00 P2

A Scanning Probe Microscope (SPM) with quasi *in-situ* Sample Treatment Capabilities: Solvent vapor treatment of thin polymer films in the presence of high electric fields — ●VIOLETTA OLSZOWKA, MARKUS HUND, LARISA TSARKOVA, ALEXANDER BÖKER, and GEORG KRAUSCH — Physikalische Chemie II, Universität Bayreuth, D-95440 Bayreuth

We have investigated a block copolymer thin film undergoing treatments with solvent vapor and high homogenous electric fields (E-fields, $\approx 40 \frac{V}{\mu m}$). E-fields can be used to control the domain orientation which in turn ends to an important role in fabricating and controlling nanostructures. Due to the high electric field it is not possible to perform *in-situ* scanning. The E-field would produce SPM image artifacts caused by additional electrostatic forces between tip and sample. Moreover the applied high voltage could destroy the microscope by flashovers and could damage the scanner. Performing the sample treatments 'ex situ' would require time-consuming re-positioning protocols. We therefore have adapted an SPM with advanced quasi *in-situ* sample treatment capabilities to effectively study the influences of high electric fields on block copolymer films exposed to a controlled solvent vapor atmosphere.

CPP 27.25 Thu 17:00 P2

Spreading of nematic liquid crystals — ●CHRISTOPHE POULARD — LPCP, Université de Mons-Hainaut, 20 place du Parc, B-7000 MONS, Belgique

The spontaneous spreading of nematic liquid crystals on silica substrates has been investigated at various scales by combining ellipsometry, profilometry and interferometry. While anchoring defects play a major role on hydrophilic substrates at the macroscopic scale, making the behaviour of films highly complex, they do not show up on these hydrophobic substrates.

Then, the main specificity of the nematic films is the elastic energy associated to the long range orientational order. Experiment shows that the macroscopic spreading laws differ from the ones of simple wetting liquids. Moreover, at the microscopic scale, a sharp transition between a mesoscopic, nematic film, and a molecularly thin precursor, is observed. The length of the precursor scales as the inverse of the macroscopic velocity, as expected for adiabatic wetting films.

CPP 27.26 Thu 17:00 P2

Effect of high-frequency oscillatory shear on the force of detachment of an AFM tip from a solid surface — ●BINYANG DU¹, SERGIY RUDENKIY¹, PATTRAWIN GASEMJIT¹, LARS-OLIVER HEIM², and DIETHELM JOHANNSMANN¹ — ¹Institute of Physical Chemistry, Clausthal University of Technology, Arnold-Sommerfeld-Str. 4, 38678, Clausthal-Zellerfeld — ²Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz

The force of detachment between an AFM-tip and a material surface, namely the pull-off-force, is a key parameter for characterization of adhesive interactions on the nanometer scale. Experiments have shown that the pull-off-force can depend on the loading rate, at which the force is ramped up. Kramer's theory also predicts a logarithmic dependence on the loading rate, which has indeed been found in various experiments. Here we report on the pull-off-force between an AFM tip and a quartz crystal under high-frequency oscillatory lateral shear as a function of shear amplitude. The pull-off-force (more precisely: the pull-off-distance) was determined repeatedly and automatically at a rate of 0.5 Hz, while the quartz crystal was swept through a resonance. The shear amplitude is typical in a range of nanometer. The pull-off-distance decreases with increasing the shear amplitude. By plotting the pull-off-distance versus the logarithm of shear amplitude, one finds a linear dependence over a range of more than a decade. This behavior can be rationalized by assuming a multicontact interface with an exponential distribution of peak heights.

CPP 27.27 Thu 17:00 P2

Formation of thermoresponsive hydrogel films via electrochemically initiated polymerization — ●JOHANNA REUBER and DIETHELM JOHANNSMANN — Institute of Physical Chemistry, Arnold-Sommerfeld-Strasse 4, 38678 Clausthal-Zellerfeld

Electrochemically initiated polymerization has previously been employed to produce coatings on metals [1], where the interest mainly was in corrosion protection. We report on the extension of this technique to films of poly-(N-isopropylacrylamide) (p-NIPAM), which is a thermoresponsive hydrogel.[2] A free-radical polymerization is initiated via an electron transfer from the electrode to an electrochemically active initiator. The progress of polymerization was monitored by means of the electrochemical quartz crystal microbalance (EQCM). Typical thicknesses are in the range of up to 100 nm. The water content varies between 20 and 80 %. AFM micrographs reveal a globular structure. The permeation of ions through the gel is possible, as proven by CV runs in the presence of K₃[Fe(CN)₆] in the bulk. First experiments have been performed to explore biomedical applications such as cell-sheet engineering [3] or stimulated drug release [4]. In cell culture, the layers show low-fouling properties. A second application are polymer metal composites: galvanic deposition of copper particles onto the polymer-covered surface has been demonstrated. References: [1] N. Baute, C. Jérôme, et al., European Journal of Inorganic Chemistry 2001, 1097. [2] H.G. Schild, Progress in Polymer Science 1992, 17, 163. [3] A. Kikuchi, T. Okano, Journal of Controlled Release 2005, 101, 69. [4] A. Kikuchi, T. Okano, Advanced Drug Delivery Reviews 2002, 54, 53.

CPP 27.28 Thu 17:00 P2

Substrate-Consuming Metal-Organic Layers (SCMOLs) from Thiol Derivatives - a combined SAXS/SEM Study. — ●BIRGIT RIEDEL¹, MATTHIAS BARCZEWSKI^{1,2}, JOCHEN GEERK³, THOMAS SCHIMMEL^{1,2}, and STEFAN WALHEIM¹ — ¹Institute for Nanotechnology, Forschungszentrum Karlsruhe, 76021 Karlsruhe (Germany) — ²Institute of Applied Physics, University of Karlsruhe, 76131 Karlsruhe (Germany) — ³Institute for Solid-State Physics, Forschungszentrum Karlsruhe, 76021 Karlsruhe (Germany)

Substrate-Consuming Metal-Organic Layers (SCMOLs) were prepared using a variety of thiol molecules. This new type of metal-organic dielectric films grow at room temperature from solution at the interface of the metal substrate and the newly formed metal-organic film. The resulting morphological characteristics of the various compounds were investigated by Small Angle X-Ray Scattering (SAXS) and Scanning Electron Microscopy (SEM). A strong correlation of the structural data and the molecular architecture could be observed and will be discussed. First results on the optical properties of these solid transparent films - with a thickness pre-selectable from a few nanometer up to 1 micrometer - will be presented.

CPP 27.29 Thu 17:00 P2

Synthesis, structure and *ab initio* calculations of three-dimensional polymers of C₆₀ fullerene. — ●NAGESH KINI, AKIRA KUBO, and SHOJI YAMANAKA — Department of Applied Chemistry, Graduate School of Engineering, Hiroshima University, Higashi Hiroshima - 739-8527, Japan.

