

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

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Overview of Invited Talks and Sessions

(lecture rooms H37, H40, and H47; Poster B)

Invited Talks

CPP 1.1	Mon	9:30–10:00	H37	Dynamic Processes in Supramolecular Nanoassemblies — ●CHRISTIAN VON BORCZYKOWSKI
CPP 4.1	Mon	14:00–14:30	H37	Direct measurement of critical Casimir forces — CHRISTOPHER HERTLEIN, LAURENT HELDEN, ●CLEMENS BECHINGER
CPP 10.1	Tue	9:30–10:00	H37	Polymer dynamics: From Synthetic Polymers to Biopolymers — ●DIETER RICHTER
CPP 10.6	Tue	11:15–11:45	H37	Time-resolved small-angle neutron scattering — ●ROLAND MAY
CPP 11.1	Tue	14:00–14:30	H37	Surface sensitive neutron scattering — ●R. STEITZ
CPP 11.6	Tue	15:45–16:15	H37	Coherent x-ray studies of polymer membrane fluctuations and colloidal dynamics near the glass transitions — ●SIMON MOCHRIE
CPP 11.10	Tue	17:15–17:45	H37	Microbeam Synchrotron Radiation Scattering Experiments in Soft Condensed Matter — ●CHRISTIAN RIEKEL
CPP 17.1	Wed	14:00–14:30	H37	Liquid distribution in a granular pile — MARIO SCHEEL, MARTIN BRINKMANN, ●STEPHAN HERMINGHAUS, RALF SEEMANN
CPP 24.1	Thu	9:30–10:00	H37	Fluctuating 2d vesicles in hydrodynamic Stokes flow — ●REIMAR FINKEN, UDO SEIFERT
CPP 25.1	Thu	17:15–17:45	H37	Coupled electro-hydrodynamic force fields for the manipulation of objects in solutions — ●MAGNUS JAEGER, MAIKA FELTEN, GUENTER FUHR, MICHAEL STUKE, CLAUS DUSCHL
CPP 26.1	Thu	10:00–10:30	H40	Efficient coupling of single molecules with light — ●VAHID SANDOGHDAR
CPP 26.2	Thu	10:30–11:00	H40	Charge and Energy Transfer in Photosynthetic Systems - Some Principles of Photosynthetic Light Harvesting — ●VILLY SUNDSTRÖM
CPP 26.5	Thu	11:30–12:00	H40	Optimal Control of Femtosecond Time-Resolved Four-Wave Mixing for the Selective Excitation of Molecular Modes — ●ARNULF MATERNY
CPP 27.1	Thu	14:30–15:00	H40	Controlling intermolecular interactions in organic semiconductors — ●LAURA HERZ
CPP 27.4	Thu	15:30–16:00	H40	Coherent control of single spins in diamond — ●FEDOR JELEZKO, JÖRG WRACHTRUP
CPP 27.7	Thu	16:30–17:00	H40	Optical spectroscopy on single carbon nanotubes — ●ACHIM HARTSCHUH, HUIHONG QIAN, TOBIAS GOKUS, MATHIAS STEINER, ALFRED MEIXNER

Invited talks of the joint symposium SYOE

See SYOE for the full program of the Symposium.

SYOE 4.1	Tue	9:30–10:15	H1	Vapor and Solution Deposited Small Molecule Organic Thin Film Transistors — ●THOMAS JACKSON
SYOE 5.1	Tue	11:15–12:00	H1	Organic electronic devices and their applications — ●PAUL HEREMANS
SYOE 6.1	Tue	14:30–15:15	H32	Theory of polymer devices: OFETs and OLEDs — ●REINDER COEHOORN

SYOE 7.1	Tue	16:30–17:15	H32	Electronic spectrum and spin states of a single organic molecule — •HERRE VAN DER ZANT
SYOE 10.1	Wed	16:45–17:30	H32	Single grain contacts — •GREGOR WITTE

Invited talks of the joint symposium SYBM

See SYBM for the full program of the Symposium.

SYBM 1.1	Thu	9:30–10:00	H1	Using Ice to Mimic Nacre: From Structural Materials to Artificial Bone — •A. P. TOMSIA, S. DEVILLE, E. SAIZ
SYBM 1.2	Thu	10:00–10:30	H1	On the structure of biogenic CaCO₃ — •B. POKROY
SYBM 1.3	Thu	10:30–11:00	H1	Bio-Inspired Hybrid Materials from Block Copolymer Assemblies and Nanoparticle Co-assemblies — •U. WIESNER
SYBM 1.4	Thu	11:15–11:45	H1	Bio-Inspired Organic-inorganic Hybrid Materials — •U. STEINER
SYBM 1.5	Thu	11:45–12:15	H1	Structural, Nanomechanical, and Nanotribological Characterization of Human Hair Using Atomic Force Microscopy and Nanoindentation — •BHARAT BHUSHAN

Invited talks of the joint symposium SYPE

See SYPE for the full program of the Symposium.

SYPE 2.1	Thu	14:00–14:30	H37	Coulomb and Flory: Fathers of SONS. Polyelectrolytes in Self Organized Nano Systems — •MARTIEN COHEN STUART
SYPE 2.7	Thu	16:00–16:30	H37	Bundling Phenomena in Semiflexible Polyelectrolytes — •CHRISTIAN HOLM, MEHMET SAYAR, BERK HESS
SYPE 3.1	Fri	10:30–11:00	H1	Behaviour of polyelectrolyte solutions under confinement — •DOMINIQUE LANGEVIN, CÉSAR MARQUEZ, HEINIG PETER, DAN QU
SYPE 3.4	Fri	11:30–12:00	H1	Polymers at Surfaces: Sticking and Gliding — •ROLAND NETZ

Sessions

CPP 1.1–1.10	Mon	9:30–12:30	H37	Supramolecular Aggregates
CPP 2.1–2.9	Mon	10:00–12:30	H40	Polymer Physics I
CPP 3.1–3.9	Mon	10:00–12:30	H47	Colloids and Nanoparticles I: Structure
CPP 4.1–4.6	Mon	14:00–15:45	H37	Colloids and Nanoparticles II: Effective Interactions
CPP 5.1–5.5	Mon	14:30–15:45	H40	Polymer Physics II
CPP 6.1–6.5	Mon	14:30–15:45	H47	Dynamics of Molecular Systems
CPP 7.1–7.32	Mon	16:00–18:00	Poster B	POSTER: INTERNAL SYMPOSIUM Scattering Experiments
CPP 8.1–8.37	Mon	16:00–18:00	Poster B	POSTER: Polymer Physics
CPP 9.1–9.25	Mon	16:00–18:00	Poster B	POSTER: Colloids and Nanoparticles
CPP 10.1–10.9	Tue	9:30–12:30	H37	INTERNAL SYMPOSIUM Scattering Experiments I
CPP 11.1–11.12	Tue	14:00–18:15	H37	INTERNAL SYMPOSIUM Scattering Experiments II
CPP 12.1–12.9	Tue	10:00–12:30	H40	Polymer Physics III: Interfaces
CPP 13.1–13.9	Tue	14:30–17:15	H40	Polymer Physics IV: Thin Films
CPP 14.1–14.9	Tue	10:00–12:30	H47	Biological Systems
CPP 15.1–15.8	Tue	14:30–16:45	H47	Diffusion and Transport Processes
CPP 16.1–16.6	Tue	17:00–18:30	H47	Colloids and Nanoparticles III
CPP 17.1–17.6	Wed	14:00–15:45	H37	Micro and Nano Fluidics I: Structured Substrates
CPP 18.1–18.5	Wed	14:30–15:45	H40	Light-Induced Phenomena
CPP 19.1–19.20	Wed	16:00–18:30	Poster B	POSTER: Micro and Nano Fluidics
CPP 20.1–20.32	Wed	16:00–18:30	Poster B	POSTER: Biological Systems + New Materials
CPP 21.1–21.11	Wed	16:00–18:30	Poster B	POSTER: Dynamics and Diffusion
CPP 22.1–22.16	Wed	16:00–18:30	Poster B	POSTER: INTERNAL SYMPOSIUM Optical Spectroscopy
CPP 23	Wed	16:00–18:30	Poster B	POSTER: JOINT SYMPOSIUM Polyelectrolytes
CPP 24.1–24.10	Thu	9:30–12:30	H37	Micro and Nano Fluidics II: Soft Objects in Flow + Slippage
CPP 25.1–25.6	Thu	17:15–19:00	H37	Micro and Nano Fluidics III: Lab-on-Chip Geometries
CPP 26.1–26.7	Thu	10:00–12:30	H40	INTERNAL SYMPOSIUM Optical Spectroscopy I

CPP 27.1–27.7	Thu	14:30–17:00	H40	INTERNAL SYMPOSIUM Optical Spectroscopy II
CPP 28.1–28.4	Thu	17:15–18:15	H40	Polymer Physics V
CPP 29	Thu	14:00–17:00	H37	JOINT SYMPOSIUM Polyelectrolytes I
CPP 30	Fri	10:30–12:30	H1	JOINT SYMPOSIUM Polyelectrolytes II
CPP 31.1–31.8	Fri	10:30–12:30	H40	New Materials

Annual General Meeting of the Section Chemical and Polymer Physics

Wed 18:30–19:30 H37

- Bericht + Tagungsnachlese
- Wahl
- Symposien 2008
- Sonstiges

CPP 1: Supramolecular Aggregates

Time: Monday 9:30–12:30

Location: H37

Invited Talk**Dynamic Processes in Supramolecular Nanoassemblies** — CPP 1.1 Mon 9:30 H37

•CHRISTIAN VON BORCZYKOWSKI — Center of nanostructured materials and analytics, TU Chemnitz, 09107 Chemnitz

Supramolecular aggregates of organic molecules have proven to be both biomimetic systems e. g. for photosynthetic reaction units and model systems for a development of model systems in bottom-up molecular electronic concepts. Due to that large range of properties such as functional groups and redox-potentials organic molecules are versatile building blocks blades of functionalized units. Complementary, semiconductor quantum dots of sizes in the nanometer range are in combination with quantum confinement tunable over a large range of broad band absorption combined with narrow band emission properties. This contribution will report the progress of the combination both of perspectives, namely chemical versatility of molecules and bandgap-tuning of semiconductor nanocrystals. Optical experiments on self-organized ensembles between dye molecules and CdSe nanocrystals will be in the center of this investigation. [1], [2].

[1] E. Zenkevich et al., *J. Phys. Chem. B* 109, 8679 (2005). [2] D. Kilin et al., *J. Photochem. Photobiol. B* (2006, in print).

CPP 1.2 Mon 10:00 H37

Controlled Fabrication of Molecular Nano-Dot Patterns —

•STEPHAN RATH, DIRK SAUER, and HELMUT PORT — 3. Physikalisches Institut, Universität Stuttgart

For applications in molecular electronics and photonics small dot-like structures are attractive objects as they can be individually addressed.

To fabricate nano-dots thin organic films are deposited at UHV conditions on helium-cooled substrates. Controlled annealing to room temperature transforms the films into homogeneous distributions of isolated dots by dewetting. This process can be quantified and optimized for different combinations of molecules and substrates.

To achieve regular and closely packed patterns of dots, we introduced topographically structured substrates as templates. In this way, we are able to control size, density and arrangement of nano-dots on mm²-sized areas. For characterization and single dot access two operation modes are applied: confocal microscopy in combination with AFM and scanning near-field optical microscopy (SNOM).

CPP 1.3 Mon 10:15 H37

The absorption spectrum of organic dye aggregates —

•ALEXANDER EISFELD and JOHN BRIGGS — Theoretische Quantendynamik, Universität Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg, Germany

Certain molecular aggregates consisting of organic dyes are remarkable in exhibiting an intense and very narrow absorption peak, known as a J-band [1], which is red-shifted away from the region of monomer absorption. Apart from those dyes showing the J-band on aggregation, there are also dyes where the absorption maximum is shifted to higher energies. The width of the resulting absorption band (called an H-band) is comparable to that of the monomeric dyes and shows a complicated vibrational structure.

Following our analysis of the J-band [2,3] spectra of polymer aggregates using the CES approximation, a theory that includes vibrations explicitly, we show that the same approximation can account for measured H-band spectra. Using simple analytical forms of the monomer spectrum the origin of the widely-different shapes of H- and J-bands is explained within the CES approximation [4].

[1] T. Kobayashi, *J-Aggregates*. World Scientific, 1996

[2] A. Eisfeld, J. S. Briggs, *Chem. Phys.* 281, 61

[3] A. Eisfeld, J. S. Briggs, *Phys. Rev. Lett.* 96, 113003

[4] A. Eisfeld, J. S. Briggs, *Chem. Phys.* 324, 376

CPP 1.4 Mon 10:30 H37

Single molecule spectroscopy of dye - quantum dot

•DANNY KOWERKO, JÖRG SCHUSTER, and CHRISTIAN VON BORCZYKOWSKI — Center of nanostructured materials and analytics, TU Chemnitz, 09107 Chemnitz

Nanoassemblies of semiconductor quantum dots (QDs) and organic molecules are promising objects of research and application in many fields of science and technology. Physics and chemistry of coupling mechanisms and possible interactions (i.e. energy transfer) are com-

plex and thus not yet fully understood. Förster resonance energy transfer has been proven to be one reason for quenching of CdSe QDs luminescence in the presence of pyridyl porphyrin molecules [1]. Already observed QD luminescence quenching in pyridyl functionalized perylenebisimide solutions promises such systems on a single molecule/single nanoparticle level. In order to be able to use such spectroscopic techniques even at cryogenic temperatures nanoassemblies need to be immobilized on surfaces. Here we report on the preparation and spectroscopic characterization of dye - QD assemblies on silica surfaces. We will show that there is clear evidence that such assemblies are formed in solution and are stable on the surface. [1] E. I. Zenkevich et al., *J. Phys. Chem. B*, 109, 8679, 2005.

15 min. break

CPP 1.5 Mon 11:00 H37

Selective mapping of the coordinate metal bonds in

supramolecular nanoarchitectures — •P. MÜLLER¹, M.S. ALAM¹, L.K. THOMPSON², U. KORTZ³, R. SAALFRANK⁴, M. RUBEN⁵, and J.-M. LEHN⁶ — ¹Physikalisches Institut III, Universität Erlangen-Nürnberg — ²Chemistry Department, Memorial University, St. Johns, Canada — ³School of Engineering and Science, International University, Bremen — ⁴Institut für Organische Chemie, Universität Erlangen-Nürnberg — ⁵Institut für Nanotechnologie, FZ Karlsruhe — ⁶ISIS, Université Louis Pasteur, Strasbourg, France

Coordinate-bonded 3d metal ions dominate the electronic density of states of organic molecules incorporating such metal centers. Supramolecular nanostructures of different structural complexity and incorporating different transition metal ions were investigated. The molecules were deposited from the solution onto HOPG surfaces. The structural and electronic properties were studied at the single-molecule level by STM and current imaging tunneling spectroscopy (CITS). This spectroscopy was applied to different types of square and star-like metal ion arrays, a supramolecular copper-oxygen assembly embedded into a polyoxotungstate wheel, and a coordination polymer based on amino acids, rendering local tunneling probabilities with submolecular resolution. These investigations allowed the localization of the positions of the incorporated transition metal centers due to a selective mapping of the coordinate metal-ligand bonds. CITS measurements of a one-dimensional, Fe containing polymer revealed a high contrast between the high-spin and the low-spin complexes.

CPP 1.6 Mon 11:15 H37

Balance of structure-building forces in aliphatic self-

assembled monolayers on metal substrates — ANDREY SHAPORENKO¹, TOBIAS WEIDNER¹, ANDREAS TERFORT², and •MICHAEL ZHARNIKOV¹ — ¹Angewandte Physikalisches Chemie, Universität Heidelberg, 69120 Heidelberg, Germany — ²Anorganische und Angewandte Chemie, Universität Hamburg, 20146 Hamburg, Germany

Using self-assembled monolayers (SAMs) of biphenyl-substituted alkaneselenols (BPnSe, where n = 2-6 is the number of the methylene units in the aliphatic linker) on gold and silver substrates as a model system, we demonstrate that the bonding configuration of the selenol headgroup is the deciding factor in the balance of structure-building interaction in the alkaneselenol SAMs. The energy associated with the persistence of this configuration is high enough to prevail over the energy gain associated with the optimal (i.e., dense) packing of the biphenyl moieties in the BPnSe SAMs. Considering, that the similar effects have been observed for the alkanethiolate SAMs, we can conclude on the generality of this phenomenon, stating that the exact bonding configuration of the headgroup is an important or, in most cases, even deciding factor in the balance of different contributions responsible for the molecular packing and structure of aliphatic self-assembled monolayers on metal substrates. This bonding configuration can be alternatively associated with a definite hybridization of the sulphur atom in the substrate-sulfur-carbon joint or a definite geometry of the adsorption site on the given substrate.

CPP 1.7 Mon 11:30 H37

Competitive Adsorption of Functionalized Molecules

on Semiconductor Nanocrystal Surfaces — KLEMENTYNA SZWAYKOWSKA^{1,2}, CHINNAPPAN RAJA^{3,4}, •THOMAS BLAUDECK^{1,3},

FRANK CICHOS^{1,5}, and CHRISTIAN VON BORCZYKOWSKI³ — ¹POM, TU Chemnitz, 09107 Chemnitz, Germany — ²Engineering and Applied Sciences, California Institute of Technology, Pasadena, CA 91125, USA — ³OSMP, TU Chemnitz, 09107 Chemnitz, Germany — ⁴ABMC, Kansas State University, Manhattan, KS 66506, USA — ⁵Molecular Nanophotonics, U Leipzig, 04103 Leipzig, Germany

Inorganic/organic aggregates from semiconductor nanocrystals and functionalized molecules such as porphyrins are considered building blocks in future nanoelectronics as they may provide control on the charge and energy transfer processes [1, 2]. We report on the formation process and the stability of aggregates comprising CdSe and CdSe/ZnS nanocrystals and TOPO ligands in toluene at ambient conditions. Applying steady-state spectroscopy to binary and ternary mixtures we compare the results in presence and absence of additional molecules. The experiments show that the formation kinetics is related to by the absolute concentration of the compounds in parallel to their molar ratio. The importance of the local TOPO concentration at the NC surface indicates a dynamic equilibrium governing the number of adsorption sites available. The findings are discussed in the light of Monte-Carlo simulations.

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

[2] D. Kilin et al., J. Photochem. Photobiol. B (2006, in print).

CPP 1.8 Mon 11:45 H37

Grazing incident scattering for the investigation of crystallization in micellar systems — ●MAX WOLFF¹, ANDREAS MAGERL², and HARTMUT ZABEL¹ — ¹Lehrstuhl für Festkörperphysik/EP IV, Ruhr-Universität Bochum, 44780 Bochum, Germany — ²Lehrstuhl für Kristallographie und Strukturphysik, Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

Small angle scattering is known to provide information on the structural arrangement of block polymers. In highly dilute systems the conformation of the monomers is accessible from the radial intensity distribution. For higher concentrations micelles may appear and in the case of crystallisation usually an isotropic three dimensional powder is formed. From the resulting Debye-Scherrer rings it is difficult to determine the crystallographic structure. One way out is to introduce anisotropy by the application of shear. However, shear may affect the structure. Alternatively, by use of near surface small angle scattering, the ordering can be investigated close to the solid-liquid interface. We extracted detailed information on the crystallization of Pluronic (PEO-PPO-PEO) micelles solved in water in the vicinity of a solid substrate. We find the crystalline structure dependent on the chemical termination of the substrate as well as on the history of the sample. In addition we generally find large crystallites when entering into a crystalline phase from a liquid one that shrink in size further away from the phase boundary.

We acknowledge financial support by the BMBF grant no.: ADAM ZAE8BO and the DFG within the priority program SPP 1164.

CPP 1.9 Mon 12:00 H37

Self-assembly of diblock-copolymer micelles for template-based preparation of PbTiO₃ nanograins — STEPHAN KRONHOLZ¹, ●SILKE RATHGEBER², SILVIA KARTHÄUSER¹, HERMANN KOHLSTEDT¹, SVEN CLEMENS³, and THEODOR SCHNELLER³ — ¹Max-Planck Institute for Polymer Science, Polymer Physics, 55128 Mainz — ²Research Center Jülich GmbH, Center of Nanoelectronic Systems for Information Technology, 52425 Jülich — ³RWTH-Aachen, Institute of Materials for Electronic Engineering 2, 52074 Aachen

A bottom-up fabrication route for ferroelectric PbTiO₃ nanograins grown on predefined TiO₂ nanostructures used as seeds is presented. [1] The structuring of the TiO₂ seeds is performed using a self-organized template constructed from a gold-loaded micellar monofilm. With this fabrication process, 12nm TiO₂ seeds and 30nm PbTiO₃ grains are prepared without any e-beam lithographic step. The dimensions of the structure imposed by the micellar template are transferred through all the processing steps to the final PbTiO₃ grains. By a combination of scattering experiments on the micellar solutions and a characterization of the monofilm we can determine whether the architecture of the diblock-copolymers in the micelles or the preparation conditions determine the quality and characteristics of the monofilm. It is shown that the intermicelle distance and the degree of order in the dried monofilm is mainly determined by the pulling velocity in the dipping process and the strength of the surface-micelle interaction, and not necessarily by the architecture of the diblock copolymers. [1] S. Kronholz et al., Adv. Funct. Mater. 16, 2346 (2006)

CPP 1.10 Mon 12:15 H37

Nanoaggregates on structured surfaces — ●HARALD GRAAF, THOMAS BAUMGÄRTEL, MAIK VIELUF, and CHRISTIAN VON BORCZYKOWSKI — Centre for nanostructured materials and analytics, TU Chemnitz, 09107 Chemnitz

Structuring of surfaces by local oxidation induced by electrical atomic force microscopy opens a way to prepare functional nanostructures. Different properties of the nanostructures compared to the surrounded surfaces can be adjusted by modifying the surface and nanostructure with various monolayers.

We report here on the selective binding of dye molecules as well as nanoparticles by non-covalent bonding. We used silicon (100) as substrates. The silicon surfaces were modified by a covalently bond alkene monolayer. The surface properties can be tuned by using functionalized alkene molecules. The monolayers are characterized by a high physical and chemical stability. By local anodic oxidation the monolayer can be locally degraded and the underlying silicon oxidized leading to silicon oxide nanostructure.[1] Dye molecules and nanoparticles were bond selectively to the nanostructure and/or the surrounding monolayer. Non-covalent interactions as ionic or hydrophobic interactions were responsible for this propose.[2]

[1] M. Ara, H. Graaf, H. Tada, Appl.Phys.Lett. 80(2002) 2565

[2] H. Graaf, M. Vieluf, C. von Borczykowski, submitted

CPP 2: Polymer Physics I

Time: Monday 10:00–12:30

Location: H40

CPP 2.1 Mon 10:00 H40

Multiscale modeling of block-copolymer-nanomaterials — ●STEPHAN ALEXANDER BAEURLE¹, TAKAO USAMI², and ANDREI GUSEV³ — ¹Department of Chemistry and Pharmacy, Institute of Physical and Theoretical Chemistry, University of Regensburg, D-93053 Regensburg, Germany — ²Polymer Design Laboratory, Mitsubishi Chemical Group Science and Technological Research Center, Yokkaichi, Mie 510-0885, Japan — ³Department of Materials, Institute of Polymers, ETH, CH-8093, Zurich, Switzerland

A detailed knowledge about the physics and chemistry of multiphase materials on different length and time scales is essential to tailor their macroscopic physical and mechanical properties. A better understanding of these issues is also highly relevant to optimize their processing and, thus, their elucidation can be determinant for their final industrial application. In this presentation we introduce an analytical and numerical multiscale modeling approach, to explain and predict the peculiar stress relaxation behavior of block-copolymer-based thermoplastic elastomers at long times, which are subjected to a nonlinear

extensional strain. We compare our theoretical results to the stress relaxation measurements performed on poly(styrene-isoprene-styrene) triblock copolymers and show that they correctly describe the crossover from power-law to stretched-exponential relaxation behavior, observed below the glass transition temperature of the polystyrene crosslinks. Our study confirm the importance of the chain-pullout mechanism in the stress relaxation process and demonstrates the involvement of multiple time- and structural-length-scales.

CPP 2.2 Mon 10:15 H40

Bicontinuous AB-diblock-copolymer mesophases: geometric arguments in favour of an "alternating" Im3m phase based on the I-WP surface — ●G.E. SCHROEDER-TURK¹, S.T. HYDE², and A. FOGDEN² — ¹Inst. für Theor. Physik I, Univ. Erlangen-Nürnberg, Staudtstraße 7, 91058 Erlangen — ²Applied Maths, Res. School of Phys. Sciences, Australian National University, 0200 ACT, Australia

Bicontinuous phases in AB-diblock-copolymers are well known. In the "coreshell" Gyroid phase, immiscibility of A and B blocks leads to two

intertwined identical networks of block A separated by a matrix of block B. The Gyroid triply-periodic minimal surface (TPMS) lines the middle of the B domain. For AB diblock copolymers, an "alternating" phase (as found in linear ABC terpolymers) with one network consisting of A and the other of B blocks does not exist. Chain stretching frustration is crucial to the phase stability analysis of these systems. Variations of the domain thickness, i.e. of the length between the TPMS and the center of the network channels, is unavoidable and incurs an entropic penalty for stretching of the polymer chains. We present an analysis of these variations for various TPMS of cubic symmetry. We demonstrate that the Gyroid is the bicontinuous geometry with the smallest frustration. The I-WP geometry is another TPMS where the two networks are not identical. The domain thickness variations are small for one network and large for the other. We argue that the I-WP may be suitable for an AB-diblock alternating phase in an asymmetrically polydisperse polymer system where one moiety has a wide and one a narrow molecular weight distribution.

CPP 2.3 Mon 10:30 H40

Core-shell filler in a block copolymer matrix: morphology and properties — ●LESZEK JAKUCZEK^{1,2}, JOCHEN GUTMANN^{2,3}, and DANUTA ZUCHOWSKA¹ — ¹Wroclaw University of Technology, Wroclaw, Poland — ²Max Planck Institute for Polymer Research, Mainz, Germany — ³J. Gutenberg University, Mainz, Germany

Physical modification of block copolymer matrices has drawn much attention due to the remarkable possibility of property tailoring. Numerous structures can be prepared by changing the properties of the matrix (e.g. block length) or those of the nanofiller (dimensions, type of modification). Simultaneously interesting research problems- e.g. possible spatial arrangements of constitutive elements- can be addressed.

PS-grafted nanoparticles (polysiloxane microgel) were used as the filler. The inorganic cores were synthesized in a sol-gel process and surface modified with ATRP initiator. Controlled polymerization allowed to obtain well-defined polymer shells (Mw- up to 30 kg/mol; Mw/Mn about 1,10).

PS-grafted nanoparticles were used to modify the PS-PI diblock and PS-PI-PS triblock copolymers. All samples were prepared via solution casting. Upon changing the filler type and loading, the influence of such parameters as Mw of grafted chains, grafting density and particle dimensions on the properties of host matrix could be extensively evaluated. Nanocomposites were thoroughly characterized- morphology changes were identified and visualized using SAXS and TEM. Additional information was obtained from rheological and thermal analyses (by the DSC).

15 min. break

CPP 2.4 Mon 11:00 H40

Thermal and chemical glass transition of two nanocomposite systems — ROLAND SANCTUARY, ●JÖRG BALLER, RAVI BACTAVATHALOU, JAN KRISTIAN KRÜGER, BARTOSZ ZIELINSKI, and MARTINE PHILIPP — Université du Luxembourg, Laboratory of Physics of Condensed Matter and Advanced Materials (LPM), 162a, avenue de la Faiënerie, L-1511 Luxembourg

Epoxy resins modified with different kind of nanoparticles, so-called nanocomposites, reveal properties which are interesting from the fundamental and technical point of view. E.g. nanoparticles of Al₂O₃ strongly increase the viscosity of the composites which leads to a modified glass transition behaviour: T_g as well as the distribution of relaxation time is changed as a function of nanoparticle content. However surface-treated SiO₂ particles almost have no effect. Addition of a suited hardener to these nanocomposites leads to reactive adhesive systems. These systems undergo a chemical glass transition during the curing process. Despite of the big difference in viscosity between the epoxy resins filled with Al₂O₃ and SiO₂ particles, curing of these systems doesn't seem to be sensitive to the type of filler particles. Moreover the kinetics of the chemical reaction is faster compared to systems without nanoparticles. Concerning the thermal glass transition, the influence of filler particles is completely different for the epoxy resin and the cured system (e.g. opposite shift of T_g). MDSC, Brillouin spectroscopy and rheology data is presented and discussed for these systems before, during and after chemical curing.

CPP 2.5 Mon 11:15 H40

Structure Property Relationships of Polymeric Nanocomposites based on Polyhedral Oligomeric Silsesquioxanes — NING

HAO, MARTIN BOEHNING, and ●ANDREAS SCHÖNHALS — Federal Institute of Materials Research and Testing (BAM), Unter den Eichen 87, D-12205 Berlin

Polymer based nanocomposites continue to receive tremendous attention for different applications. They show remarkable property improvement (increased tensile properties, decreased gas permeability, decreased solvent uptake, increased thermal stability and flame retardance) when compared to conventionally scaled composites. Different polymer based nanocomposites are prepared where, polycarbonate and polystyrene are used as polymer matrices. As molecular nanofillers polyhedral oligomeric silsesquioxanes (POSS) with different substituents (Phenethyl-, Chlorpropyl-) are used. The property structure relationships of these nanocomposites are investigated by dielectric spectroscopy, gas transport measurements (permeation, sorption) and density measurements as well. The results are discussed with regard to the phase structure of the nanocomposites and the properties of the different POSS. This includes the construction of phase diagrams. Especial attention is paid to characterize the interfacial region between the polymeric matrix and nanoparticles. This regards also to estimate the length scale of interaction between the nanoparticle and the matrix.

CPP 2.6 Mon 11:30 H40

Shear and elongational properties of melts of reactively compatibilized PA 6/ABS blends — CHRISTIAN SAILER and ●ULRICH ALEXANDER HANDGE — Institute of Polymers, Department of Materials, ETH Zurich, Wolfgang-Pauli-Strasse 10, CH-8093 Zurich

Reactive compatibilization is a technologically commonly applied method in order to improve the interfacial adhesion in multiphase polymer blends. In this study, we investigated the influence of reactive compatibilization on the rheological properties and the morphology of polyamide 6/acrylonitrile-butadiene-styrene (PA 6/ABS) blends in the melt. Three different blends with different types of morphology (disperse morphology and cocontinuous structure) were prepared. Then linear viscoelastic shear, melt elongation and subsequent recovery experiments were performed. The linear viscoelastic shear properties of the blends were discussed using the fractional Zener model. In melt elongation, we investigated the deformation of the blend morphology using atomic force microscopy and quantified the stretch ratio of the extended drops and domains. The analysis of our recovery experiments after melt elongation revealed that the interfacial tension and reactive compatibilization strongly influence the elasticity of the blends (C. Sailer, U.A. Handge, submitted). We discuss our experimental results for the blends by taking into account the formation of polymer chains grafted with PA 6 via reactive compatibilization.

CPP 2.7 Mon 11:45 H40

Collective rearrangement under shear of a polycrystalline soft material — ●TERESA BAUER^{1,2}, JULIAN OBERDISSE¹, and LAURENCE RAMOS¹ — ¹Laboratoire des Colloïdes, Verres et Nanomatériaux (UMR CNRS-UM2 5587), CC26, Université Montpellier 2, France — ²Lehrstuhl für Biophysik E22, Technische Universität München, Germany

Polycrystalline soft materials show interesting rheological behaviour in creep experiments. Initially the instantaneous shear rate decreases as a power law with time in a similar manner as a solid. This power law regime is followed by an abrupt increase of the shear rate, indicating a fluidization of the sample, and finally reaches a stationary flow with a high constant shear rate. Here we studied how this behaviour is coupled to a structural rearrangement of the sample by conducting in situ rheology and Synchrotron (ID2 ESRF) SAXS measurements on a polycrystalline surfactant hexagonal columnar phase simultaneously. We show that a collective reorientation of the crystallites occurs at the onset of flow. We discuss how the fluidization time, which scales with the shear modulus and the applied stress, is related to structural changes.

CPP 2.8 Mon 12:00 H40

Skotometrical Investigation of Volume Changes during Rapid Deformation of Elastomers — ●MICHAEL KERSCHER, GERALD JOHANNES SCHNEIDER, and DIETMAR GÖRITZ — Institut für Physik, Universität Regensburg, 93040 Regensburg

Polymer composites consisting of a filler and an elastomer are indispensable for daily life. Thus, an enormous effort is done to understand their properties. When trying to derive constitutive equations for elastomers, the constance of volume on deformation is one of the major

assumptions to be made. Already several decades ago, however, experiments showed a volume expansion, albeit very small. Therefore, a constant volume has still been assumed even though these experiments were only performed at small strain rates or with slow measuring processes not considering a possible effect at short time intervals.