Solid C₆₀ fullerene is known to polymerise in one, two or three dimensions under high pressure and high temperature (HPHT) conditions. Earlier, we have reported structures of orthorhombic and rhombohedral two-dimensional (2D) polymers determined by x-ray diffraction of single crystals synthesised under HPHT conditions. Recently we have obtained good quality single crystals of three-dimensional (3D) polymers of C₆₀ fullerenes by a topochemical conversion under HPHT conditions. The three different types of single crystals of 3D polymers obtained are: an orthorhombic 3D polymer (polymerised from orthorhombic 2D polymer), a rhombohedral 3D polymer (polymerised from rhombohedral 2D polymer) and a 3D cubic (fcc) polymer (polymerised from monomer (fcc) C₆₀). The structures of these 3D polymers were determined by single crystal x-ray diffraction using a Rigaku R-axis diffractometer attached with an imaging plate (IP). The structures were geometrically optimised by *ab initio* calculations and the relative stabilities of the 3D polymer structures were compared.

CPP 27.30 Thu 17:00 P2

Chemisorption of PTCDA on Ag(110): A quantum chemical study — ●AFSHIN ABBASI, MICHAEL SCHREIBER, and REINHARD SCHOLZ — Institut für Physik, Technische Universität Chemnitz

Experimental studies of PTCDA monolayers on Ag(110) have revealed an adsorption geometry where each molecule is placed on top of 12 substrate atoms [1]. In the present work, we investigate a non-periodic approximant of this interface, including one PTCDA molecule and one or two layers of silver. Both in Hartree-Fock and DFT calculations, the anhydride oxygen atoms experience a strong interaction with the substrate, resulting in a bended geometry with an Ag-O bond length of about 2.4 Å. Several orbitals delocalized over the molecule and the topmost substrate layer result in a large positive net charge of the adsorbate. As most of the negative charge in the topmost layer of the substrate resides below the positively charged perylene core, the Coulomb interaction between substrate and adsorbate contributes a substantial part to the total binding energy.

The calculated adsorption geometry is analysed in terms of the chemical hardness of the electronic orbitals, electronic excitations, and the infrared activity of the molecule along the substrate normal.

[1] C. Seidel, J. Poppensieker, and H. Fuchs, Surf. Sci. **408**, 223 (1998); M. Böhringer, W. D. Schneider, K. Glöckler, E. Umbach, and R. Berndt, Surf. Sci. **419**, L 95 (1998).

CPP 27.31 Thu 17:00 P2

Fabrication and electrical characterization of Polypyrrole nanowires — ●JÖRN-HOLGER FRANKE, BIN DONG, LIFENG CHI, and HARALD FUCHS — Physikalisches Institut and CENTech, Wilhelm-Klemm Str. 10, WWU Münster

E-Beam Lithography is used to pattern a resist structure (PMMA-Resist on Silicon-Wafer) which is subsequently used as a mask for copoly-

merization of Pyrrole and N-(3-Trimethoxysilyl-Propyl) Pyrrole. The Trimethoxysilyl group of the latter one binds covalently to the Silicon Dioxide of the Wafer, thereby enabling the generated Polypyrrole nanowires to survive the following Lift-Off Process. Gold electrodes are evaporated on top of the resulting Polypyrrole to form easily accessible electrodes for conductivity measurements. The dependence of specific conductivity on nanowire diameter is studied.

CPP 27.32 Thu 17:00 P2

Electrode Stability in Electrochromic Systems Based On Flexible Substrates — ●ROLAND WAGNER^{1,2}, ROLAND WEISS¹, GOTTHARD RIEGER¹, and JÜRGEN R. NIKLAS² — ¹Siemens AG Corporate Technology, Dept. CT MM 1, Erlangen, Germany — ²Technical University Bergakademie Freiberg, Freiberg, Germany

Electrochromic (EC) systems use materials that change their color when an electrical voltage is applied. Due to redox processes the intra molecular electron configuration is affected causing different absorption spectra. Electrodes of this EC system are exposed to an aggressive environment, as electrons are exchanged at the interface of solvent based electrolytic EC material and flexible electrodes. Especially the transparent top electrode, which is typically ITO on thin PET films, degrades during device operation. Metals (e.g. Cu), TCO and polymer (e.g. PEDOT) based materials are tested as back and top electrode for its degradation under different conditions, e.g. accelerated lifetime tests and voltage cycling. Optical and electrical properties like contrast and current behavior are discussed as well as degradation processes and mechanisms.

CPP 27.33 Thu 17:00 P2

Cyclo-olefin-polymer ferroelectrets: Electric charging, piezoelectric activity and thermal stability — ●OLENA VORONINA, MICHAEL WEGENER, WERNER WIRGES, and REIMUND GERHARD-MULTHAUPT — University of Potsdam, Department of Physics, Am Neuen Palais 10, D-14469 Potsdam, Germany

Non-cellular cyclo-olefins are known for their good charge-trapping properties. Their charge stability is quite comparable to that of the best known polymer electrets FEP and PTFE [1]. Thus, cyclo-olefins are interesting candidates for the development of piezoelectric polymer foams, so-called ferroelectrets. Ferroelectrets are cellular polymer films containing air-filled voids. Their piezoelectricity is based on an optimized combination of bipolar internal charging of the voids (which thus become giant electric dipoles) and of a rather low elastic modulus. An applied mechanical stress changes the void size and leads to an electrical signal.

Recently, cyclo-olefin polymers were developed into ferroelectret polymer films [2]. We briefly describe the preparation process and discuss the electric charging, the piezoelectric properties and the thermal stability of the new ferroelectrets. The results demonstrate that the piezoelectric activity is thermally stable at least up to 110°C, which is a significant improvement of the service temperature in comparison to other ferroelectret polymers.

[1] G. M. Sessler, G. M. Yang and W. Hatke, Annual Report CEIDP, IEEE Service Center, Piscataway NJ, 467-470 (1997). [2] A.-M. Savijärvi, M. Pääjänen, E. Saarimäki, and H. Minkkinen, Proc. 12th Intern. Symp. on Electrets (ISE12), IEEE Service Center, Piscataway NJ, 75-78 (2005).

CPP 27.34 Thu 17:00 P2

Electromechanics of organic Schottky like contacts, in between piezoelectricity and electrostriction — ●REINHARD SCHWÖDIAUER¹, SIEGFRIED BAUER¹, GILLES DENNLER², CHRISTOPH LUNGENSCHMIED², NIYAZI SARICIFTCI², and HOWARD REISS³ — ¹Soft Matter Physics, Johannes Kepler University, Altenbergerstrasse 69, A-4040 Linz, Austria — ²Linz Institute for Organic Solar Cells (LIOS), Physical Chemistry, Johannes Kepler University, Altenbergerstrasse 69, A-4040 Linz, Austria — ³Department of Chemistry and Biochemistry, University of California, 600 Charls E. Young Drive East, Los Angeles, CA90095, USA

Piezoelectricity and electrostriction are electromechanical effects at the heart of a variety of applications in transducers. In organic semiconductors an unusual voltage dependence of the electromechanical strain is observed: The converse electromechanical response follows a power law dependence $S \sim V^a$ of the mechanical strain S versus the applied voltage V , with an exponent $a=1.5$. The power law exponent is in-between traditional linear piezoelectricity and quadratic electrostriction. The experimental finding is a direct consequence of the strongly nonuniform electric field distribution within the Schottky contact arrangement. Electromechanical responses of organic Schottky devices appear to be of fundamen-

tal interest for the investigation of non-uniform electric field distributions, and for potential practical applications as electromechanical transducers.