In our contribution, we show the influence of deformation velocity on volume expansion at high deformation rates. For this purpose, in our experiments we use an optical dilatometer based on the principle of a scotometer (from greek “σκότᾶδι”: darkness) which allows measurement of volume changes in the range of a few milliseconds.

Our experiments point to a by far higher volume change than expected from slow deformation which then relaxate in the range of several milliseconds. These new results have to be taken into consideration when trying to fully understand the laws behind the deformation of elastomers.

CPP 2.9 Mon 12:15 H40

How to stop ageing of biosynthetic PHB - 'melt irradiation' — ●ANTJE BERGMANN^{1,2} and ANTHONY OWEN¹ — ¹Fakultät für Physik, Universität Regensburg — ²Fakultät für Physik, Universität Karlsruhe

(TH)

Bacterially processed polyhydroxybutyrate (PHB) is a semicrystalline polymer. Its properties are similar to those of some conventional plastics such as polyethylene (PE). Unfortunately, it undergoes an ageing process, which is characterised by an increasing embrittlement while stored at room temperature. Using various structural analysis methods and comparing the results with those obtained by mechanical measurements we investigated the mechanisms of ageing and found that both a progressive crystallisation process and physical ageing are responsible for the ageing phenomenon.

On the basis of that knowledge we tried out different treatments on the samples in order to prevent the progressive embrittlement. Whereas annealing treatments and the use of plastizisers were not suitable to stop the ageing process completely, irradiation of amorphous PHB with electrons turned out to be a successful method - we call this procedure 'melt irradiation'. An elastic network can be established within the amorphous regions, even though the samples are highly crystalline. This new PHB morphology shows the desired elastic mechanical properties, and the samples are no longer prone to ageing.

CPP 3: Colloids and Nanoparticles I: Structure

Time: Monday 10:00–12:30

Location: H47

CPP 3.1 Mon 10:00 H47

Structural crossover and connectivity in binary colloidal hard-sphere mixtures — JÖRG BAUMGARTL¹, ●ROEL DULLENS¹, MARJOLEIN DIJKSTRA², ROLAND ROTH³, and CLEMENS BECHINGER¹ — ¹Physikalisches Institut, Universität Stuttgart, Germany — ²Soft Condensed Matter Group, Utrecht University, The Netherlands — ³Max-Planck-Institut für Metallforschung und Institut für Theoretische und Angewandte Physik, Stuttgart, Germany

Already the simplest conceivable multi-component system, i.e. a binary mixture of hard spheres, exhibits an exceedingly rich phenomenology in comparison to single-component systems. Recently, it has been predicted that the phase diagram is divided by a crossover line which distinguishes two regions where the oscillation wavelength of the pair correlation function in the asymptotic limit is either dominated by the diameter of the big spheres or that of the small spheres. Despite the generic character of this structural crossover, this effect has not been observed experimentally. This is the more surprising, because recent calculations demonstrate that the asymptotic regime starts already at intermediate ranges, implying that structural crossover should be visible at relatively small distances. In this work, we use confocal microscopy to investigate the structural crossover in a (high-packing fraction) binary colloidal model system. Furthermore, we address the question as to what the repercussions of the crossover on the structure of a binary fluid are. To this end, we analyze the fluid structure in terms of connectivity based on Delaunay triangulations. This analysis is extended to lower packing fractions using Monte-Carlo simulations.

CPP 3.2 Mon 10:15 H47

Scattering by Self-Affine Fractals — ●GERALD JOHANNES SCHNEIDER and DIETMAR GÖRITZ — Institut für Physik, Universität Regensburg, 93040 Regensburg

The structure, i. e. the size and the shape, of colloidsized objects at a length scale of nanometers is of fundamental interest for elementary science and for applications. Due to its statistical relevance and its easy appliance scattering methods are very suitable to study the structure of samples at the nanoscale. However, the information content obtained, strongly relies on models of the structure.

Generally, in order to model colloidal objects, the clusters are considered as spherically symmetric. Although, this assumption simplifies the underlying mathematics, it does not work if external forces acting on the sample and thus the experimental results could not interpreted within standard theories.

In our contribution we introduce a new model, based only on the mathematical framework of self affine fractals, which is able to describe the scattering experiment on both isotropic and anisotropic clusters.

CPP 3.3 Mon 10:30 H47

Novel crystal phase in suspensions of hard ellipsoids — ●PATRICK PFLEIDERER and TANJA SCHILLING — Institut für Physik,

Johannes Gutenberg-Universität, Staudingerweg 7, 55099 Mainz

Hard ellipsoids serve as a popular model system for granular materials, and colloidal and molecular liquids, solids, and glasses. We present a Monte Carlo simulation study on the crystalline phases of hard ellipsoids of revolution. For aspect ratios ≥ 3 we have found a novel crystal, which replaces the previously suggested stretched-fcc phase [D. Frenkel and B. M. Mulder, *Mol. Phys.* **55**, 1171 (1985)]. The unit cell of the new solid contains two ellipsoids with unequal orientations. The lattice is simple monoclinic. The crystal possesses a rheological specialty: The angle of inclination of the lattice, β , is a very soft degree of freedom, while the two right angles are stiff. Further, we have determined that for one particular value of β , the close-packed version of this crystal is a specimen of the family of superdense packings recently reported [A. Donev et al., *Phys. Rev. Lett.* **92**, 255506 (2004)]. Our update of the phase diagram is relevant for studies of nucleation and glassy dynamics of colloidal suspensions of ellipsoids; the rheology may inspire new materials with tailor-made properties.

15 min. break

CPP 3.4 Mon 11:00 H47

Director Tumbling of Nematic Wormlike Micelles Under Shear: Time-Resolved Rheo-NMR Experiments — NIKOLAY SINYAVSKY¹, ISABEL QUIJADA-GARRIDO², and ●CLAUDIA SCHMIDT³ — ¹Department of Physics, Baltic State Academy, Molodiozhnaya str. 6, 36029 Kaliningrad, Russia — ²Instituto de Ciencia y Tecnologia de Polimeros, Consejo Superior de Investigaciones Científicas, Juan de la Cervera 3, 28006 Madrid, Spain — ³Department Chemie, Universität Paderborn, Warburger Str. 100, 33098 Paderborn, Germany

Nematic liquid crystals show a complex flow behavior due to the coupling between orientation and flow. Some materials show a stable director orientation in steady shear flow (flow aligning), while for others no stable director orientation exists (tumbling). Director tumbling gives rise to oscillations of shear and normal stresses in rheological experiments and can be detected by optical methods, for example by microscopy or birefringence measurements. We have used deuterium NMR spectroscopy to observe shear-induced director orientations [1,2]. In the lyotropic system cetylpyridinium chloride/hexanol/brine, which forms a nematic phase of wormlike micelles, time-resolved observations of the director orientation by means of deuterium NMR spectroscopy of D₂O have been possible for the first time. The time-dependence of the director orientations in both shear start-up and flow-reversal experiments will be presented.

[1] D. A. Grabowski, C. Schmidt, *Macromolecules*, **27**, 2632 (1994).

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

CPP 3.5 Mon 11:15 H47

Precise structure determination of ZnO and CdSe/ZnS

core-shell nanoparticles — ●FRANZISKA NIEDERDRAENK¹, KNUD SEUFERT¹, PAWEŁ LUCZAK¹, CHRISTIAN KUMPF¹, REINHARD NEDER², and EBERHARD UMBACH¹ — ¹Universität Würzburg, Experimentelle Physik II, Am Hubland, 97074 Würzburg — ²Universität Würzburg, Mineralogisches Institut, Am Hubland, 97074 Würzburg

In order to obtain an appropriate picture of very small nanoparticles (< 5 nm) and their properties a precise geometric structure determination is essential. X-ray diffraction, in principle, is well suited for this purpose. However, well established methods like powder diffraction including Rietveld refinement are not sufficiently reliable for very small particles, since they are based on solid state approaches. One alternative way is to model the entire nanoparticle and use the Debye formula for calculating its diffraction pattern. As this technique imposes no restrictions on the particle, intrinsic parameters like the particle shape, stacking faults or surface strain can easily be considered. Furthermore, modeling of core-shell particles and consideration of parameter distributions is enabled. Modeling of the nanoparticles, calculation of the diffraction pattern and ensemble averaging are embedded in an evolutionary algorithm for an automated fit procedure.

We present data obtained from ZnO particles and CdSe/ZnS core-shell particles. In order to test the sensitivity of individual parameters many different parameter combinations were considered for the ZnO system. For the core-shell particles we will demonstrate that the consideration of a shell is essential for obtaining proper fit results.

CPP 3.6 Mon 11:30 H47

Template-Directed Self-Assembly of Nanoparticles — ●ALEXANDER BÖKER, GÜNTHER JUTZ, NATHALIE MOUGIN, and SERGEJ KOUTOUZOV — Physikalische Chemie II, Universität Bayreuth, 95440 Bayreuth, Germany

We report on the general concept of nanoparticle self-assembly at templating interfaces. Inorganic cadmium selenide as well as organic particles like ferritin and cow pea mosaic virus (CPMV) are employed as building blocks for three-dimensional assemblies. The self-assembly kinetics is followed by in-situ GISAXS or pendant drop tensiometry depending on the type of interface. The resulting structures are imaged using cross sectional TEM. In addition, several methods (crosslinking, mineralization, etc.) are described to lock the particle assembly into place and construct mechanically robust nanoporous capsules and membranes which are characterized using TEM and SEM.

CPP 3.7 Mon 11:45 H47

Streuung weicher Röntgenstrahlung an freien Nanopartikeln — ●HARALD BRESCH¹, BURKHARD LANGER², BERHARD WASSERMANN¹, CHRISTINA GRAF¹, MATHIAS BARTHEL¹, ROMAN FLESC¹ und ECKHART RÜHL¹ — ¹Institut für Chemie und Biochemie, Freie Universität Berlin, Takustr. 3, 14195 Berlin — ²Max-Born-Institut für Nichtlineare Optik und Kurzzeitspektroskopie, Max-Born-Straße 2A, 12489 Berlin

Winkelaufgelöste Lichtstreuung an freien Nanopartikeln wird mittels Synchrotronstrahlung im Bereich weicher Röntgenstrahlung untersucht. Durch einen Aerosolgenerator werden Partikel, die in der flüssigen Phase mit Methoden der Kolloidchemie hergestellt werden, in die Gasphase überführt. Eine aerodynamische Linse erlaubt die Fokussierung des kontinuierlichen Teilchenstrahls im Hochvakuum auf die Synchrotronstrahlung. Mit diesem Ansatz kann Lichtstreuung an frei-

en Nanopartikeln ohne Kontakt zu einem Substrat unter Vermeidung von Strahlenschäden untersucht werden.

Zwei verschiedene Experimente wurden an gröbenselektierten SiO₂-Nanopartikeln durchgeführt: Winkelaufgelöste Lichtstreuung im Bereich der Innerschalenanregung, sowie energieaufgelöste Lichtstreuung, wobei der Detektor auf einen festen Winkel gestellt und die Photonenenergie im Bereich der Innerschalenabsorptionskante (Si 2p, O 1s) variiert wurde.

Es lassen sich mit hoher Genauigkeit Größenverteilungen aus den Experimenten ableiten. Der Einfluss des Brechungsindex und der Zusammensetzung der Oberfläche der Nanopartikel wird diskutiert.

CPP 3.8 Mon 12:00 H47

Smart Multifunctional Hybrid Microgels for Biological Applications — ●JORGE RUBIO-RETAMA, NIKOLAOS ZAFEIROPOULOS, and MANFRED STAMM — Leibniz-Institute für Polymerforschung e.V. Dresden

In summary, a simple chemical route to synthesize multifunctional smart microgels for bio-applications is discussed in the present study. Magnetic iron oxide nanoparticles were incorporated on the surface of P(NIPAM-AA) microgels rendering materials which are both magnetically and thermally responsive. SEM analysis revealed that the composite microgels have a dense "raspberry" type morphology, whilst TEM and SAED confirmed the presence of cubic gamma-Fe₂O₃ nanoparticles mostly on the surface of the microgels. SQUID experiments corroborated the results of SAED showing that indeed the iron oxide nanoparticles are superparamagnetic cubic gamma-Fe₂O₃. The incorporation of the iron oxide on the P(NIPAM-AA) microgels shifted their volume transition temperature from 36 to 40 °C, yielding a material that is biocompatible and potentially well suited as carrier for controlled drug release.

CPP 3.9 Mon 12:15 H47

Miniemulsionen als Basis hochgeordneter Nanopartikel-Ensembles und ihre Anwendung als Ätzmaste — ●ACHIM MANZKE¹, FABIAN ENDERLE¹, CHRISTIAN PFAHLER¹, ALFRED PLETTL¹, PAUL ZIEMANN¹, EYK SCHREIBER², DANIEL CRESPIY², ULRICH ZIENER² und KATHARINA LANDFESTER² — ¹Institut für Festkörperphysik, Universität Ulm, D-89069 Ulm — ²Institut für Organische Chemie III, Universität Ulm, D-89069 Ulm

Die Miniemulsionstechnik erlaubt die Herstellung kolloidaler Polystyrol-Partikeln in wässriger Lösung, die mit metallischen Precursoren beladen sind. Wir berichten über Kolloide und Kern-Schale-Kolloide mit Pt-Komplex-Beladung. Auf hydrophile Si/SiO_x-Substrate aufgetropft, bilden sich hexagonale hochgeordnete Partikel-Monolagen aus. Optimierte Plasma- und Temperprozesse erzeugen Pt-Nanopartikel unter Beibehaltung der ursprünglichen Ordnung. Die Größe der Partikel wird durch die Metallkonzentration im Kolloid bestimmt und konnte bisher zwischen 6 und 13 nm variiert werden. Diese neue Technik besitzt das Potential, die Grenzen der Mizellaren Technik [1] hinsichtlich Ordnung und Teilchenabstand deutlich zu übertreffen. Als Anwendung wird gezeigt, wie sich diese Nanopartikel als direkte oder invertierte Ätzmasten in RIE-Prozessen verwenden lassen.

[1] Micellar Nanoreactors - Preparation and Characterization of hexagonally ordered Arrays of Metallic Nanodots, G. Kästle et al. Adv. Funct. Mat. 13, 853 (2003).

CPP 4: Colloids and Nanoparticles II: Effective Interactions

Time: Monday 14:00–15:45

Location: H37

Invited Talk

CPP 4.1 Mon 14:00 H37

Direct measurement of critical Casimir forces — CHRISTOPHER HERTLEIN, LAURENT HELDEN, and ●CLEMENS BECHINGER — 2. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart

Similar to electromagnetic vacuum fluctuations which can induce long-ranged interactions between uncharged, conducting surfaces, a rather similar effect was predicted almost 30 years ago to occur in confined binary mixtures close to their critical point. This so-called critical Casimir effect has attracted considerable attention because it can strongly modify the interaction potential of colloidal particles immersed in a binary fluid. We present the first direct measurement of such critical Casimir forces between a colloidal particle and a flat

surface in a water - 2,6-lutidine mixture. With total internal reflection microscopy (TIRM) which is capable to resolve forces down to 5fN, we obtain distance resolved particle-wall interaction profiles. Upon approaching the critical point we observe long-ranged interactions which are attractive or repulsive depending on the specific boundary conditions of the walls. This behavior is in good agreement with recent theoretical predictions.

CPP 4.2 Mon 14:30 H37

Testing a morphological theorem for the solvation energy of non trivially shaped objects — ●FLORIAN PESTH and MARTIN OETTEL — Institute of Physics, Johannes Gutenberg-University, 55099 Mainz

For a given solvent, the grand potential in a finite volume in general depends in a complex way on the shape of the container, or alternatively, the solvation energy of a large solute depends in a similarly complex way on the shape of the molecule. A morphological theorem states [1], that if some physical restrictions are imposed on the container or the solute, the grand potential depends on only four quantities, namely the volume, the surface area, the integrated mean curvature and the Euler characteristic of the container or the solute. We test this theorem in an approach which combines integral equation methods with density functional theory which allows to calculate the solvation energy of large molecules. This appears to be relevant for applications of this morphological theorem to the configuration dependent solvation energy of macromolecules [2].

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

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

CPP 4.3 Mon 14:45 H37

Theoretical study of a liquid-vapor interface and effective interactions between colloids at interface — ●VITALIE BOTAN and MARTIN OETTEL — Institut für Physik, WA 331, Johannes-Gutenberg-Universität Mainz, D-55099 Mainz, Germany

We present a microscopic theory combined of integral equations and density functional theory to study the liquid-vapor interfacial properties of simple liquids. The asymptotic behavior of the density profiles, inhomogeneous two-body correlation functions and their implication for the surface tension are analyzed with respect to the mesoscopic capillary wave picture. In contrast to mean-field theories of the interface we observe fairly strong feedback of the pair correlation function to the density profile. The developed methods are applied to the study of interfacial effects in the effective interaction between colloids trapped at the interface.

CPP 4.4 Mon 15:00 H37

Structure of charged colloids in three dimensions and in films: How important is the salt ? — ●SABINE KLAPP^{1,2}, DAN QU¹, and REGINE VON KLITZING¹ — ¹Stranski-Laboratorium für Physikalische und Theoretische Chemie, Technische Universität Berlin — ²Institut für Theoretische Physik, Technische Universität Berlin

Using computer simulations and (hypernetted chain) integral equations we investigate the structure of charged colloidal suspensions in bulk and in spatial confinement (film geometry), focusing on the identification of characteristic length scales. The calculations are based on an effective description of the multicomponent colloidal suspension via a screened Coulomb (DLVO) potential between the macroions. The range of the interaction is controlled by the inverse Debye length κ determined by the concentrations of counterions and the ionic strength of additional salt (if present). Concerning bulk properties, we find that the commonly accepted power law $\xi \propto \phi^{-1/3}$ for the average particle

distance $\xi = 2\pi/q_{\max}$ in three spatial dimensions describes the results only for low ionic strength, that is for relatively long-ranged potentials characterized by small values of κ . On the other hand, systems with larger ionic strengths do not obey such power-law behavior and rather resemble an uncharged hard-sphere fluid, where the relevant length scale is the particle diameter. Similar observations hold in a film geometry. For both geometries, our results for suspensions with low salt concentration are in excellent quantitative agreement with experimental results for charged Silica particles.

S. H. L. Klapp, D. Qu, and R. v. Klitzing, J. Phys. Chem. B, in press.

CPP 4.5 Mon 15:15 H37

Effect of confinement on the structuring within colloidal suspensions: A comparison between theory and experiment —

●REGINE V. KLITZING, DAN QU, YAN ZENG, and SABINE KLAPP — TU Berlin, Stranski-Laboratorium, D-10623 Berlin

Small angle neutron scattering experiments at suspensions containing Silica particles show a structure peak which indicates interactions between the particles. The position of the structure peak scales with the concentration c with an exponent $1/3$. In order to study the effect of geometrical confinement the solutions are confined between a microsphere and a flat interface in a Colloidal-probe AFM. Oscillatory forces are measured due to layer-by-layer expulsion of the particles. The period has the same value as the particle distance in the corresponding bulk solution calculated from the position of the structure peak. The addition of salt reduces the amplitude, i.e. the ordering of the particles, and the scaling exponent of the particle distance in dependence of the concentration. The latter effect is observed for the first time. All results can be perfectly fitted by a theoretical model assuming a DLVO potential.

CPP 4.6 Mon 15:30 H37

A Pre-Wetting Transition on Colloidal Particles — ANDREAS ERBE¹, KLAUS TAUER², and ●REINHARD SIGEL² — ¹Institute of Physics, Academia Sinica, Taiwan — ²MPI of Colloids and Interfaces, D-14476 Golm

The salt concentration around charged colloidal particles is traditionally described by the Poisson-Boltzmann equation. Not predicted by this equation is a sudden transition to a layer of high salt concentration around the colloids when the average salt concentration is enhanced. This transition has been found experimentally by ellipsometric light scattering [1]. The observation is interpreted as a first order pre-wetting transition. The interactions stabilizing the layer of enhanced concentration as well as the extent and the softness of the layer are discussed. The pre-wetting by a highly concentrated salt solution can also explain an experimental finding for charged spherical brushes composed of polyelectrolytes around colloidal particles. Here, a concentration profile similar to uncharged spherical brushes is detected, instead of the stretched chain behavior predicted by theory.

[1] A. Erbe, K. Tauer, R. Sigel, Langmuir, in press.

CPP 5: Polymer Physics II

Time: Monday 14:30–15:45

Location: H40

CPP 5.1 Mon 14:30 H40

Characterizing knots in polymer coil and globule phases — ●PETER VIRNAU¹, MEHRAN KARDAR², and YACOV KANTOR³ — ¹Uni Mainz — ²Massachusetts Institute of Technology, Department of Physics — ³Tel Aviv University, School of Physics and Astronomy

We examine the statistics of knots with numerical simulations of a model polymer, spanning high temperature (coil) and low temperature (globule) phases. All monomers in the model interact via a Lennard-Jones potential, while adjacent beads are connected by flexible springs. Although relatively simple, this model provides a realistic description of polyethylene, thus relating the simulation results to specific polymers. We find that knots are common in the globule phase and under confinement, but rare in coils. We also associate a typical size with the knots, and find knots to be small (tight) in the swollen phase, and large (loose) in the dense phase.

CPP 5.2 Mon 14:45 H40

Dynamics of melts consisting of circular and linear polymers — ●MICHAEL LANG and MICHAEL RUBINSTEIN — Department of Chem-

istry, University of North Carolina at Chapel Hill, Venable Hall, 27599 Chapel Hill, N.C., United States of America

Recent experimental results indicate that small contaminations of linear polymers with 0.1% volume fraction or less in ring polymer melts lead to dramatic changes in the rheology of the melt. These volume fractions are clearly below overlap concentration of the linear species. Thus, the experimental observations cannot be explained by a simple picture based on a percolating cluster of linear chains penetrating rings. The goal of our computer simulation studies of comparable systems is to solve this puzzle. We use the bond fluctuation method on a lattice as introduced by Carmesin and Kremer (Macromolecules 21, 2819-2823 (1988)) to model homopolymer melts ranging from 32 to 1024 monomers per chain. The volume fraction of linear polymer is varied from $1/16$ to zero. We simulate small melts of 16384 monomers in order to have access to the long-time behavior of the samples. We will present and discuss simulation data on diffusion, ring and linear polymer conformations, mobility and contact statistics of different samples with varying volume fraction of linear polymer.

CPP 5.3 Mon 15:00 H40

On the influence of excluded volume in polymer melts — ●HENDRIK MEYER, JOACHIM WITTMER, and JÖRG BASCHNAGEL — Institut Charles Sadron, CNRS, 67083 Strasbourg, France

Flory's ideality hypothesis states that polymer chains in the melt have random walk like conformations as if there would be no excluded volume. However, it was shown recently that the excluded volume interaction induces corrections to scaling which are long range and which give rise to a power law decay of bond-bond correlation function [1] as well as to corrections to the Kratky plateau of the form factor [2]. In this presentation, we extend the study to dynamic quantities: The excluded volume potential is switched on gradually to study the crossover from phantom chains (representing perfect random walks described by the Rouse model) to real polymer melts. This gives evidence that subdiffusive behaviour found in contradiction to the Rouse model [3] is also caused by the excluded volume interaction.

[1] J. Wittmer, H. Meyer, J. Baschnagel et. al. Phys. Rev. Lett. **93** (2004) 147801.

[2] J. Wittmer et. al. cond-mat/0610359, cond-mat/0611322

[3] W. Paul, Chem. Phys. **284** (2002) 59.

CPP 5.4 Mon 15:15 H40

Untangling polymer systems: Structure prediction in polymer networks with quenched disorder — ●ABIGAIL KLOPPER¹, RALF EVERAERS², and CARSTEN SVANEBOG³ — ¹Max-Planck-Institut fuer Physik komplexer Systeme, Dresden — ²Laboratoire de Physique, Ecole Normale Supérieure Lyon, France — ³Department of Chemistry, University of Aarhus, Denmark

Highly concentrated liquids comprising long polymeric chains can undergo processes of cross-linking and entanglement, giving rise to intriguing macroscopic properties. The key ingredient is connective quenched disorder, which freezes the topology of the liquid in the form of a polymer network. The translational invariance in the system is spontaneously broken and the phase space is divided into disjoint ergodic regions.

Such behaviour is well-known from a large class of systems exhibit-

ing the so-called glassy phase, characterised by randomness and slow dynamics. This opens the door to an extensive analytic formalism for structure prediction in cross-linked polymer systems. By constructing a theoretical framework which makes use of simulation data, one can draw from these techniques without resorting to microscopic detail and otherwise unphysical assumptions. In the study presented, the spin-glass replica formalism is applied to data from molecular dynamics simulations of ideal non-interacting cross-linked polymer systems in order to describe neutron scattering measurements in interacting systems.

CPP 5.5 Mon 15:30 H40

The scattering of polymer gels and networks: Origin and relation to network structure — ●MICHAEL LANG¹ and JENS-UWE SOMMER² — ¹University of North Carolina, Department of Chemistry, Venable Hall, 27599 Chapel Hill, N.C., United States of America — ²Leibniz Institut für Polymerforschung Dresden e.V., Hohe Strasse 6, 01069 Dresden

We utilize computer simulations to directly relate connective and topological structure, density, and particle fluctuations with the scattering of polymer gels. We observe density fluctuations on three different length scales upon swelling independent of whether the original sample was homogeneous or heterogeneous in the dry state. The observed density fluctuations and length scales are a) dynamic fluctuations on the length scale of single monomers or substrands of the polymer chains due to thermal fluctuations, b) static density fluctuations on the length scale comparable to the size of prime network rings which result from network connectivity, and c) static density fluctuations on length scales larger than the size of network rings due to frozen in density fluctuations of the elastically active material, whereby origin, length scale, and amplitude of these longest fluctuations depend mostly on the preparation conditions of the sample. Connective and topological analysis, scattering curves, dynamic as well as static spatial density profiles, and the pair correlations of cross-links and polymers are compared and discussed with the results obtained from polymer solutions at the same concentrations.

CPP 6: Dynamics of Molecular Systems

Time: Monday 14:30–15:45

Location: H47

CPP 6.1 Mon 14:30 H47

Confinement effects on the molecular dynamics of thin polymer films — ●ANATOLI SERGHEI and FRIEDRICH KREMER — Universität Leipzig, Institut für experimentelle Physik I, Linnestr. 5, 04103 Leipzig

The molecular dynamics in thin films of polymers having different (linear, hyperbranched and dendritic) macromolecular architectures is discussed. Based on measurements by means of Broadband Dielectric Spectroscopy, capacitive scanning dilatometry and AC-calorimetry, the following issues are addressed: (i) What is the molecular mechanism of the confinement-effects? (ii) What role plays the macromolecular architecture in the dynamics of confined polymers? (iii) Do different experimental techniques deliver similar results when applied to investigate the dynamics of confined polymers? (iv) Does the presence of a free interface lead to shifts in the dynamics glass transition of thin polymer films? In order to address the last question, a novel experimental approach is demonstrated, which enables one to measure the molecular dynamics in ultra-thin organic layers having one free interface. [1] A. Serghei, F. Kremer, Phys. Rev. Lett. **91**, 165702 (2003). [2] A. Serghei et al., Phys. Rev. E **71**, 061801 (2005). [3] A. Serghei et al., Eur. Phys. J. E **17**, 199 (2005). [4] A. Serghei et al., J. Polym. Sci. B **44**, 3006 (2006). [5] A. Serghei, M. Tress, and F. Kremer, Macromolecules, in press (2006). [6] A. Serghei, and F. Kremer, Rev. Sci. Instrum. **77**, 116108 (2006).

CPP 6.2 Mon 14:45 H47

Low-temperature spectral dynamics of single TDI molecules in alkane matrixes — ●SEBASTIAN MACKOWSKI, STEPHAN WÖRMKE, MORITZ EHRL, and CHRISTOPH BRÄUCHLE — Department of Chemistry and Biochemistry and Center for Nanoscience, Ludwig-Maximilian-University, D-81377 Munich, Germany

We use vibronic excitation approach to study the low-temperature

(1.6K) fluorescence dynamics of the single TDI molecules in alkane matrixes. Four hosts were used, characterized with different length and parity: heptane, hexane, pentadecane and hexadecane. For every matrix, fluorescence trajectories of several tens of single molecules were measured. In the case of long-chain alkanes (pentadecane and hexadecane), the fluorescence of single TDI molecules has been found to be stable, showing only occasional spectral jumps of moderate energy (<10cm⁻¹). An average time between the jumps is 10 seconds and the jumps occur between well resolved levels. We have not observed any difference between the two matrixes. On the other hand, the spectral dynamics of TDI molecules embedded within the short-length alkane matrixes (heptane and hexane) is dramatically different. In these cases the spectral jumps are much more frequent, with average time between the two jumps being less than 1 second. In addition, we also observe significant, threefold increase in average energy of the jump. No qualitative differences between the two matrixes with short chain length were observed. The results suggest that matrixes composed of short chain molecules are more susceptible for translations and/or rotations which influence the spectral properties of single chromophores.

CPP 6.3 Mon 15:00 H47

The electronic structure and the hydrogen bond network of H₂O and D₂O studied by X-ray emission (XES) and X-ray absorption spectroscopy (XAS) in the soft X-ray range — ●MONIKA BLUM¹, OLIVER FUCHS¹, MARKUS WEIGAND¹, FLORIAN MAIER¹, EBERHARD UMBACH¹, LOTHAR WEINHARDT², MARCUS BÄR², CLEMENS HESKE², MICHAEL ZHARNIKOV³, MICHAEL GRUNZE³, and JONATHAN DENLINGER⁴ — ¹Universität Würzburg, Experimentelle Physik II, 97074 Würzburg — ²Dept. of Chem., University 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 H₂O, D₂O, NaOH and NaOD.

The molecular dynamics within the time scale of the core hole lifetime (a few femtoseconds) lead to isotope and temperature effects of the measured liquids in both, XES and XAS spectra. These effects can be analyzed by the comparison of the XES spectra of H₂O and D₂O. Two different species can thus be identified. The observed isotope, energy and temperature dependent effects can be explained by these species involving tunneling processes within the hydrogen bond network.

CPP 6.4 Mon 15:15 H47

Investigation of the electronic structure of NH₃ and ND₃ in aqueous solution using x-ray absorption spectroscopy (XAS) and resonant inelastic x-ray scattering (RIXS) — ●M. WEIGAND¹, O. FUCHS¹, M. BLUM¹, F. MAIER¹, E. UMBACH¹, L. WEINHARDT², M. BÄR², C. HESKE², M. ZHARNIKOV³, M. GRUNZE³, and J. DENLINGER⁴ — ¹Universität Würzburg, Experimentelle Physik II, 97074 Würzburg — ²Dept. of Chem., University of Nevada, Las Vegas — ³Ang. Phys. Chemie, Uni Heidelberg — ⁴ALS, Berkeley

Soft x-ray spectroscopy of aqueous solutions at the carbon-, nitrogen- and oxygen-edge is a promising technique to investigate the electronic structure of biological systems in natural environment. Precise measurements require the use of a flow-through liquid cell to ensure thermodynamic equilibrium and to reduce beam-induced damage effects. Hitherto used Si₃N₄-windows denied access to the N-edge and showed contaminations limiting the viability of spectroscopy of solutions at the C- and O-edge. Using new ultra-thin SiC-membranes, the N-edge energy window is now open to measurements.

NH₃ and ND₃ provide an excellent test system to study the influence of H-bonds in aqueous solution, providing complementary information compared to the O-edge of H₂O and D₂O, which is currently in the focus of extensive investigations. XAS showed pronounced differences to the gas phase as well as strong isotopic effects, mirroring the behaviour of the water O-edge. RIXS results demonstrate excellent membrane properties and provide evidence of spectator and shake-up processes in NH₃ solutions.