CPP 27.35 Thu 17:00 P2

Luminescent characterization of perovskite-like layered strontium lanthanum titanate compounds — ●VOLODYMYR CHUMAK¹, YU TITOV¹, M SLOBODYANIK¹, S NEDILKO², O CHUKOVA², and P SMOLYAR² — ¹Chemistry faculty of Kyiv National Taras Shevchenko University, 64, Volodymyrska str., 01033, Kyiv, Ukraine — ²Physics faculty of Kyiv National Taras Shevchenko University, 64, Volodymyrska str., 01033, Kyiv, Ukraine

First the peculiarities of the luminescent emission of the five-slab perovskite-like $SrLa_{4-x}Ln_xTi_3O_{17}$ ($Ln = Pr, Yb$) compounds belonged to the $A_nB_nO_{3n+2}$ -family are found and described. Photoluminescence and excitation spectra were obtained at 4.2, 77 and 300 K. Luminescence was excited by radiation from the N_2 -laser, the Ar-laser, powerful xenon lamp DKsL-1000. The luminescence was registered using MDR-2 and DFS-12 diffraction spectrometers which cover wide spectral region. Reflection, excitation and luminescence spectra were also investigated using synchrotron radiation in the energy region 3.5-20 eV. Experiments with synchrotron radiation were carried on at SUPERLUMI station at HASYLAB (DESY), Hamburg, Germany. Results of experimental studies allowed us to conclude that mentioned above the sets of compound could be regarded as perspective phosphors, i. e. the transformers of the UV or IR emission into visible light, or the white-light-emitting and storage phosphors, perspective laser materials. When doped with the rare earth ions Pr^{3+} or Yb^{3+} they are considered as perspective fast-scintillation materials.

CPP 27.36 Thu 17:00 P2

Ion Irradiation of Polystyrene - Sol Molecular Weight Distribution — ●RALF DELTO and RÜDIGER BRENN — Physikalisches Institut, Universität Freiburg, Hermann-Herder-Str.3, 79104 Freiburg

Irradiation of polymers with high energetic ions results in a change of molecular weight distribution. The formation of crosslinks produces a gel fraction (network) while breaking of chains leads to a soluble sol fraction. The change of the Mw distribution depends on the applied ion dose.

Theoretical and experimental work has been done on the production of networks. Here we concentrate on the sol part. Sol-Mw distributions are calculated with statistical methods and with numerical simulations. Measurements are performed on polystyrene (PS) thin films using 1 MeV protons for irradiation. The films consist of a deuterated and a protonated layer (dPS-hPS). The irradiated sol (dPS and hPS) diffuses into the opposite layer while heating above T_g . As the tracer diffusion constant depends on the molecular weight, chains of different length diffuse unequally fast. Thus the diffusion profiles contain information about the abundance of chains of different degrees of polymerisation in the sol. Diffusion depths profiles for the deuterated component are determined with 3He nuclear reaction analysis.

CPP 27.37 Thu 17:00 P2

Struktur und mechanische Festigkeit eines nanostrukturierten Biomaterials zum Knochenaufbau — ●SVEN RADEFELDT and THOMAS GERBER — Universität Rostock, August-Bebel-Str. 55, 18055 Rostock

Nanostrukturierte Biomaterialien, die dadurch charakterisiert sind, eine extrem hohe innere Oberfläche zu besitzen und deren innere Oberfläche so modifiziert ist, dass körpereigene Proteine während der Anwendung angelagert werden, bieten vollkommen neue Möglichkeiten in der regenerativen Medizin. Es wird eine im Sol-Gel-Verfahren hergestellte Hydroxylapatit-Keramik vorgestellt, die von den Zellen nicht als Fremdkörper angesehen wird und sofort in den natürlichen remodelling-Prozess des Körpers eingebunden wird. Dieses hochporöse Material, dessen Nanostruktur der des natürlichen Knochens nachempfunden ist, wurde in seiner Zusammensetzung so optimiert, dass zukünftig auch die Heilung von Defekten ermöglicht werden soll, die an sehr stark belasteten Knochen (z.B. Wirbelkörper der Wirbelsäule) aufgetreten sind. Zum Nachweis der Korrelation zwischen Struktur und Eigenschaften des Biomaterials wurden Untersuchungen mittels SAXS, WAXS, TGA, DTA, REM und TEM durchgeführt.

CPP 27.38 Thu 17:00 P2

Nanofibrillar structure and molecular mobility in spider dragline silk — ●TILO SEYDEL¹, DANIEL SAPEDE^{1,2}, TREVOR FORSYTH¹, MAREK KOZA¹, RALF SCHWEINS¹, FRITZ VOLLRATH³, and CHRISTIAN RIEKEL² — ¹Institut Laue-Langevin, B.P.156, F-38042 Grenoble, France — ²European Synchrotron Radiation Facility, B.P.220, F-38043 Grenoble, France — ³Dept. of Zoology, University of Oxford, Oxford OX1 3PS, U.K.

Spider silk is a protein biopolymer known for its outstanding mechanical properties combining elasticity and strength. Spider dragline silk has been investigated by neutron diffraction and neutron spectroscopy techniques [1]. The results support a three-phase hierarchical model of the structure consisting of semicrystalline nanofibrils embedded in an amorphous polymer matrix. The mechanical properties of spider dragline silk fibres are strongly affected by the water content, and neutron spectroscopy provides information on the humidity-dependent polymer chain mobility as well as on a gradual melting of confined water. New instrumental developments in neutron spectroscopy will be presented alongside, as the feasibility of neutron experiments is often limited by the small available sample quantities.

[1] D.Sapede, T.Seydel, V.T.Forsyth, M.M.Koza, R.Schweins, F.Vollrath, and C.Riekel; *Macromolecules* Vol.38, p.8447 (2005).

CPP 27.39 Thu 17:00 P2

Gas Induced Dilation in Glassy Polymers - Combining Experiment, Phenomenological Models and Simulation — ●OLE HÖLCK¹, MARTIN BÖHNING¹, MATTHIAS HEUCHEL², and MARTIN R. SIEGERT² — ¹Bundesanstalt für Materialforschung und -prüfung (BAM), Unter den Eichen 87, 12205 Berlin, Germany — ²GKSS Forschungszentrum, Institut für Polymerforschung, Kantstrasse 55, 14513 Teltow, Germany

Dense amorphous polymers are utilised as barrier materials or membranes in a variety of applications. Considerable efforts have been made to describe and characterise solution and diffusion of small penetrants constituting the permeation process. However, little is known about the mechanisms which - at elevated concentrations and long term exposure - lead to plasticisation of the polymer matrix and subsequent structural rearrangements. In this joint research project a thorough kinetic analysis of sorptive dilation along with the evaluation in the framework of phenomenological models, such as the Site Distribution-model of Kirchheim, is utilised to relate the results of laboratory experiments to complementary investigations of detailed atomistic MM/MD-packing models. The results are based on established analysis methods as well as promising new approaches to overcome the discrepancies due to the different time scales of observation in experiment and modelling. Comparison is made between measured and simulated characteristics relevant to gas transport and dilation, such as diffusivity and solubility of the penetrant and free volume distribution of the polymer matrix.