CPP 6.5 Mon 15:30 H47

²H-NMR-Untersuchungen an hochdichtem amorphem Eis — ●MARCO SCHEUERMANN¹, BURKHARD GEIL², KATRIN WINKEL³ and FRANZ FUJARA¹ — ¹Institut für Festkörperphysik, TU Darmstadt, Hochschulstr. 6, 64289 Darmstadt — ²Lehrstuhl für Experimentelle Physik III, Universität Dortmund, Otto-Hahn-Str. 4, 44221 Dortmund — ³Allgemeine, Anorganische & Theoretische Chemie Universität Innsbruck, Innrain 52a, A-6020 Innsbruck, Österreich

In dieser Arbeit¹ werden ²H-Spin-Gitter-Relaxationsmessungen in Abhängigkeit von der Temperatur an den amorphen Eisformen Low-Density Amorphous (LDA), High-Density Amorphous (HDA) und Very-High-Density Amorphous (VHDA) vorgestellt. Die T₁-Relaxationszeiten werden als Monitor-Parameter verwendet, um die Kinetik der Übergänge von HDA nach LDA und VHDA nach LDA bei ambientem Druck zu untersuchen. Die Übergangstemperaturen von 108 K (HDA/LDA) und 120 K (VHDA/LDA) stimmen mit den Ergebnissen aus Neutronen-Streu-Experimenten überein². Im Übergang von VHDA nach LDA wird ein Zwischenzustand identifiziert, dessen dynamische Eigenschaften denen des HDA gleichen. Dieser HDA-ähnliche Zustand tritt jedoch bei Temperaturen auf, die höher sind als die Stabilitätsgrenze von HDA.

¹M. Scheuermann et al, J. Chem. Phys. 124, 224503 (2006)

²M. Koza et al, Phys. Rev. Lett. 94, 125506 (2005)

CPP 7: POSTER: INTERNAL SYMPOSIUM Scattering Experiments

Time: Monday 16:00–18:00

Location: Poster B

CPP 7.1 Mon 16:00 Poster B

Electric field effects on alignment of lamellar structures in diblock copolymer thin films studied by neutron scattering — ●XU LI 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

Self-assembled block copolymers have attracted much attention in recent years for their potential use as nanostructure templates. In this context, it is of interest to control the order and orientation of block copolymer thin films by means of external electric fields. In order to gain additional understanding of the alignment process, we studied the effect of a weak electric field on a lamellar microphase structure oriented perpendicular to the electric field by neutron diffuse scattering in reflection geometry. It has been predicted that the electric field induces periodic structural undulations which lead to a disruption of the original structure and facilitate reorientation to set in. In our experiments on lamellar PS-PMMA block copolymers these field-induced undulations were not observed. Rather, already after preparation the films displayed a diffuse intensity interpreted as corresponding to a mosaic structure of domains with a typical correlation length of about 1-2 μm. This diffuse intensity increases after the application of the field, even if the field is too weak to induce alignment. The lateral length scale of the mosaicity remains unaffected by the electric field.

CPP 7.2 Mon 16:00 Poster B

Extending the possibilities of a Kratky-Compact-Camera by use of focussing multilayer X-ray optics — ●THOMAS HENZE, KLAUS SCHRÖTER, and THOMAS THURN-ALBRECHT — Martin-Luther-Universität Halle-Wittenberg, Institut für Physik, Polymerphysik

The use of focussing multilayer x-ray optics in laboratory x-ray equipment offers the potential of a substantial gain in primary beam intensity without a significant loss of resolution. We present the result of a refurbishment of Kratky-Compact-Camera, a classical setup for small angle x-ray scattering on isotropic samples, with an elliptically bent focussing multilayer. The advantages of the Kratky collimation system are ease of alignment, high intensity and low background. A further

gain in intensity is highly desirable for time dependent experiments as well as for measurements of weakly scattering samples. The performance of the revised setup is analyzed quantitatively by comparing intensity and full width at half maximum of the primary beam, as well as the minimal accessible scattering vector with the corresponding parameters of the simple setup without optics. A gain in intensity of a factor of 2 up to 10 is achieved, depending on the details of the alignment. In addition the multilayer produces a monochromatic beam. First measurements on exemplary polymer systems are shown.

CPP 7.3 Mon 16:00 Poster B

Structural investigation of casein micelles in thin films — ●E. METWALLI¹, R. GEBHARDT¹, A. TOLKACH², J.-F. MOULIN¹, V. KÖRSTGENS¹, S.V. ROTH³, R. CUBITT⁴, and P. MÜLLER-BUSCHBAUM¹ — ¹Physikdepartment E13, TU München, 85747 Garching. — ²Chair for Food Process Engineering and Dairy Technology, TU München, Weihenstephan — ³HASYLAB at DESY, Hamburg — ⁴Institut Laue-Langevin, Grenoble, France

Casein micellar films on solid supports have interesting applications in labeling of glass containers and adhesion technology. Gaining structural information on these films will help to optimize the appropriate physical properties for the desired application. Casein micelles thin films were applied from aqueous solutions on pre-cleaned glass slides by spin coating technique. The effect of transglutaminase enzyme concentrations on the thin film structures was investigated using atomic force microscopy (AFM) and grazing incidence small-angle X-ray scattering (GISAXS). The AFM images can only give information on the top surface structure with low statistical significance. In contrary, GISAXS provides information on the in-plane structures of the casein thin film with much higher statistical significance. The GISAXS data on the thin films were compared with those obtained by dynamic light scattering from the solution phase. The swelling behavior of some selected casein films in deuterated water vapor was also investigated using grazing incidence small-angle neutron scattering (GISANS). The results were discussed and compared with various proposed models on the casein micelle structures.

CPP 7.4 Mon 16:00 Poster B

Dielectric and neutron spectroscopy on nano-confined liquid crystals — STEFAN FRUNZA¹, LIGIA FRUNZA¹, ●ANDREAS SCHOENHALS², MARIA MAYOROVA³, REINER ZORN³, and BERNHARD FRICK⁴ — ¹National Institute of Materials Physics, R-76900-Bucharest-Magurele — ²Federal Institute for Materials Research and Testing (BAM), — ³Research Center Jülich, Institute for Solid State Research, D-52425 Jülich — ⁴Institut Max von Laue - Paul Langevin, B.P. 156, F-38042 Grenoble

The liquid crystals E7 and 8CB are confined to the nanopores of the molecular sieve Al-MCM-41 with a mean diameter of the pores of 2.5 nm. Dielectric spectroscopy shows that for the confined system one relaxation process is observed. Its characteristic relaxation time is much lower compared to that of the bulk. The temperature dependence of the relaxation time of this relaxation process shows some similarities to glassy dynamics. Moreover excess contributions to the vibrational densities of state (Boson-Peak) were found by neutron scattering using the time-of-flight spectrometer IN4 at the ILL in Grenoble. The Boson-Peak is a characteristic feature of glassy behaviour. In addition elastic scans are carried out at the backscattering spectrometer IN10 (ILL) These measurements show a signature for glass transition.

CPP 7.5 Mon 16:00 Poster B

Influence of spacer length and density on the vertical structures of supported membranes studied by neutron reflectivity — ●PETER SEITZ¹, OLIVER PURRUCKER², ANTON FÖRTIG³, RAIMUND GLEIXNER⁴, GIOVANNA FRAGNETO⁵, RAINER JORDAN³, and MOTOMU TANAKA^{1,2} — ¹Physikalisch-Chemisches Institut, Universität Heidelberg, Germany — ²Physik-Department E22, Technische Universität München, Germany — ³Institut für Technische Chemie, Technische Universität München, Germany — ⁴Max Planck Institute of Biochemistry, Martinsried, Germany — ⁵Institut Laue-Langevin, Grenoble, France

We studied the structure of a new class of polymer-supported membranes, which are separated from the solid substrate via poly(2-methyl-2-oxazoline) spacers of defined length, functionalized with a surface coupling group and hydrophobic membrane anchors. The proximal leaflet was deposited via Langmuir-Blodgett transfer, followed by vesicle fusion to deposit the distal layer. Precise control of the polymer chain length and its lateral density enables the quantitative adjustment of the thickness and the viscosity of the polymer interlayer. Previously, we measured the membrane-substrate distance with fluorescence interference contrast microscopy (FLIC). To gain a deeper insight to the vertical structure of the membrane, we conducted specular neutron reflectivity experiments under a systematic variation of the spacer length and density, and calculated the static roughness and the volume fraction of water in the polymer interlayer.

CPP 7.6 Mon 16:00 Poster B

Formation of lateral structures in thin diblock copolymer films by vapor treatment — ●CHRISTINE PAPADAKIS¹, PETER ČERNOCH², CHARLES DARKO¹, EZZ METWALLI¹, PETR ŠTĚPÁNEK², DETLEF-M. SMILGIES³, and STEPHAN V. ROTH⁴ — ¹Physikdepartment E13, TU München, James-Frank-Str. 1, 85747 Garching — ²Inst. Macromoleculare Chemistry, Prague, Czech Republic — ³Cornell University, Ithaca NY, USA — ⁴HASYLAB at DESY, Hamburg

Diblock copolymers in the melt spontaneously self-organize into mesoscopically ordered structures. In order to understand their response to changes of the environment, in-situ and real-time methods are of great value. We have performed grazing-incidence small-angle X-ray scattering (GISAXS) measurements on thin films of poly(4-octylstyrene-*b*-butyl methacrylate) (OB) and poly(4-octylstyrene-*b*-methyl methacrylate) (OM) before and after vapor treatment with different solvents. In the bulk, OB is lamellar, whereas OM forms connected struts [1]. The solvent quality and selectivity were found to have a strong influence on the inner film structure. Solvents which are poor for one block and good for the other block preferentially lead to the formation of lateral structures. Time-resolved in-situ GISAXS measurements allowed us to follow the formation of lateral structures in the vapor, giving insight into the time scales and the mechanisms involved.

1. P. Černoch, P. Štěpánek et al., Eur. Polym. J., accepted.

CPP 7.7 Mon 16:00 Poster B

Recent developments at BW4 / HASYLAB — ●A. TIMMANN, S.V. ROTH, R. GEHRKE, S. HU, F.-U. DILL, M. DOMMACH, R. DÖHRMANN, and T. SCHUBERT — HASYLAB at DESY, Notkestr. 85, D-22607 Hamburg, Germany

The beamline BW4 of HASYLAB, Hamburg (Germany), is a dedicated materials science beamline [1]. The main experimental techniques used are transmission small-angle x-ray scattering (TSAXS) and grazing-incidence SAXS (GISAXS). With the implementation of the microfocus option at BW4 scanning experiments have become possible [1]. After the major refurbishment of the beamline in 2004 and 2005, we focussed on upgrading and introducing necessary sample environments. This includes a new stretching cell allowing to draw film shaped samples to elongations up to 640mm with drawing velocities from 0.1 up to 1200 mm/min keeping the beam position on the sample fixed. Presently, several force sensors with a measuring range up to 500N are available now, which will be upgraded to 1kN. For GISAXS, a heating stage for polymeric samples has been commissioned. In-situ sample observation is now possible with a high-resolution video camera. Based on recent experimental results, we present the upgraded capabilities of BW4.

[1] S.V. Roth et al., Rev. Sci. Instr. 77, 085106 (2006)

CPP 7.8 Mon 16:00 Poster B

Structure and changes of thin block copolymer films during vapor treatment — ●ZHENYU DI¹, CHRISTINE PAPADAKIS¹, DORTHE POSSELT², and DETLEF-M SMILGIES³ — ¹Physikdepartment E13, TU München, 85747 Garching, Germany — ²IMFUFA, Roskilde University, Denmark — ³CHESS, Cornell University, Ithaca NY, USA

The mesoscopic structures formed by diblock copolymers in thin film geometry are interesting for a variety of applications. However, self-assembly leads to domain structures with domain walls and defects. Vapor treatment has been shown to be an efficient way to increase the long-range order.

We have studied the structural changes in thin films of poly(styrene-*b*-butadiene) (PS-PB) diblock copolymers and their kinetics during vapor treatment. In this system, the initial lamellar orientation (parallel or perpendicular) can be controlled by the block copolymer molar mass [1]. We have investigated both initial orientations as well as the influence of the solvent selectivity and the film thickness. In-situ grazing-incidence small-angle x-ray scattering (GISAXS) is ideally suited because of its good time resolution (~sec) [2]. We found that in addition to swelling of the films, lamellar reorientation takes place on the time scale of minutes. Complex processes and transient states were encountered. In some cases, improved long-range order was achieved.

[1] P. Busch, D. Posselt, D.-M. Smilgies, C.M. Papadakis et al. Macromolecules 36, 8717 (2003) and Macromolecules, in press.

[2] D.-M. Smilgies, P. Busch, C.M. Papadakis, D. Posselt, Synchr. Rad. News 15(5), p. 35 (2002).

CPP 7.9 Mon 16:00 Poster B

Thin films of diblock copolymers having one crystalline block — ●CHARLES DARKO¹, EZZELDIN METWALLI¹, IOAN BOTIZ², GÜNTER REITER², DAG W BREIBY³, STEPHAN V ROTH⁴, DETLEF-M SMILGIES⁵, and CHRISTINE M PAPADAKIS¹ — ¹Physikdepartment E13, TU München, James-Frank-Str. 1, D-85747 Garching — ²Institut de Chimie de Surfaces et Interfaces, CNRS, Mulhouse, France — ³Niels Bohr Institute, University of Copenhagen, Denmark — ⁴HASYLAB at DESY, Hamburg — ⁵CHESS, Cornell University, Ithaca NY, USA

In thin films of semicrystalline diblock copolymers, the final structure formed depends on the competition between (i) the order-disorder transition of the diblock copolymer, (ii) the crystallization of the crystallisable block, and (iii) the vitrification of the amorphous block. We have studied lamellae-forming poly(styrene-*b*-ethylene oxide) diblock copolymers differing in molar mass. Combining grazing-incidence small and wide-angle X-ray scattering with high-resolution grazing-incidence X-ray diffraction, we obtain information on the inner structures on a large range of length scales and can compare them to the surface textures from optical and atomic-force microscopy. For the lowest molar mass sample, we find that the surface textures are different from the ones of poly(ethylene oxide) homopolymer films and that, depending on crystallization temperature, confined crystallization or breakout occur.

CPP 7.10 Mon 16:00 Poster B

The microfocus SAXS/WAXS beamline at PETRA III / DESY — ●S.V. ROTH, R. DÖHRMANN, H. FRANZ, R. GEHRKE, U. HAHN, R. RÖHLSBERGER, H. SCHULTE-SCHREPPING, N. SCHWARZ, and E. WECKERT — HASYLAB at DESY, Notkestr. 85, D-22607 Hamburg, Germany

Among the first beamlines to be built at PETRA III is the microfo-

cus small- and wide-angle x-ray scattering beamline μ SAXS/WAXS. This beamline will exploit the excellent photon beam properties of the low emittance source PETRA III to provide micro- and nanofocused beams in dedicated end-stations with ultra-high intensity and resolution in real and reciprocal space. Targeting at scanning investigations at multiple length scales, the areas of research include in-situ experiments as well as brilliance demanding novel methods like microbeam grazing incidence small-angle x-ray scattering (μ GISAXS) [1] and microbeam SAXS tomography [2]. The current layout foresees a large-offset double crystal monochromator and compound refractive on-axis optics for microfocusing. The projected beam sizes for routine user operation range from 110nm-40 μ m. The design of the beamline especially allows for combining ultra small-angle x-ray scattering (USAXS) with a microfocused beam (μ USAXS). We will present the present layout of the μ SAXS/WAXS beamline introducing the projected capabilities of this new micro- and nanofocus scattering beamline at PETRA III.

[1] S.V. Roth et al., Appl. Phys. Lett. 88 (2006) 021910

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

CPP 7.11 Mon 16:00 Poster B

High Pressure SAXS/WAXS using a Diamond Anvil Cell — ●RONALD GEBHARDT, MANFRED BURGHAMMER, MICHAEL HANFLAND, MOHAMED MEZOUAR, and CHRISTIAN RIEKEL — European Synchrotron Radiation Facility, B.P. 220, F-38043 Grenoble Cedex, France

The possibility of using a diamond anvil cell for SAXS/WAXS studies on small confined volumes has been explored at the ESRF ID13 beamline. As a demonstration experiment, single potato starch granules were pressurized up to 700 MPa at 20°C. In this pressure range a two-phase process was proposed (1,2). Scanning SAXS/WAXS experiments were performed with an about 1 micron beam. A Raman spectrometer was used to determine the pressure from the ruby fluorescence. The experimental setup is explained and first experimental results are shown. 1) Svensson E., Eliasson A. C. (1995) Carbohydrate Research, 26, 171-176 2) Rubens P., Heremans K. (2000) Biopolymers, 54, 524-530

CPP 7.12 Mon 16:00 Poster B

Spin-Echo Neutron Reflectivity on Diblock-Copolymer Films — ●MAX NÜLLE, ADRIAN RÜHM, MARTON MAJOR, JÁNOS MAJOR, and HELMUT DOSCH — Max Planck Institut für Metallforschung, Heisenbergstr. 3, 70569 Stuttgart

SERGIS (Spin-Echo Resolved Grazing Incidence neutron Scattering) is a recently developed novel neutron scattering technique which we employ at the new neutron/X-ray 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 yields novel information about both equilibrium and time-dependent phenomena on these length scales. As an example, we employ SERGIS to study morphologies produced by dewetting phenomena in thin polymer films. These experiments are complemented by detailed atomic force microscopy investigations. First results on thin diblock-copolymer films will be presented.

CPP 7.13 Mon 16:00 Poster B

Ellipsometric Light Scattering: The Spectroscopic Approach — ●ARNE STARK¹, ANDREAS ERBE², KLAUS TAUER¹, and REINHARD SIGEL¹ — ¹MPI of Colloids and Interfaces, D-14476 Golm — ²Institute of Physics, Academia Sinica, Taiwan

We present first results obtained by Spectroscopic Ellipsometric Light Scattering (SELS). The discussion is complemented by an analysis of the general robustness of ELS against polydispersity effects.

Ellipsometric light scattering is based on Mie theory to analyze the scattering of polarized light by suspended particles in the colloidal range. Similar to standard ellipsometry this technique has an enhanced sensitivity to interface effects, allowing to investigate e.g. (multiple) coatings on particles or adsorbed surface layers.

First experimental results obtained with a multi-wavelength apparatus are presented: augmenting the method to a spectroscopic technique extends the resolution considerably. The camera detector allows a simultaneous investigation of a range of scattering angles and speeds up the measurements. Light of different wavelengths is selected by

interference filters from a mercury lamp. Thus, it is established experimentally that coherence of the light source is not required.

All ellipsometric methods yield ratios of eigenvalues of the optical system under investigation. Consequently ELS exhibits an averaging behavior that is distinctly different from normal static light scattering. It is shown theoretically and experimentally that information regarding structural details of the suspended particles is robustly preserved in the presence of moderate sample polydispersity.

CPP 7.14 Mon 16:00 Poster B

Polymer coated micro mechanical cantilever arrays — ●SEBASTIAN K. NETT^{1,2}, GUNNAR KIRCHER¹, and JOCHEN S. GUTMANN^{1,2} — ¹Max Planck Institute for Polymer Research, Ackermannweg 10, D-55128 Mainz, Germany — ²Institute for Physical Chemistry, Johannes Gutenberg University, Jakob-Welder-Weg 10, D-55099 Mainz

Functional layers can turn micro mechanical sensors consisting of an array of eight cantilevers into specific sensing systems for chemical or biological applications. We showed before that tethered polymers are robust and sensitive for analytes. To access individual cantilevers inkjet printing is a versatile approach. Using the automatic pipetting system, Nano-PlotterTM (GeSiM) the solution for tethering is applied contact less in small droplets directly onto the cantilever. Small droplets tend to evaporate in a few seconds. On the other hand anchoring the molecules to the surface need some time due to kinetic and diffusion processes. Therefore room temperature Ionic Liquids which have a negligible vapour pressure are incorporated in the coating step. The small geometry of the cantilever (500 to 1000 μ m length, 90 μ m width, 1 to 5 μ m of thickness) rises problems with the standard techniques for characterising the functional layer. To overcome these characterization problems, we used the μ -focus option at the GISAXS Line BW4 at the HASYLAB in Hamburg for detailed studies.

CPP 7.15 Mon 16:00 Poster B

Investigation of lubrication in natural joints by neutron reflectometry — ●THOMAS KALTOFEN¹, THOMAS GUTBERLET², MAXIMILIAN WOLFF³, ROLAND STEITZ⁴, and REINER DAHINT¹ — ¹Angewandte Physikalische Chemie, Universität Heidelberg — ²Paul-Scherrer-Institut, Villigen, Schweiz — ³Experimentalphysik IV - Festkörperphysik, Universität Bochum — ⁴Hahn-Meitner-Institut, Berlin

Despite their high medical relevance, the principles of lubrication in natural joints are still unclear. It is generally accepted, that the presence of hyaluronic acid (HA), the main component of the synovial liquid, plays an important role for the low friction observed. Furthermore, it is assumed that surface active lipids participate in the lubrication. Using a model system of lipid bilayers deposited on a polyelectrolyte (PE) cushion and in contact with HA solution, we started to investigate the effects of pressure and shear forces, as experienced by natural joints, on the internal structure of the SiO₂/PE/lipid/HA interface and the bulk HA solution by neutron reflectometry (NR), complemented by in situ ellipsometry and quartz crystal microbalance (QCM-D) measurements. Only on positively charged polyelectrolyte surfaces, the successful build-up of the model system could be demonstrated. By NR, the existence of an irreversibly absorbed, highly hydrated HA layer on top of the lipid membrane was proven. For shear rates above 2.5 min⁻¹ a swelling of the HA layer has been observed. Pressure dependent studies are presently underway.

CPP 7.16 Mon 16:00 Poster B

Influence of degree of branching in LLDPE on its physical properties — ●STEFAN FISCHER¹, DIETER MEINHARDT², BERNHARD RIEGER², and OTHMAR MARTI¹ — ¹Institute of Experimental Physics, University of Ulm, 89069 Ulm, Germany — ²Institute of Inorganic Chemistry II, University of Ulm, 89069 Ulm, Germany

Novel metallocene catalysts allow the polymerization of linear low density polyethylene (LLDPE) with controlled molecular weight directly from ethylene without the need for (more expensive) higher alkanes [1]. The influence of the degree of branching and the molecular weight on the physical properties has been analyzed with several methods, including tensile tests, AFM (atomic force microscopy), DSC (differential scanning microscopy), WAXS (wide angle x-ray scattering) and SAXS (small angle x-ray scattering). The LLDPE samples have been compared with commercially available high and low density polyethylenes (HDPE and LDPE). The results will be presented.

[1] Dieter Meinhard, Marcus Wegner, Georgy Kipiani, Andrew Hearley, Peter Reuter, Stefan Fischer, Othmar Marti and Bernhard Rieger;

JACS; submitted

CPP 7.17 Mon 16:00 Poster B

Modelling the structure of fillers in rubber and their small angle scattering — ●KLAUS NUSSER, GERALD JOHANNES SCHNEIDER, and DIETMAR GÖRITZ — Universität Regensburg, Universitätsstr. 31, 93053 Regensburg

Silicas are technically important fillers for elastomers with respect to several applications. In such a filler-rubber system the mechanical properties strongly depend on the kind and the concentration of the filler. Despite being crucial for the adjustment of high performance materials, the exact correlation between the morphology of the filler and the related reinforcement of the material is still unknown.

An up-to-date constitutive model suggests that isotropic silica primary particles form fractal clusters, which work as a basic unit for larger cluster structures. This notion was gained by the analysis of small angle X-ray scattering curves, which show regions of constant slope in a log-log plot. However, conclusions from scattering curves are not unique. In order to examine the assumptions made in constitutive models, numerical investigations were performed. Scattering structures were generated and their scattering curves were calculated by means of a computer. In particular, the origin of regions of constant slope in log-log depicted scattering curves was investigated.

CPP 7.18 Mon 16:00 Poster B

Side chain crystallization in soft and rigid confinement — ●E. HEMPEL¹, H. BUDE², M. HAHN², and M. BEINER¹ — ¹Martin-Luther-Universität Halle-Wittenberg, Institut für Physik, D-06099 Halle (Saale), Germany — ²Fraunhofer Pilotanlagencentrum für Polymer-synthese und -verarbeitung, Value Park, Bau A74, D-06258 Schkopau, Germany

The side chain crystallization of poly(*n*-octadecyl methacrylate) [PODMA] under confinement is studied in a series of microphase-separated block copolymers containing PODMA cylinders with diameters in the range 10-20nm. The glass temperature of the matrix is systematically varied in the range 50...-30°C by choosing amorphous poly(*n*-alkyl methacrylates) with three to eight alkyl carbons per side chain as second component of the block copolymer. Since the crystallization temperature of the PODMA block is about 25°C crystallization occurs either in a glassy or in a highly viscous environment. The influence of the matrix properties on crystallization kinetics and internal structure of the PODMA domains is investigated by DSC and X-ray scattering. A central question of this study is whether or not the block copolymer morphology is changing due to side chain crystallization in the PODMA domains under conditions where the matrix material is soft and chemically not too different from the crystallizable component.

CPP 7.19 Mon 16:00 Poster B

Reversible Tuning of Block Copolymer Domain Spacings via Electric Fields — ●KRISTIN SCHMIDT¹, HEIKO SCHOBERTH¹, HELMUT HÄNSEL¹, THOMAS WEISS², VOLKER URBAN³, 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 Lab (ORNL), Oak Ridge, TN 37831, USA

We investigate the influence of electric fields on the domain spacing of a lamellar forming diblock copolymer solution by time-resolved synchrotron small angle X-ray scattering. As a model system we use a polystyrene-*b*-polyisoprene block copolymer dissolved in toluene or tetrahydrofuran. We find a significant dependence of the characteristic spacing on the electric field strength. For lamellae aligned parallel to the electric field direction we observe a decreasing lamellar distance with increasing field strength, while for perpendicularly orientated lamellae the domain size is increasing. We investigate the influence of the electric field strength, the degree of phase separation, molecular weight, composition and the polarity of the solvent. Furthermore we monitor the relaxation kinetics and show the reversibility of the changes in domain spacing on application and turn off of the electric field.

CPP 7.20 Mon 16:00 Poster B

Scaling behavior of the reorientation kinetics and changes in the phase behavior of block copolymers exposed to electric fields — ●HEIKO G. SCHOBERTH¹, KRISTIN SCHMIDT¹, THOMAS M. WEISS², AGUR SEVINK³, ANDREI V. ZVELINDOVSKY⁴, 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 — ³Leiden Institute of Chemistry, Universiteit Leiden, The Netherlands — ⁴Department of Physics, Astronomy & Mathematics, University of Central Lancashire, Preston PR1 2HE, United Kingdom

We have followed the reorientation kinetics of various block copolymer solutions exposed to an external electric DC field by time-resolved synchrotron small-angle X-ray scattering (SAXS). The characteristic time constants follow a power law indicating that the reorientation is driven by a decrease in electrostatic energy. Moreover, the observed exponent suggests an activated process in line with the expectations for a nucleation and growth process. When properly scaled, the data collapse onto a single master curve spanning several orders of magnitude both in reduced time and in reduced energy. The power law dependence of the rate of reorientation derived from computer simulations based on dynamic density functional theory (MesoDyn) agrees well with the experimental observations. In addition, we observe an influence of the electric field on the order disorder temperature and phase separation in our block copolymer solutions. For further investigations we study this effect by birefringence and SAXS.

CPP 7.21 Mon 16:00 Poster B

Characterisation of structural changes during deformation and relaxation of semi-crystalline polymers by SAXS — ●KONRAD SCHNEIDER¹ and PETER BÖSECKE² — ¹Leibniz-Institut für Polymerforschung Dresden, Hohe Str. 6, 01069 Dresden — ²European Synchrotron Radiation Facility (ESRF), BP 220, F38043 Grenoble, France

Time resolved small angle x-ray scattering using synchrotron radiation allows to follow up structural changes during deformation and relaxation of semi-crystalline polymers. On the example of polypropylene as well as high-density polyethylene copolymers the changes of the structure in the crystalline and in the amorphous domains were followed during the three characteristic stages of the load-displacement curves: The elastic stage and the plastic range composed of the stage of the lowering load in the force-displacement-curve (yielding) and the strain hardening. It is found that most rigorous changes are observed during yielding, whereas changes on a scale of second during relaxation are more pronounced than during the loading steps.

CPP 7.22 Mon 16:00 Poster B

Upgrades of two SANS diffractometers at the Munich reactor FRM-II — ●HENRICH FRIELINGHAUS, AUREL RADULESCU, PETER BUSCH, VITALY PIPICH, ALEXANDER IOFFE, DIETMAR SCHWAHN, and DIETER RICHTER — Forschungszentrum Jülich GmbH, Jülich Centre of Neutron Science, D-52425 Jülich

Political decisions made the Jülich reactor FRJ-2 shut down, and the high performance instruments are moved to Munich now. The two SANS diffractometers are transferred, and refurbished in a second step in order to meet the world leading machines. Neutron polarization and polarization analysis will be possible to study magnetic samples. Supermirrors and ³He filters will be installed. Aspherical neutron MgF₂ lenses aim at two goals: 10 to 20 times higher intensity and a resolution of $\Delta Q = 10^{-4} \text{ \AA}^{-1}$. The lenses will be cooled to minimize the thermal diffuse scattering. A high resolution detector ($\Delta x = 0.5 \text{ mm}$) allows to collect the high resolution scattering patterns. To operate with high resolution at finite *Q* a chopper placed behind the selector will reduce the wavelength uncertainty to 1% and better by a TOF analysis. The newly developed TiSANE mode will be possible: The neutron pulses will be triggered by a periodic external field at the sample in concert with the projected time-dependent scattering collected by the detector. We expect to resolve kinematic processes in the range of 2μs to 5ms and above. In this mode the *Q*-resolution typically is not improved. The GISANS option allows to study the lateral structure of thin films in the range of 10 to 1000Å with a free depth resolution. Here we aim at soft condensed matter and magnetic films.

CPP 7.23 Mon 16:00 Poster B

Focusing-mirror ultra-small-angle neutron scattering (US-ANS) instrument of Research Centre Jülich at FRM-2 Reactor — EMMANUEL KENTZINGER¹, ●AUREL RADULESCU^{1,2}, ALEXANDER IOFFE^{1,2}, PETER-PAUL STRONCIWILK^{1,2}, JÖRG STELLBRINK¹, DIETMAR SCHWAHN¹, THOMAS BRÜCKEL^{1,2}, and DIETER RICHTER^{1,2} — ¹Institute for Solid State Research, Research Centre Jülich, 52425 Jülich, Germany — ²Jülich Centre for Neutron Sciences (JCNS), Research Centre Jülich, 52425 Jülich, Germany

Biological, colloidal and macromolecular samples presenting characteristic length scales from nanometer up to micron-scale are usually investigated by combining USANS at double-crystal diffractometers (DCD) and SANS at conventional pinhole cameras. In principle, the Q-range of both classes of instruments overlaps but the required instrumental settings push both techniques to their limits, mainly due to signal-to-noise level and the reduced flux at sample position. The KWS3 USANS instrument of Research Centre Jülich is the worldwide unique instrument running on the principle of a one-to-one image of an entrance aperture on a two-dimensional position sensitive detector by neutron reflection from a double-focusing toroidal mirror. The instrument is just relocated at the FRM-2 reactor in Garching where it will permit to perform SANS studies within a Q-range between 4×10^{-5} and 10^{-3} \AA^{-1} with considerable advantages over the DCD and conventional SANS instruments. The working principle and recent use of KWS3 in investigations of multiscale aggregates formed by poly(ethylene-butene) random copolymers in solution are reported.

CPP 7.24 Mon 16:00 Poster B

Microbeam GISAXS investigation of sol-gel templated nanocomposite films — ●J. PERLICH¹, M. MEMESA², J.S. GUTMANN^{2,3}, S.V. ROTH⁴, and P. MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik-Department LS E13, James-Frank-Str. 1, D-85748 Garching (Germany) — ²Max-Planck Institute for Polymer Research, Ackermannweg 10, D-55128 Mainz (Germany) — ³Institute for Physical Chemistry, Johannes Gutenberg University, Jakob-Welder-Weg 10, D-55099 Mainz (Germany) — ⁴HASYLAB at DESY, Notkestr. 85, D-22603 Hamburg (Germany)

We focus on the creation of nanostructured TiO₂ thin films, which are of great interest for many applications, due to their electrical performance. The performance is strongly dependent on the morphology of the nanocomposite films. For the preparation of the TiO₂ nanocomposite films we combine the amphiphilic diblock-copolymer PS-b-PEO with an inorganic sol-gel chemistry. Under these conditions a so-called good-poor-solvent pair induced phase separation leads to the formation of the nanostructures by film preparation via spin-coating. The different morphologies can be controlled by the solvent concentration. In order to obtain crystalline TiO₂ films as the final step calcination is conducted at higher temperature in air. For the investigation of the morphologies of the sol-gel templated nanocomposite films microbeam grazing incidence small angle x-ray scattering (μ GISAXS) is performed at the synchrotron beamline BW4 of the DESY HASYLAB. The investigation is complemented by surface and thin film sensitive probes. We acknowledge financial support by the project MU 1487/5-1.