CPP 27.40 Thu 17:00 P2

Ion mobility in PMMA doped with small amounts of a Lithium salt — ●P. KOHN, K. SCHRÖTER, and T. THURN-ALBRECHT — Department of Physics, Martin Luther University, Hoher Weg 8, 06120 Halle, Germany

Normally NMR techniques are used to determine the mobilities of ions in polymer electrolytes (via determination of diffusion coefficients and use of the Einstein relation). We discuss Time Of Flight (TOF) measurements in an electric field and parallel plate geometry as an alternative method to determine mobilities of ions. In a first step the ions of opposite charge are forced to separate and accumulate at the different electrodes by applying a constant voltage. As a consequence of a reversed voltage in the second step the ions migrate from one electrode to the other. The current measured during this process gives the transit time which is directly related to the mobilities of the charge carriers.

For an exemplary application we used this method to study ion mobility in polymethylmethacrylate (PMMA) doped with lithiumtrifluoromethanesulfonate (LiCF₃SO₃). The measurements were complemented by dielectric spectroscopy in the frequency domain. While the TOF measurements give the mobilities, the frequency dependent dielectric measurements give the temperature and salt-concentration dependence of the ohmic conductivity of the electrolyte.

CPP 27.41 Thu 17:00 P2

Tailoring the material properties of Polypropylene by blending — ●STEFAN FISCHER¹, OTHMAR MARTI¹, TOBIAS DIESNER², and BERND RIEGER² — ¹Department of Experimental Physics, University of Ulm, 89069 Ulm, Germany — ²Department of Inorganic Chemistry II, University of Ulm, 89069 Ulm, Germany

Tailoring material properties like mechanical deformation behavior is of special interest for possible applications. Isotactic Polypropylene (iPP) is a low-cost polymer, showing a high modulus with the drawback of being brittle. By blending commercial available iPP with high molecular iPP (synthesized with metallocene catalysts) we intended to influence material properties like failure behavior, such broadening the range of accessible applications. This approach additionally has special advantages in the recycling process since there is no mixture of chemical different materials. We will present the results of different blending experiments, analyzed by DSC and mechanical measurements. For a target-oriented approach to tailoring material properties it is crucial to know the processes taking place on a microscopic level like crystallization. Preliminary results of measurements with AFM and X-ray scattering and their connection to the macroscopic behavior will be discussed.

CPP 27.42 Thu 17:00 P2

Side chain crystallization in random copolymers containing octadecylmethacrylate — ●E. HEMPEL¹, H. BUDDE^{2,3}, C. SCHICK-TANZ⁴, S. HÖRING², and M. BEINER¹ — ¹FB Physik und — ²FB Chemie, Universität Halle, D-06099 Halle/Saale — ³Fraunhofer Pilotanlagenzentrum für Polymersynthese und -verarbeitung Schkopau, D-06258 Schkopau — ⁴FB INW, Fachhochschule Merseburg, D-06217 Merseburg

The crystallization behavior of two series of random copolymers, poly(styrene-*stat*-octadecylmethacrylate) [P(S-*stat*-ODMA)] and poly(methylmethacrylate-*stat*-octadecylmethacrylate) [P(MMA-*stat*-ODMA)], has been studied by DSC and scattering techniques. Interestingly, side chain crystallization occurs in all copolymers containing more than 25mol% ODMA while only a single glass transition is observed for lower ODMA contents. This indicates that the alkyl groups of different ODMA units can aggregate and form small crystals if the ODMA content is large enough. Isothermal crystallization experiments show that the crystallization kinetics slows down and that the transformation interval broadens if the ODMA content decreases. The crystallization temperature T_c for samples containing 25mol% ODMA is 40K reduced as compared to values for PODMA homopolymers. This can be interpreted as a consequence of crystallization occurring in isolated ODMA compartments which must be nucleated separately. Scattering data measured during the isothermal crystallization process of P(S-*stat*-ODMA) copolymers are included in the discussion. The results for random copolymers are compared with the findings for PODMA homopolymers as well as P(S-*block*-ODMA) block copolymers.

CPP 27.43 Thu 17:00 P2

Probing Micromechanical Behavior of Semicrystalline Polypropylene Films by Brillouin Spectroscopy — ●OLGA PRIADILOVA¹, WEI CHENG¹, WERNER STEFFEN¹, JOCHEN GUTMANN¹, and GEORGE FYTAS^{1,2} — ¹Max-Planck for Polymer Research, D-55128 Mainz, Germany — ²Department of Materials Science and Technology, University of Crete and FO.R.T.H P.O.Box 1527, 71110 Heraklion, Greece

The elastic properties of polypropylene films crystallized under different conditions were investigated via Brillouin spectroscopy measurements. It was found that elastic constants of the polypropylene films are dependent on their microstructure. Inelastic Brillouin light scattering from films reveals the presence of up to four bulk and surface phonons. The coexistence of amorphous and crystalline regions with at least submicron sizes allow for the propagation of two longitudinal and transverse elastic excitations. The relation of the acoustic excitations to the surface and bulk morphology of the semicrystalline films is supported by X-ray scattering techniques and optical microscopy images. Inelastic (Brillouin) light scattering from semicrystalline homopolymers can measure the high frequency elastic constant of the two microphases if the formed spherulites exceed the size of the wavelength of the probed phonons. In this case, the film is inhomogeneous over the relevant length scales and there is an access to the transverse phonon in the crystalline phase yielding the elastic constant as well.

CPP 27.44 Thu 17:00 P2

Kinetics of isothermal crystallisation and melting-recrystallisation of iPP, iPS, PET and PBT — ●J. HEEG, A. MINAKOV, and C. SCHICK — University of Rostock, Institute of Physics, Universitätsplatz 3, 18051 Rostock, Germany

Isothermal crystallisation and melting-recrystallisation were investigated by the help of Fast Scanning Chip Calorimetry and DSC (Differential Scanning Calorimetry). For the purpose of fast scanning a commercially available chip calorimeter was used. The implanted heater in combination with non-adiabatic operation gave the possibility for both controlled fast heating and cooling. Crystallization kinetics of the slowly crystallising iPS and PET were studied on a PerkinElmer PYRIS 1 DSC. PBT and iPP were investigated with the fast scanning chip calorimeter. In the case of iPP, in accordance with de Santis [1], two minima in isothermal melt crystallisation half time were observed. These can be explained by the formation of two different phases in iPP. Namely, the crystalline alpha-modification and the mesomorphic phase. Additionally isothermal cold crystallisation experiments gave no evidence for preferring a certain crystallising temperature in case of the alpha-modification. Only the mesomorphic phase gave again a pronounced peak in crystallisation half time. Surprisingly, for PBT two minima in crystallisation half time were found too, for both melt and cold crystallisation. The reason for this is not yet understood. Beside crystallization kinetics recrystallization kinetics will be discussed too.

[1] F. de Santis, C. Schick, in preparation for publication.

CPP 27.45 Thu 17:00 P2

Crystallization/melting transition of polymer thin films probed by ellipsometry — ●CHRISTA H.M. WEBER, ADRIANA M. MIHUT, SVEN HÜTTNER, ARNAUD CHICHE, and GEORG KRAUSCH — Physikalische Chemie II, Universität Bayreuth, 95440 Bayreuth

Ellipsometry has been used to investigate crystallization and melting of thin polymer films. This technique is sensitive to the sharp changes in film density and thickness that occur during these transitions. As a result, precise melting and crystallization points can be measured in-situ during thermal or solvent vapor treatments. We present example studies of model crystalline polymers and block copolymers thin films.

CPP 27.46 Thu 17:00 P2

Relaxation behavior, physical aging and crystallization kinetics — ●T.R. GOPALAKRISHNAN and M. BEINER — FB Physik, Universität Halle, D-06099 Halle/Saale, Germany

Recently the properties of amorphous pharmaceuticals attracted a lot of attention. We have studied the relaxation and crystallization behavior of amorphous acetaminophen produced by rapid quenching. DSC heating curves for this sample show a pronounced glass transition at $T_g=23^\circ\text{C}$ before spherulites are formed during the cold crystallization process at temperatures around $T_c=85^\circ\text{C}$. Weak exothermal contributions in the range 110-130°C indicate a solid-to-solid transition to another polymorphic state which finally melts at $T_m \approx 158^\circ\text{C}$. In order to get more detailed information about the relaxation behavior of amorphous acetaminophen we have investigated the dynamic glass transition (α) between T_g and T_c by dielectric spectroscopy. A weak secondary relaxation (β) has been found in ϵ'' isotherms measured at temperatures below T_g . The crystallization kinetics will be described based on isothermal crystallization experiments by dielectric spectroscopy at temperatures between 30°C and 55°C. We observed that isothermal crystallization affects mainly the α relaxation strength $\Delta\epsilon$ while shape and position of the α peak in ϵ'' isotherms are nearly unaffected. This shows that the situation can be approximated by a two phase model. The dielectric results are consistent with data from calorimetric measurements detecting the change of the strength of the thermal glass transition ΔC_p after different periods of isothermal crystallization at T_c . Characteristic crystallization times τ_c obtained by both methods are nearly identical.

CPP 27.47 Thu 17:00 P2

Semi-flexible star-shaped molecules — ●SIBYLLE GEMMING^{1,2}, MICHAEL SCHREIBER², MATTHIAS LEHMANN³, IGOR POPOV¹, and GOTTHARD SEIFERT¹ — ¹Physikalische Chemie und Elektrochemie, TU Dresden, D-01062 Dresden — ²Institut für Physik, Technische Universität, D-09107 Chemnitz — ³Institut für Chemie, Technische Universität, D-09107 Chemnitz

The structural prerequisites are investigated, which make star-shaped molecules suitable precursors for the formation of columnar liquid crystalline phases. Electronic structure calculations on smaller mesogens

show, that not all conformers exhibit the atomistic structure, the stability against distortion, and additional dipole moments, which favour columnar stacking. For the presently studied compounds with short terminating alkyl chains, the calculations indicate that the steric factor becomes dominant with increasing star size. Thus, the optimised geometric structures were employed to generate a simplified mathematical model of the structures, which accounts only for the steric interaction in the larger stars. With the help of these diagrams, the most common conformers of star-shaped molecules can be derived in a systematic fashion.

CPP 27.48 Thu 17:00 P2

Polymer-surfactant interactions: Effect of temperature on aggregation — ●JOHN BOSCO STANISLAUS¹, HEIKO ZETTL¹, JEROME CRASSOUS², MATHIAS BALLAUFF², and GEORG KRAUSCH¹ — ¹Physical Chemistry II, Universität Bayreuth, Universitätstraße 30, 95440, Bayreuth, Germany — ²Physical Chemistry I, Universität Bayreuth, Universitätstraße 30, 95440, Bayreuth, Germany

The interactions between an anionic surfactant sodium dodecyl sulphate (SDS) and hydrophobically modified non ionic polymer, methylcellulose (MC), in water have been investigated by fluorescence correlation spectroscopy (FCS) and rheology. FCS is used to study the dynamics of the aggregates. We are able to follow the solution properties over a wide concentration range of both polymer and surfactant via measurement of the diffusion time of single dye molecules. At constant MC concentration the diffusion time increases gradually with SDS concentration. Starting from certain SDS concentration it decreases again to a minimum when the SDS concentration is further increased. This behaviour is coinciding with the behaviour of the zero shear viscosity. Two possible aggregations can be identified above the critical aggregation concentration (CAC). The changes in diffusion time and aggregation states are studied as a function of temperature. Moreover the gelation of MC is studied by piezoelectric axial vibrator.

CPP 27.49 Thu 17:00 P2

ATRP-Synthesis of Polymer Brushes in aqueous Solution for Silicon Surface Modification — ●SEBASTIAN NETT¹, GUNNAR KIRCHER¹, MARKUS WOLKENHAUER¹, and JOCHEN S. GUTMANN^{1,2} — ¹Max Planck Institute for Polymer Research, Ackermannweg 11, D-55128 Mainz — ²Institute for Physical Chemistry, Johannes Gutenberg University, Welderweg 11, D-55099 Mainz

The aim of this project is the chemical modification of Micromechanical Sensors (MMS) for the use as temperature and chemical probes. The silicon-surface properties are changed by growing polymer brushes on top of the MMS.

Our approach make use of a Nanoplotter (GESIM) to "print" microstructures on micro cantilever sensors. The Nanoplotter is optimized for water as system liquid. Therefore the synthesis of the covalently bound polymer brushes has to be in aqueous solution. We performed ATRP (Atom Transfer Radical Polymerization) -Synthesis of PNIPAM (Poly(N-Isopropylacrylamide)) in a mixture of H₂O and DMF both in bulk solution and small droplets. Ellipsometry measurements provided the characterization of the film. The brush thickness varies with molecular weight from 5 to 40 nm.

The synthesized PNIPAM shows a LCST (lower critical solution temperature) behavior at a critical temperature of 32°C.

CPP 27.50 Thu 17:00 P2

Single DNA Molecules in Shear Flow — ●DAVID STEINMETZ¹ and CHRISTIAN WAGNER² — ¹Geb. 38, 3. OG, Zi. 3.19, Universität des Saarlandes, 66041 Saarbrücken — ²Geb. 38, 3. OG, Zi. 3.20, Universität des Saarlandes, 66041 Saarbrücken

We present investigations of single DNA molecules in an oscillatory shear flow, that is a typical form of a time dependent rheometric flow. The molecules are labelled with a fluorescent dye (POPO-3) and observed with a EPI fluorescence microscope. The viscosity of DNA solutions in oscillatory flows is a complex quantity and at the frequency corresponding to the inverse relaxation time of the single molecules, the elastic part of the viscosity should have a maximum. The microscopic response of the molecules to the oscillatory shear flow should also be maximal at this frequency. Our goal is to associate macroscopic behaviours with microscopic ones.