CPP 7.25 Mon 16:00 Poster B

The new Jülich Neutron Spin Echo Spectrometer J-NSE at the FRM-II — ●OLAF HOLDERER^{1,2}, MICHAEL MONKENBUSCH^{1,2}, REINHARD SCHÄTZLER^{1,2}, and DIETER RICHTER^{1,2} — ¹Jülich Centre for Neutron Science (JCNS), Forschungszentrum Jülich GmbH, D-52425 Jülich, Germany — ²Institut für Festkörperforschung, Forschungszentrum Jülich GmbH, D-52425 Jülich, Germany

Neutron spin echo (NSE) spectroscopy is a well-suited method for studying the dynamics of soft matter systems such as glasses, polymers and complex liquids and paramagnetic properties of e.g. spin glasses. The Jülich NSE spectrometer has been in operation at the Jülich research reactor FRJ-2 since 1996. It has been transferred now to the new research reactor FRM-II of the TU München, where it is in the commissioning phase and will continue with user service this year. The J-NSE will operate at a neutron guide end position, giving access to the wavelength band of about 4.5 to 16 Å. New correction coils have been designed and manufactured, allowing to use higher currents in the main precession coils.

A larger neutron guide exit of 60x60 mm, the higher neutron flux and the better correction elements push the performance of the instrument to fourtimes $\lambda=1$ ps to about 350 ns, with a q-range of $q=0.02 - 1.5 \text{ 1/\AA}$.

CPP 7.26 Mon 16:00 Poster B

GISAXS studies on titania ultrathin films with different morphologies — YAJUN CHENG¹, MARKUS WOLKENHAUER¹, GINA BUMBU¹, STEPHAN ROTH³, JOCHEN GUTMANN^{1,2}, and ●YAJUN CHENG¹ — ¹Max Planck Institute for Polymer Research, Ackermannweg 10, D-55128 Mainz, Germany — ²Institute for Physical Chemistry, Johannes Gutenberg University, Welder Weg 11, D-55099 Mainz — ³HASYLAB at DESY, Notkestr. 85, D-22603 Hamburg

Ultrathin TiO₂ films showing rich morphologies are achieved by us-

ing sol-gel chemistry coupled with an amphiphilic polystyrene-block-poly(ethylene oxide) (PS-b-PEO) diblock copolymer as a structure-directing agent. The block copolymer undergoes a good-poor-solvent pair induced phase separation in a mixed solution of 1,4-dioxane, concentrated hydrochloric acid (HCl) and Titanium tetraisopropoxide (TTIP). By adjusting the weight fractions of 1,4-dioxane, HCl, and TTIP, inorganic-block-copolymer composite films containing a variety of different morphologies are obtained. Through calcination the amorphous Titania composite films can be converted to crystalline anatase phase. Based on the local characterization of AFM and SEM on the various different morphologies of the film. Grazing incidence small angle x-ray scattering (GISAXS) is further conducted to study the lateral structure of the film over large length scale. As a complementary method, x-ray reflectivity experiment is made to investigate the electron density gradient normal to the substrate. As a result, the combination of local imaging characterization and average x-ray scattering experiment provide a deep insight into the structure of the film.

CPP 7.27 Mon 16:00 Poster B

Beitrag abgesagt — ●XXX XXX —

CPP 7.28 Mon 16:00 Poster B

Nanostructure evolution during melting and oriented crystallization of polypropylene studied by in-situ SAXS — ●ULRICH NÖCHEL¹, ARMANDO ALMENDÁREZ CAMARILLO¹, NORBERT STRIBECK¹, and STEPHAN VOLKHER ROTH² — ¹University of Hamburg, Institute TMC, Hamburg, Germany — ²HASYLAB at DESY, Hamburg, Germany

Polypropylene film with high uniaxial orientation and lamellar structure is melt-annealed at temperatures between 168°C and 175°C followed by different cooling programs during which 2D SAXS patterns are continuously taken in order to identify the mechanisms of crystallization. Peculiar "cross-patterns" observed during the early stages of crystallization clearly demonstrate the mechanism of "building of lamellae from blocks" as proposed by Strobl. The evolution of the patterns under quiescent conditions shows that the complementary model of a "cross-hatched structure" cannot be applied. 2D SAXS data from various crystallization series[1] are evaluated by means of the CDF method[2] for a quantitative description of the crystallization mechanisms.

[1] Fibr. Text. EE (2005), 13(5), 27-29

[2] J. Appl. Cryst. (2001), 34(4), 496-503

CPP 7.29 Mon 16:00 Poster B

Optical diffraction measures the filling of superhydrophobic surfaces. — ●HELMUT RATHGEN and FRIEDER MUGELE — University of Twente, Physics of Complex Fluids, Postbus 217, 7500AE Enschede, The Netherlands

A hydrophobic surface with a periodic texture of period of order $1 \mu\text{m}$ is a superhydrophobic surface and an optical grating at the same time. A drop deposited on such a superhydrophobic optical grating can float on the texture like a fakir (*Cassie-Baxter* state) or it can penetrate the texture, soaking the grooves of the grating completely (*Wenzel* state). In the prior case, micrometer size liquid-gas interfaces are formed at the rims of the grooves. The diffractive properties of the optical grating (diffraction efficiencies of all diffraction orders) now depend on position and curvature of these micro menisci. Realspace information can be obtained by comparing measured diffraction data to a theoretical model based on Multilayer Rigorous Coupled Wave Analysis. We use this to investigate filling state and microscopic curvature at a superhydrophobic surface for a true water-vapor two phase system as a function of external pressure. We find: 1. The surfaces fill (transition from Cassie-Baxter to Wenzel state) at a critical pressure that depends on geometry and hydrophobicity in agreement with a prediction based on capillary theory. 2. Filling cannot be reversed by decreasing the external pressure to the vapor pressure. Our method is relevant as a technique of optical detection for a range of problems in micro- and nanofluidics, such as tracer free liquid detection in nanochannels or surface cavitation.

CPP 7.30 Mon 16:00 Poster B

Microemulsion-Polymer Systems Studied with Elastic and Inelastic Neutron Scattering — ●TINKA SPEHR^{1,2}, BERNHARD FRICK¹, and BERND STUEHN² — ¹Institut Laue-Langevin, Grenoble, France — ²Institute of Solid State Physics, TU Darmstadt, Germany

We study a microemulsion consisting of water, decane or toluene and

AOT forming water-in-oil droplets. The addition of amphiphilic triblock copolymer leads to the interconnection of the droplets. We are investigating the structural and dynamical behavior of this model system for a transiently linked network with different neutron scattering techniques. Also this system is used to realize soft confinement of the water. Neutron Small Angle Scattering showed increasing ordering of the droplets upon polymer addition. Measurements on pure microemulsions have been carried out on a time-of-flight and a neutron backscattering instrument to study the effect of spatial soft confinement on water. Two different droplet sizes have been investigated (diameters of about 3 and 10 nm). Elastic scans from 315 K to 2 K showed a deeper undercooling of the water confined in the smaller droplets. Inelastic scans have been carried out at temperatures between 300 K and 250 K. The dynamic structure factor displays a complex shape clearly deviating from one single Lorentzian. The combination of spatial restriction and wall effects on the dynamics will be discussed. Neutron Spin Echo can probe shape fluctuations of the droplet shell [3]. We investigated the effect of polymer addition on the elastic properties of the surfactant shells.

[2] J. Huang, S. Milner, B. Farago, D. Richter (1987), PRL 59, 2600

CPP 7.31 Mon 16:00 Poster B

Water uptake and exchange kinetics of polyelectrolyte films: A neutron reflectometry study — ●REGINE V. KLITZING¹, JOHN WONG¹, and ROLAND STEITZ² — ¹TU Berlin, Stranski-Laboratorium, Straße des 17. Juni 124, D-10623 Berlin — ²Hahn-Meitner-Institut, SF1, Glienicke Str. 100, D-14109 Berlin

The sequential layer-by-layer adsorption of polyanions and polycations to build polyelectrolyte multilayers has triggered enormous interest in their potential uses in a wide range of fields, from photonic to pharmaceutical applications. We will show that the conformation of the solvent swollen films – prior to drying – is determined by the initial adsorption conditions, but can be altered ex-situ by exposure to a liquid phase of very high ionic strength. Recently it has been observed that the swelling depends on the charge of the outermost layer. In the PAH/PSS system we saw that assemblies with PSS as the outermost

layer swell more than those with PAH outside. A neutron reflectivity study of this effect in addition indicated the existence of two kinds of water, bound with different strength within the films. Beside an unexpected two-step kinetics of swelling, the reflectivity curves of the layers against vacuum before and after re-hydration in D2O vapor did not agree. It was only after subsequent re-hydration in saturated H2O vapor that the initial and final reflectivity curves against vacuum superimposed. We will discuss our findings in the context of polyion complex formation, interdigitation and film imperfections.

CPP 7.32 Mon 16:00 Poster B

Horizontal ToF-Neutron Reflectometer REFSANS at FRM II Munich: Potential and First Experimental Results — ●REINHARD KAMPMANN¹, MARTIN HAESE-SEILLER¹, VALERI KUDRYASHOV¹, BERT NICKEL², PETER MÜLLER-BUSCHBAUM⁴, CHRISTINE PAPADAKIS⁴, WILHELM FENZL², ANDREAS SCHREYER¹, ERICH SACKMANN³, and JOACHIM RÄDLER² — ¹GKSS-Forschungszentrum Geesthacht GmbH, D-21502 Geesthacht, Germany — ²Department für Physik, Ludwig-Maximilians-Universität, D-80539 München, Germany — ³Physik-Department E22, TU-München, D-85748 Garching, Germany — ⁴Physik-Department E13, TU-München, D-85748 Garching, Germany

The reflectometer REFSANS allows to perform comprehensive analyses of vertical and lateral surface and interface structures by means of specular and off-specular neutron reflectivity as well as small-angle neutron scattering at grazing incidence (GISANS). All measurements can be performed on the air-water interface (horizontally aligned sample). REFSANS has been put into operation in 2005/06. Its performance is demonstrated by results of first reflectivity as well as GISANS measurements on nanostructured polymer and metallic films. The potential of this novel instrument for measuring weak off-specular scattering, GI-SANS and extremely low specular reflectivity including the case of a strongly incoherently scattering substrate is discussed.

This work has been supported by the German Federal Ministry of Education, Research and Technology (BMBF) under contracts 03-KA5FRM-1 and 03-KAE8X-3.

CPP 8: POSTER: Polymer Physics

Time: Monday 16:00–18:00

Location: Poster B

CPP 8.1 Mon 16:00 Poster B

A Monte Carlo study of a chain in a periodic potential — ●MIRCEA GALICEANU¹, JENS-UWE SOMMER², and ALEXANDER BLUMEN¹ — ¹Theoretische Polymerphysik, Universität Freiburg, Hermann-Herder-Straße 3, D-79104 Freiburg, Germany — ²Leibniz-Institut für Polymerforschung Dresden e. V., Hohe Strasse 6, D-01069 Dresden, Germany

We present Monte Carlo simulations of polymer chains of length N in a periodic array of traps. The static quantities, like the effective segment length and the end-to-end distance are controlled by the scaling variable $E = \delta\xi$, where δ is the strength of adsorption and ξ is the distance between two neighboring traps. We study chains with $N = 500$ and 1000 monomers and different values of δ and ξ . That the static quantities depend only on $E = \delta\xi$ is in very good agreement with former results[1]. The dynamic quantities which we study are the mean square displacement of all monomers, the mean square displacement of the center of mass and of the middle monomers relative to the center of mass. Using these results we are able to obtain the relaxation time as a function of the scaling variable E , and can show that at low values of E a chain in a periodic environment obeys a Rouse-like dynamics.

[1] J.-U. Sommer and A. Blumen, *J. Chem. Phys.* **105**, 6008, (1996)

CPP 8.2 Mon 16:00 Poster B

Simulations of Flexible and Semiflexible Polymers: Dynamic and Viscoelastic Properties — ●JULIAN SCHNEIDER^{1,2}, ALEXANDER BLUMEN¹, and MARTIN STEINHAUSER² — ¹Albert-Ludwigs-Universität, Theoretische Polymerphysik, Freiburg — ²Fraunhofer Institut für Kurzzeitdynamik (EMI), Freiburg

Using Molecular-Dynamics-Simulations we investigate the dynamic and viscoelastic properties of single chains and of melt systems consisting of flexible and semiflexible units. In order to find a unified description for such chains we performed simulations with different polymer

models and compared the numerical results to standard models. We find good agreement with the scaling-predictions of the Rouse-Model for flexible chains with no significant dependence of the spring-type connecting the beads. For semiflexible chains we observe a $t^{-5/4}$ -decay in the time-dependent shear modulus as recently predicted.

CPP 8.3 Mon 16:00 Poster B

Advanced ultrafast nanocalorimetry: superheating in linear polymers — ●ALEXANDER MINAKOV¹, ANDREAS WURM², and CHRISTOPH SCHICK² — ¹A.M. Prokhorov General Physics Institute, Vavilov 38, 119991 Moscow, Russia — ²University of Rostock, Institute of Physics, Universitätsplatz 3, 18051 Rostock, Germany

To study phase transition kinetics on submillisecond time scale a set of new membrane gauges for ultrafast scanning nanocalorimetry were constructed. Controlled ultrafast cooling, as well as heating, up to 1 million K/s was attained. The dynamic model describing the temperature distribution at ultrafast temperature change in the membrane-gas system was developed. The characteristic rate corresponding to the quasi-static limit of the temperature change in the membrane-gas system was determined. The rate equals 0.1 million K/s for different gauges in helium gas. The method was applied for the measurements of the superheating phenomenon in a set of linear polymers iPS, PBT, PET, iPP. A power law relation between the superheating and the heating rate was observed in the range 0.01 - 10000 K/s of heating rates. A superheating limit about 10% of the melting temperature was fined out at the rates above 0.01 - 0.1 millions K/s. This limit depends on the sample crystallization temperature. The observed superheating limit, as well as the power law, can be accounted for the internal stress induced by the superheating near the crystalline-amorphous interfaces in the semicrystalline polymers.

CPP 8.4 Mon 16:00 Poster B

Neue Einsichten in die Strukturbildung von elastomerem

Polypropylen — ●MECHTHILD DÖRING, CHRISTIAN DIETZ, SABINE SCHERDEL, NICOLAUS REHSE und ROBERT MAGERLE — Chemische Physik, TU Chemnitz, D-09107 Chemnitz

In unseren Experimenten untersuchen wir dünne Filme von elastomerem Polypropylen (ePP) mit einem sehr niedrigen Polymerisationsgrad. Mit Hilfe des Rasterkraftmikroskops können wir die Kristallisation des zuvor aufgeschmolzenen Materials *in situ* bei Raumtemperatur beobachten. Anschließend bilden wir die räumliche Struktur mittels Nanotomographie ab. Auf diese Weise lässt sich der Zusammenhang zwischen dem Prozess der Kristallisation und der räumlichen Struktur der Kristallite besser verstehen. Während der Kristallisation beobachteten wir zahlreiche Phänomene, die sich mit derzeitigen, einfachen Modellen der Strukturbildung nicht vollständig beschreiben lassen, wie zum Beispiel das Aufspalten einer Lamelle. Um diese und andere Beobachtungen näher zu untersuchen, wurde von der Probe mittels Nanotomographie ein Volumenbild des entsprechenden Bereichs erstellt und mit den so erhaltenen Erkenntnissen ein Modell für die jeweiligen Phänomene aufgestellt. Neben dem Effekt der Aufspaltung werden in unserem Beitrag weitere Beobachtungen des Wachstums und der Struktur von ePP-Kristalliten mit den dazugehörigen Modellen vorgestellt und diskutiert.

CPP 8.5 Mon 16:00 Poster B

Dynamik und Struktur von Defekten in dünnen Blockcopolymerfilmen — ●EIKE-CHRISTIAN SPITZNER, MARCUS BÖHME, MARTIN KREIS, CHRISTIAN DIETZ, SABINE SCHERDEL, NICOLAUS REHSE und ROBERT MAGERLE — Chemische Physik, TU Chemnitz, D-09107 Chemnitz

Wir untersuchen Dynamik in Systemen dünner Schichten von Polystyrol-*block*-Polybutadien Copolymeren, die im Volumen hexagonal geordnete Zylinderstrukturen bilden. Die Mikrodomänendynamik der in Chloroformdampf gequollenen Filme verfolgen wir *in situ* mit Hilfe der Tapping Mode Rasterkraftmikroskopie. Hierbei kommt es zu einer Reihe von charakteristischen Defekten, die teilweise über längere Zeit stabil sind. Beispielsweise sind ringförmige Defekte mit einem Punkt in der Mitte außerordentlich stabil. Ihre Volumenstruktur ist jedoch unbekannt. Die räumliche Abbildung der Defektstrukturen mit der Nanotomographie kann helfen, die Ursachen für ihre Stabilität besser zu erklären. Zudem wird somit auch ein Vergleich mit Ergebnissen aus Simulationen der Strukturbildung ermöglicht.