CPP 27.51 Thu 17:00 P2

Molecular Dynamics of the Glass Relaxation Process of Block — ●S. Z. MOHAMMADY¹ and S. KAHLE² — ¹Chemistry Department, Faculty of Science, Cairo University, P.O.12613 Giza, Egypt — ²Max-Planck-Institut für Polymerforschung, Postfach 3148, D-55021 Mainz

The molecular dynamics of the relaxation processes of the soft blocks in different types of block copolymers having different molecular architectures have been investigated. Four model examples of block copolymers are investigated, namely, two styrene-butadiene-styrene (SBS) block copolymers and two styrene-styrene butadiene-styrene (S-SB-S). Samples were chosen, so that, in each pair of block copolymers one of them is linear triblock and the other is star asymmetric. In addition, two polybutadiene, PB, homopolymer samples having similar chain lengths to the PB blocks present in the SBS block copolymers have been investigated. Dynamic mechanical measurements have been done for the real and imaginary parts of the complex shear modulus (G' , G'') in the temperature and frequency ranges from -110 to 30°C and 10-2 to 15.9 Hz, respectively. Complete master curves have been constructed for all samples. Moreover, broad band dielectric spectroscopy has been carried out in wide temperature and frequency windows, -120 to 0°C and 10-1 to 107 Hz, respectively. Stress – strain and transmission electron microscopic (TEM) measurements were also conducted. The results show that the molecular dynamics of the glass process in the soft phase in block copolymers is dramatically changed as compared to the behavior in the bulk (for instance, PB homopolymers). In addition, the molecular architecture is found to be an important factor in determining the molecular mobility of the soft blocks. The results are explained in terms of the applied confinement of the counter phase (PS phase), block lengths,

domain thicknesses and the type of end to end junctions between the different blocks. A correlation between the macroscopic and microscopic properties in the block copolymers was done.

CPP 27.52 Thu 17:00 P2

Preparation and characterisation of Polystyrene-ZnO hybrid polymer particles. — ●MUKESH AGRAWAL¹, ANDRIJ PICH², NICK ZAFEIROPOULOS¹, and MANFRED STAMM¹ — ¹Leibniz Institut für Polymerforschung Dresden e.V., Hohe Straße 6, 01069 Dresden, Germany — ²Institute of Macromolecular Chemistry and Textile Chemistry, Dresden University of Technology, Mommsen Straße 4, 01062 Dresden, Germany

We report on the preparation and characterisation of ZnO nanoparticles and PS-ZnO polymeric composite particles. ZnO nanoparticles with diameters from 8-50 nm are formed depending on the reaction time, temperature and NaOH concentration. Polymeric composite particles are prepared by two step method in which first step consists of preparation of the functionalised core polystyrene particles and during second step prepared ZnO particles were deposited on to core particles surface. The core particles PS/AAEM with a high monodispersity are prepared by the surfactant free emulsion polymerisation. Prepared ZnO particles are deposited in the form of nano crystals on to the PS/AAEM particle surface by heterocoagulation process. Effect of reaction parameters such as reaction temperature, Zn(CH₃CO₂)₂ concentration and NaOH concentration, on the thickness of inorganic shell is investigated. ZnO particles are characterised by SEM, AFM and WAXS. Morphology of polymeric composite particles is characterised by SEM and AFM. Inorganic content in the polymeric composite is determined by thermogravimetric analysis.

CPP 28 Biological Systems

Time: Friday 10:30–12:30

Room: ZEU Lich

CPP 28.1 Fri 10:30 ZEU Lich

Can hydrophobically lined channels be gated by water? — ●K. MYRIAM KROLL^{1,2} and ROLAND ROTH^{1,2} — ¹Max-Planck-Institut für Metallforschung, Heisenbergstr. 3, 70569 Stuttgart — ²ITAP, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart

Pores of KcsA ion channels possess a hydrophobic region which changes its conformation between a wide pore, when open, to a narrower pore, when closed. Recent studies indicate that a hydrophobic pore can "gate" by capillary evaporation. With this mechanism water is expelled from the permeation pathway and ion flow is thereby stopped although the pore remains wider than the water or ion diameters. We study the connection between geometrical change of a hydrophobic pore and capillary evaporation to estimate the energetics of this gating mechanism in a realistic pore geometry, e.g. the energy it takes to remove the water from the pore and the force exerted by the water on the wall of the pore.

To this end we perform, in a first step, microscopic density functional theory (DFT) calculations, in which we focus on the density profile of water as capillary evaporation takes place. The insight gained from these DFT calculations we transfer and exploit, in a second step, in our mesoscopic morphometric approach. In morphometry the free energy of a liquid confined in a pore is expressed by four terms that describe the geometry of the pore and corresponding thermodynamic coefficients. This separation of geometry and thermodynamics makes calculations very efficient so that effects due to change in geometry can be studied in depth. Both DFT and morphometry have been applied with great success in studies of the physics of confined fluids.

CPP 28.2 Fri 10:45 ZEU Lich

Force-induced desorption and unzipping of semiflexible polymers — ●JAN KIERFELD — Max Planck Institute of Colloids and Interfaces, Science Park Golm, 14424 Potsdam

The thermally assisted force-induced desorption of semiflexible polymers from an adhesive surface or the unzipping of two bound semiflexible polymers by a localized force are investigated. The phase diagram in the force-temperature plane is calculated both analytically and by Monte Carlo simulations. Force-induced desorption and unzipping of semiflexible polymers are first order phase transitions. A characteristic energy barrier for desorption is predicted, which scales with the square root of the polymer bending rigidity and governs the initial separation process before a plateau of constant separation force is reached. This leads to activated desorption and unzipping kinetics accessible in single molecule

experiments.

CPP 28.3 Fri 11:00 ZEU Lich

Thin Casein films as prepared by spin-coating: Influence of film thickness and of pH — ●P. MÜLLER-BUSCHBAUM¹, R. GEBHARDT¹, E. MAURER¹, E. BAUER¹, R. GEHRKE², and W. DOSTER¹ — ¹TU München, Physik-Department E13, James-Frank-Str. 1, D-85747 Garching, Germany — ²HASYLAB at DESY, Notkestr. 85, D-22603 Hamburg, Germany

Casein films are successfully prepared by spin-coating water based casein solution on base treated glass surfaces. The film structure is investigated in real space by optical microscopy and atomic force microscopy and in reciprocal space by grazing incidence small angle X-ray scattering (GISAXS). Due to the changed electrostatic repulsion, with increasing pH value the size of the casein micelles increases. Dynamic light scattering confirms good agreement of the micelle size in solution and building a bulk like casein film as determined with GISAXS. As long as homogeneous casein films are producible, with decreasing film thickness the micelle size is reduced. At the moderate pressure introduced by spin-coating the micelles rearrange in a more compact size.

CPP 28.4 Fri 11:15 ZEU Lich

Thermodynamic stability of proteins — ●JOHANNES WIEDERSICH¹, SIMONE KÖHLER¹, JOSEF FRIEDRICH¹, and ARNE SKERRA² — ¹Physikdepartment E14, Lehrstuhl für Physik Weihenstephan, TU München, Germany — ²Lehrstuhl für Biologische Chemie, TU München

The folding 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 study the stability of the anticallin FluA-fluorescein complex, a small protein specifically tailored to bind the fluorophore fluorescein, as a function of pressure and temperature.

Although it is known that protein folding follows a complex path, the temperature and pressure denaturation of FluA is well described by a simple two-state model. The observed elliptic shape of the p - T phase diagram implies that—despite the complexity of protein folding—the thermodynamic parameters (namely specific heat capacity, compressibility, thermal expansion) are rather well defined and do not significantly depend on pressure and temperature. We discuss the implications of our findings on the understanding of generic features of the protein folding transition, especially on its similarities to the glass transition.

CPP 28.5 Fri 11:30 ZEU Lich

In-situ Studies of Protein Resistance of Oligo(Ethylene Glycol) Self-Assembled Monolayers — ●MAXIMILIAN SKODA^{1,2}, FRANK SCHREIBER¹, JAMES WILLIS², ROBERT JACOBS², REINER DAHNT³, MICHAEL GRUNZE³, and MAXIMILIAN WOLFF⁴ — ¹Universität Tübingen — ²Oxford University — ³Universität Heidelberg — ⁴Institut Laue-Langevin

The structure of the interface between organic matter, such as self-assembled monolayers (SAMs), and water is currently subject of intensive studies due to its importance for the understanding of surface-solvent and surface-surface interactions [1,2]. We report results from Polarisation Modulated (PM) Fourier Transform Infrared Spectroscopy (FTIR) studies that enable us to address the local interaction of water with OEG groups. Our data suggest a rather strong interaction of water molecules with the EG section of the SAM, potentially the penetration of water into the SAM. We will also discuss the potential of true in-situ investigations (i.e. under a layer of water) using PM-FTIR. In addition, we will discuss neutron reflectivity (NR) measurements on the same system. NR provides insight to the structure of the solid-liquid interface in-situ and without perturbation of the system. The measurements reveal changes in the structure of water and the protein solution in the vicinity of the SAM upon changes in temperature.

- [1] F. Schreiber, *J. Phys.: Cond. Matter* 16 (2004) R881
 [2] D. Schwendel et al., *Langmuir* 19 (2003) 2284

CPP 28.6 Fri 11:45 ZEU Lich

Solvent induced forces on bio-molecules — ●HENDRIK HANSEN-GOOS^{1,2}, ROLAND ROTH^{1,2}, KLAUS MECKE³, and SIEGFRIED DIETRICH^{1,2} — ¹MPI für Metallforschung, Heisenbergstr. 3, 70569 Stuttgart — ²ITAP, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart — ³ITP, Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen

Understanding conformations of complex molecules in organisms requires to account for solvent induced forces. The most elementary of these being the depletion force which arises even in absence of internal energy contributions from a system's tendency to maximise entropy. Additionally, solvent-solvent and solvent-molecule interactions can strongly influence the conformation of the solved molecule. A first step towards the understanding of depletion forces is the Asakura-Oosawa (AO) model which neglects solvent-solvent interactions. More realistic solvent models like the hard-sphere fluid or attractive (water-like) solvents can be realised within the context of morphological thermodynamics recently put forward. The approach is based on the Hadwiger theorem which implies that (under certain assumptions) the change in free energy upon insertion of a molecule into the solvent is a linear function of the molecule's Minkowski measures with interaction specific coefficients. We introduce a self-consistent scaled particle calculation yielding quasi-exact coefficients for the hard-sphere fluid. The morphological approach is applied for different interactions, illustrating that conclusions drawn from the AO model for phenomena such as helix formation are somewhat misleading. Limits of the approach are discussed by comparison with density func-

tional theory calculations.

CPP 28.7 Fri 12:00 ZEU Lich

Experimental and Theoretical Investigation of the Elasticity of Poly(azobenzene-peptides) — ●GREGOR NEUERT^{1,2}, THORSTEN HUGEL^{2,3,4}, ROLAND R. NETZ^{2,3}, and HERMANN E. GAUB^{1,2} — ¹Lehrstuhl für Angewandte Physik — ²Center for Nanoscience (CeNS), Ludwig-Maximilians-Universität, Amalienstrasse 54, 80799 München — ³Physics Department — ⁴Zentralinstitut für Medizintechnik, TU-München, 85748 Garching

Since the mechanical properties of individual polymers have become accessible with single molecule force spectroscopy, detailed insight was gained into the molecular origin of their elasticity. Active, optically switchable polymers were introduced as photonic muscles and used in single molecule motors. Here, we present experimental data and calculations to describe the mechanical properties of poly(azobenzene-peptides) in the complete force regime accessible by AFM. The high force regime is very well described by ab-initio quantum mechanical calculations, while for the low force regime we combine ab-initio calculations with a description of the entropic forces based on the freely rotating chain model. Finally, a one-parameter fit for the different configurations of the poly(azobenzene-peptide) and a quantitative description of the optically induced actuation are given [1-2].

- [1]Holland, N. B.; Hugel, T.; Neuert, G.; Cattani-Scholz, A.; Renner, C.; Oesterhelt, D.; Moroder, L.; Seitz, M.; Gaub, H. E. *Macromolecules* 2003, 36, 2015-2023
 [2]Neuert, G.; Hugel, T.; Netz, R. R., Gaub, H. E., *Macromolecules* accepted

CPP 28.8 Fri 12:15 ZEU Lich

Nanofriction: Pulling polymers along surfaces — ●ANDREAS SERR^{1,2} and ROLAND R. NETZ¹ — ¹Physik Department, Technische Universität München, James-Frank-Str., D-85748 Garching, Germany — ²serr@ph.tum.de

Over the last decade the method of AFM force spectroscopy has been used to extract single polymer data, e.g. on protein unfolding dynamics, polymer elasticity, covalent bond breaking and adsorption strengths. When pulling on polymers physisorbed to surfaces, a transition from stick to slip has been noted by change of pH, ionic strength or solvent conditions, which is yet not understood. Using a simple, parameterized model for polymer-surface interactions we predict the lateral and vertical forces for both pulling the polymer off from the surface and for pulling laterally alongside the surface [1]. In principle, the friction coefficient can be extracted from such experiments and its dependence on polymer & surface type, pH, etc. could be mapped out. Microscopic models and simulations provide insight into the fundamental dissipation processes for different types of polymer-surface interactions.

- [1] A. Serr, R. R. Netz, *Pulling adsorbed polymers from surfaces with the AFM: stick versus slip, peeling versus gliding*, submitted to *Europhys. Lett.*, 2005.

CPP 29 Computational Techniques

Time: Friday 10:30-11:45

Room: ZEU 160

CPP 29.1 Fri 10:30 ZEU 160

First-principles calculation of noncovalent interactions - Diffusion Monte Carlo applied to hydrogen bonding and aromatic stacking — ●M. FUCHS¹, C. FILIPPI², J. IRETA¹, and M. SCHEFFLER¹ — ¹Fritz-Haber-Institut der MPG, Berlin — ²Universiteit Leiden (NL)

Van der Waals (dispersion) forces are important in many molecular phenomena, such as self-assembly of molecular crystals and peptide folding. Calculating this nonlocal correlation effect requires accurate electronic structure methods. Usual density-functional theory (DFT) with generalized gradient functionals fails unless empirical corrections are added that still need extensive validation. Quantum chemical approaches like MP2 or coupled cluster (CCSD(T)) are accurate, yet their unfavorable computational scaling limits them to rather small systems. Diffusion Monte Carlo (DMC) can provide accurate molecular total energies and remains feasible also for larger systems. Hence DMC promises to be useful for benchmarking simpler but more approximate approaches. Here we apply the fixed-node DMC method to (bio-)molecular model systems where dispersion forces are significant. Our DMC binding energies

for (dimethyl-) formamide dimers and adenine-thymine DNA base pairs fully agree with data from CCSD(T), in particular for stacked DNA base pairs where MP2 is insufficient. In addition we consider benzene dimers in the stacked, slipped parallel, and T-shaped structures. Resolving their relative energies requires carefully optimized DMC trial wavefunctions. We discuss the role of the determinantal part and the correlation factor, optimizing them simultaneously using a fluctuation potential approach.

CPP 29.2 Fri 10:45 ZEU 160

Modeling multi-body effects in ionic solutions with a concentration dependent dielectric permittivity — ●BERK HESS¹, CHRISTIAN HOLM^{2,1}, and NICO VAN DER VEGT¹ — ¹Max-Planck Institute for Polymer Research, Ackermannweg 10, D-55128 Mainz, Germany — ²Frankfurt Institute for Advanced Study (FIAS), J.W. Goethe Universität, Max-von-Laue Strasse 1, D-60438 Frankfurt/Main, Germany

We report a new strategy to parameterize effective ion-ion potentials for large-scale implicit solvent simulations of charge systems. The effective potential includes a pair term, derived from explicit solvent simula-

tion of a single ion pair, and a Coulomb term that by means of a concentration dependent dielectric permittivity takes into account all multi-body effects. We show that, for aqueous NaCl as an example system, this approach allows to accurately predict the solution osmotic properties up to concentrations of 2.8 molar salt. Replacing the pair term with a Weeks-Chandler-Andersen potential leads to equally good predictions, which indicates that ion-specific hydration effects featuring in the effective potential need not be included. The use of a concentration dependent dielectric permittivity opens new ways to study systems with inhomogeneous charges distributions.

CPP 29.3 Fri 11:00 ZEU 160

Some computational techniques for first-principles simulations on condensed matter systems — ●ALBERTO CASTRO¹, M. A. L. MARQUES², HEIKO APPEL¹, ANGEL RUBIO^{3,1}, and E. K. U. GROSS¹ — ¹Institut für Theoretische Physik, Arnimallee 14, Fachbereich Physik, 14195 Berlin (Germany). — ²Laboratoire de Minéralogie-Cristallographie de Paris (France). — ³Donostia International Physics Center and Departamento de Física de Materiales, Facultad de Ciencias Químicas, 20018 San Sebastián (Spain).

The real-space techniques for computational simulations in the condensed matter realm are usually praised for, at least, two strong advantages: On the first hand, the intrinsically local character of the "basis set" should permit, in principle, to allow for large scale parallelization by dividing the space in domains. This locality is also the basis for the use of techniques aiming at the linear-scaling of the computational effort. On the second hand, the real space mesh on which the magnitudes are represented may be locally adapted to the needs of each region – one feature difficult to translate to the more traditional plane wave representation. We will present our approach to these two time-saving computational techniques: (i) One possible route to implement curvilinear coordinates, able to adapt the local resolution to the needs of each region in space; (ii) A multiple-way parallelization scheme that may divide the work among a given number of processors, splitting the tasks either in k-points, in Kohn-Sham states (assuming a density functional formulation of the condensed matter problem), in regions in real-space, or in a combination of all of them.

CPP 29.4 Fri 11:15 ZEU 160

Monte Carlo algorithms for electrostatic interactions in dielectric media — ●IGOR PASICHNYK¹, RALF EVERAERS¹, and ANTHONY MAGGS² — ¹Max Planck Institute for the Physics of Complex Systems, Noethnitzer Str. 38, D-01187 Dresden, Germany — ²Laboratoire de Physico-Chimie Théorique, UMR CNRS-ESPCI 7083, 10 rue Vauquelin, F-75231 Paris Cedex 05, France

Due to the magnitude and long-range nature of Coulomb forces, the accurate representation of electrostatic interactions in classical computer simulations is a difficult task and an area of on-going research.

Maggs and collaborators [1] have suggested rewriting the problem of a Coulomb system in a local lattice framework which admits also the effective treatment of nonhomogeneous dielectric medium.

The quenched version of the algorithm is applied for the construction of field lines and equipotential surfaces. The algorithm correctly reproduces fluctuations in the electrostatic field that correspond to the zero-frequency component of the van der Waals interaction. Fluctuations in the field produces inhomogeneous polarization, which in turn generates an induced charge density. This charge density interacts electrostatically and produces thermally dependent force between dielectrics. It is shown that these fluctuations lead to a Casimir-like attraction in the triple-slab dielectric system.

[1] A.C. Maggs and V. Rossetto, Phys. Rev. Lett., 88,196402, 2002

CPP 29.5 Fri 11:30 ZEU 160

Investigation of the condensation kinetics of methanol by molecular dynamics simulation — ●BJÖRN FISCHER and THOMAS KRASKA — Physical Chemistry, University Cologne, Luxemburger Str. 116, D-50939 Köln, Germany

The nucleation kinetics and the liquid cluster growth in the condensation process of supersaturated methanol vapour in a carrier gas is investigated. Methanol is chosen as an associating substance and also as the smallest member of the series of the 1-alkanols. For the modelling of the thermophysical properties of methanol several molecular models of differing complexity exist [1,2]. The suitability of these models for the direct simulation of the nucleation process has not been investigated yet.

The simulations performed here start with an equilibrated stable vapour state. The supersaturation is induced by a temperature jump to a state point in the metastable region of the phase diagram. Shortly after the jump clusters are formed by homogeneous nucleation which continue to grow by surface growth or coalescence.

The simulation results are analysed with respect to the nucleation rates at different state conditions and supersaturation and compared with experimental data. Furthermore, the cluster size distribution and the temperature development of the simulated systems are studied.

[1] M. E. van Leeuwen, B. Smit, J. Phys. Chem. 99, 1831 (1995)

[2] W. D. Cornell et al., J. Am. Chem. Soc. 117, 5179 (1995)