CPP 8.6 Mon 16:00 Poster B

Nanotomographie an Polypropylen mit hohem Kristallinitätsgrad — ●MARIO ZERSON, MECHTHILD DÖRING, CHRISTIAN DIETZ, NICOLAUS REHSE und ROBERT MAGERLE — Chemische Physik, TU Chemnitz, D-09107

Polypropylen (PP) bildet bei der Kristallisation lamellare Nanostrukturen aus. Die Form, die Ausrichtung und die Konnektivität der Kristallite bestimmen die Eigenschaften des Materials. Für die Charakterisierung der Volumenstruktur verwenden wir die Nanotomographie, die auf der Kombination von Rasterkraftmikroskopie (AFM) und geeigneten Ätzverfahren beruht. Bei dieser Methode wird die Oberfläche wiederholt schrittweise durch ein nasschemisches Ätzverfahren abgetragen und mit dem AFM abgebildet. Auf diese Weise erhält man eine Reihe von Bildern, die die Rekonstruktion der Struktur des PP ermöglicht. Eine Herausforderung stellt dabei der geringe Anteil an amorphen Material dar, der die Zuordnung der individuellen Lamellen nach jedem Ätzschritt erschwert. Wir zeigen unsere aktuellen Ergebnisse zur Nanotomographie an semikristallinen PP. Schwerpunkt der Arbeit ist es das Ätzverfahren zu optimieren, um die räumliche Struktur von PP mit höherem Kristallinitätsgrad abzubilden.

CPP 8.7 Mon 16:00 Poster B

Chemical confinement: Additional modes in the relaxation spectrum of a copolymer — ●JÖRG HACHENBERG¹, BJÖRN STEISEL², DENNIS BEDORF¹, MICHAEL BUBACK², and KONRAD SAMWER¹ — ¹I. Physikalisches Institut, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — ²Institut für Physikalische Chemie, Universität Göttingen, Tammannstr. 6, 37077 Göttingen, Germany

Copolymers with different monomer distributions but of comparable composition and comparable degree of polymerization have been investigated by mechanical spectroscopy and differential scanning calorimetry. An additional mode occurs in the relaxation spectra of copolymers with a non-random monomer distribution which is absent in those with a random distribution. This is interpreted as the motion of soft block-

like segments between rigid segments in the non-random copolymer. These unique features can be found in poly(ethylene-co-methacrylic acid) (EMAA) synthesized by high pressure free radical polymerization under steady state conditions. Two hydrogen bonds can tighten the methacrylic acid functions forming a chemical confinement in samples with a non-random distribution. The sample properties are controlled by SEC, FTIR and NMR.

This work is supported by DFG, Graduiertenkolleg 782.

CPP 8.8 Mon 16:00 Poster B

Rouse Dynamics in a Random Medium — ●MICHAEL STRAUCH and EKKEHARD STRAUBE — Martin-Luther-Universität Halle-Wittenberg, Institut für Physik, D-06099 Halle (Saale), Germany
We have studied the dynamics of a Rouse chain with randomly distributed segmental mobilities and were able to calculate the dynamic structure factor rigorously.

Introducing a *time step* opens up the possibility to extend this model so that the description of the motion of polymer chains inside random media becomes possible. The (randomly distributed) mobilities are no longer constant. Rather, the average mean square displacement (MSD) of the segments between two consecutive time steps is taken as a measure for the mean free path length. After comparing each segment's individual MSD (between consecutive time steps) with this mean free path length a decision is made whether this segment's mobility is altered (because it has moved a sufficient distance within the medium) or not (because it is still in the vicinity of its previous position).

In our poster we present results from our numerical simulations and compare them with experimental data.

CPP 8.9 Mon 16:00 Poster B

Kernspinrelaxationsverhalten und mechanische Eigenschaften von SBS-Blockcopolymeren — ●NIKOLAUS NESTLE, WALTER HECKMANN, KONRAD KNOLL und HELMUT STEININGER — BASF AG Ludwigshafen

SBS-Blockcopolymeren werden bereits seit langem als Mischungskomponente bei der Herstellung schlagzäher und hochtransparenter Styrolkunststoffe eingesetzt. Neben dem Gehalt an Butadienkauschuk sind dabei die Topologie der Ketten und die Verteilung des Butadienanteils über die einzelnen Blöcke des Polymers hinweg entscheidend für die mechanischen Eigenschaften im Gemisch mit reinem Polystyrol. Bei der Analyse von an den reinen Blockcopolymeren gemessenen TD-NMR-Daten und den mechanischen Eigenschaften der mit Polystyrol abgemischten SBS-Materialien zeigen sich deutliche Korrelationen zwischen den Parametern der Magnetisierungsabfallkurven und wichtigen anwendungstechnischen Größen wie z.B. dem E-Modul. Wegen des stärkeren Einflusses unterschiedlicher Mikrophasentopologien sind die keine vergleichbar deutlichen Zusammenhänge zwischen NMR-Größen und mechanischen Eigenschaften bei den reinen SBS-Blockcopolymeren zu beobachten.

CPP 8.10 Mon 16:00 Poster B

Atomic Force Microscopy of Polymer Networks — ●ALEXANDER SCHMATULLA and OTHMAR MARTI — University of Ulm, Institute of Experimental Physics, 89069 Ulm, Germany

We demonstrate the option of a custom built Atomic Force Microscope (AFM) for detection, nanomanipulating and pulling on strains of molecular polymer networks with a resolution on the nanometer scale.

By using contact mode, tapping mode and pulsed force mode we have imaged the polymer network. After detection of the network structure we have moved the AFM tip to a point x/y on the specimen, then we have bent and moved the cantilever in contact well defined distances over the surface. After pulling in contact we have imaged the same area which we have scanned before. The result was that molecular polymer strains of a branched polyethylene have been pulled over well defined distances. In addition we have analyzed the forces while pulling the molecule strains. After pulling the strains we have detected variances not only in the nearer periphery of the pulling area. We will compare our results with other measurement and detection methods (Raman spectroscopy, SEM).

CPP 8.11 Mon 16:00 Poster B

Phase contrast in AFM images of hard-soft polymeric systems — ●ALBRECHT PETZOLD, KLAUS SCHRÖTER, and THOMAS THURN-ALBRECHT — Martin-Luther-University Halle-Wittenberg, Institute of Physics, Experimental Polymer Physics

Tapping mode atomic force microscopy (TMAFM) is widely used to obtain height and phase images of heterogeneous polymeric systems. The influence of sample properties and imaging parameters on the phase image is still an active area of research. We here present a detailed study about the origin of the phase contrast in polyethylene (PE) as a typical semi-crystalline polymer with a liquid like amorphous phase. The phase signal obtained during imaging of PE is compared to measurements on hard and soft model systems, namely glassy polystyrene (PS) and crosslinked poly(dimethylsiloxane) (PDMS). Force spectroscopy curves of both model polymers were taken to obtain amplitude and phase information depending on the tip-sample distance. The phase signal of PE can be qualitatively understood in comparison to the different phase-distance curves obtained on PS and PDMS. Additionally the influence of several imaging parameters, like excitation frequency, free amplitude and stiffness of the cantilever on the shape of the force spectroscopy curves was investigated. As a result empirical suggestions for imaging of semi-crystalline polymers are made.

CPP 8.12 Mon 16:00 Poster B

Investigation of Internal Energy Change in Strain Experiments — ●SUSANNA HERZOG, GERALD JOHANNES SCHNEIDER, and DIETMAR GÖRITZ — Institut für Physik, Universität Regensburg, 93040 Regensburg

Due to the deformation of an elastomer the deformation energy and the heat energy change. One fundamental assumption of polymer physics is the total conversion of both energies, which implies no change of the internal energy by the first law of thermodynamics. There is however a change of the internal energy in deformation experiments. A possible explanation for this effect is the modification of the sample's volume.

In our measurement we can determine the amount of the internal energy by measuring the expended work and heat for the deformation.

CPP 8.13 Mon 16:00 Poster B

Diblock copolymer systems with boundaries and electric fields — ●MARIANNE BREUER and BARBARA DROSSEL — Institut für Festkörperphysik, Technische Universität Darmstadt, Deutschland

Block copolymer melts are a good model system for the study of molecular self-assembly. We investigate the nature, stability and dynamics of formation of diblock copolymer structures under different boundary conditions. We examine the effects of strong electric fields. We employ both numerical and approximate analytical treatments which are based on mean-field theory of the standard Gaussian model.

CPP 8.14 Mon 16:00 Poster B

Surface characterization of electron-beam irradiated polymer brushes — ●SINA BURKERT, FRANK SIMON, CORNELIA BELLMANN, PETRA UHLMANN, and MANFRED STAMM — Leibniz Institute of Polymer Research Dresden, Hohe Strasse 6, D-01069 Dresden, Germany

Polymer brushes out of PS, P2VP, PNIPAM and PAA were used to modify and control the surface potential of Si-wafers. The polymers brushes formed layers of thickness of less than 20 nm and significantly changed the surface potential of the substrate, which was investigated with contact angle measurements. Their chemical composition was studied by XPS. Electron irradiation was employed to modify the brushes by different radiation doses. With XPS and Zeta-potential measurements we were able to specify the surface composition after electron beam treatment. Changes in surface composition and the structure of the grafted polymer brushes allowed to qualify cross-linkages and degradation processes. By varying the dose we could adjust on the one hand the decomposition of the polymer and on the other hand the amount of hydrophilic groups. We know that the adsorption of proteins on polymers highly depends on the surface potential. This work could be used to control the surface potential of the polymer brush as well as the adsorption of proteins, only by varying the radiation dose. The chosen substrate silicon is also attractive for lab-on-chip applications of those modified brushes.

CPP 8.15 Mon 16:00 Poster B

Adiabatic crystallization of polycaprolactone — ●ANDREAS WURM¹, YUJI MIYAZAKI², KUMIKO MIWA², AKIRA INABA², and CHRISTOPH SCHICK² — ¹University of Rostock, Institute of Physics, Polymerphysics, 18051 Rostock, Germany — ²The Research Center for Molecular Thermodynamics, Graduate School of Science, Osaka University TOYONAKA, OSAKA 560 0043 JAPAN

Existence and formation of pre-ordered structures as the initial step of

polymer crystallization are discussed controversially. Most of the findings and interpretations are based on scattering experiments, which test small density differences between the assumed precursors of the crystals and the surrounding melt. Because of the low contrast the interpretation of experimental results becomes often speculative. Contrary relaxation experiments are probing motions in the sample and are therefore independent on density contrast. During crystallization material is transformed from the liquid to the solid state. Consequently, motions (fluctuations) typical for a liquid become impossible and do not longer contribute to the measured relaxing signal. For pre-ordered structures we expect some changes in mobility too because of the changes in conformation on pre-ordering. Adiabatic calorimetry is suitable to detect temperature changes in the sample, which can be related to crystallinities below one thousandth. In this study we compare crystallinity data from adiabatic calorimetry in the sub-percent range with complex dielectric permittivity of ϵ -polycaprolactone (PCL) during isothermal crystallization.

CPP 8.16 Mon 16:00 Poster B

Monte Carlo Simulations for Associate Formation in Semi-Dilute Polymer Solutions — ●MARIAN BRANDAU, STEFFEN TRIMPER, and EKKEHARD STRAUBE — Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle (Saale)

The results of a lattice-free dynamic Monte Carlo simulation for a semi-dilute polymer rod-bead system are presented.

We assume that the associate formation is determined by a small number of attractive saturable groups. Furthermore, the reactive monomers are supposed to be distributed randomly over the chains and are able to react mutually.

Starting from a dense well equilibrated melt configuration we extract a certain amount of chains, again randomly, which are subjected to the dynamic simulation according to a Metropolis algorithm.

The quantity of interest is the time evolution of the cluster structure depending on the chain density, the density of the reactive groups and the reaction rate. In particular, we find a cluster distribution function.

CPP 8.17 Mon 16:00 Poster B

Fluctuation Effects in the Theory of Microphase Separation in Diblock Copolymers in the Presence of an Electric Field — ●ILJA GUNKEL, SEMJON STEPANOW, THOMAS THURN-ALBRECHT, and STEFFEN TRIMPER — Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle

We generalize the Fredrickson-Helfand theory of the microphase separation in symmetric diblock copolymer melts by taking into account the influence of a time-independent homogeneous electric field on the composition fluctuations within the self-consistent Hartree approximation. We predict that electric fields suppress composition fluctuations, and consequently weaken the first-order transition. In the presence of an electric field the critical temperature of the order-disorder transition is shifted towards its mean-field value.

We also compute the collective structure factor in the disordered phase, which becomes anisotropic in the presence of the electric field. Fluctuational modulations of the order parameter along the field direction are suppressed. The latter correlates with the parallel orientation of the lamellae in the ordered state.

CPP 8.18 Mon 16:00 Poster B

Texture control in PVDF nanotubes — ●NITIN SHINGNE^{1,2}, MARKUS GEUSS², LILI ZHAO², MARTIN STEINHART², ULRICH GÖSELE², ELKE HEMPEL¹, and THOMAS THURN-ALBRECHT¹ — ¹Department of Physics, Martin Luther University, D-06120, Halle — ²Max-Planck-Institute of Microstructure Physics, D-06120, Halle

Using DSC and WAXS we studied the crystallization of poly(vinylidene fluoride) nanotubes templated inside the pores of ordered porous alumina. The crystal texture resulting from isothermal crystallization strongly depends on the crystallization temperature. We observed that crystallization at lower temperatures led to statistical orientation of the crystallites modified by growth under the conditions of 2D confinement. However, at high crystallization temperatures the 1D nanostructures shows a uniform crystal orientation with the (020)-direction pointing along the pore axes. Crystallization has to be initiated independently in each of the separated nanotubes, most likely by homogeneous nucleation. We assume that the orientation observed at low crystallization temperature reflects the random orientation of the nuclei and additionally a selection of growth direction along the pore axes, whereas at high crystallization temperatures the growth along different crystal directions seems to be highly selective leading to the

well defined crystal orientation within the nanotubes. Therefore, by choosing the crystallization temperature, control of crystal orientation within the 1D nanostructures is possible. This approach could pave the way for the reversible adjustment of ferro- and piezoelectric properties of the 1D polymeric nanostructures.

CPP 8.19 Mon 16:00 Poster B

Phase behaviour and transition of polymer-brushes on Microcantilevers — ●SEBASTIAN LENZ and JOCHEN GUTMANN — Max Planck Institute for Polymeric Research, Mainz

Polymer brush coatings are well known for their ability to tailor surface properties in a wide range of applications. In most cases, brushes are used in solution. Here we show that the micromechanical cantilever (MC) sensor technique is a tool to perform time-resolved physico-chemical investigations of the phase behaviour and phase transition of thin polymeric layers. Complementary to scattering techniques for measuring the thickness, MC sensor technique provides information about changes in the internal pressure of brushes during a phase-transition.

CPP 8.20 Mon 16:00 Poster B

Combined AC and fast scanning chip calorimetry — ●HEIKO HUTH, ALEXANDER MINAKOV, and CHRISTOPH SCHICK — Universität Rostock, Institute für Physik, Universitätsplatz 3 18051 Rostock

In the recent years new calorimetric techniques were developed using chip calorimeter based on thin film and silicon technology. Using these chips it is possible to reach fast heating and cooling rates up to 100.000 K/s. This gives new insight in the kinetic of polymer crystallization and reorganization processes not available with standard DSC devices. Another possibility is an extreme sensitive AC calorimetry for very small samples. Due to the fact of the small addenda heat capacity the measured sample is also in the range of nanogram. Here it is possible to measure thin polymer films below 10 nm. The next task was the combination of the advantage of both methods. Using the AC method the investigation of slow processes is possible with high sensitivity. Using fast scanning calorimetry the preparation of the sample prior to the measurement as avoiding crystallization is possible. This gives access to the crystallization kinetics from glass transition to melt for most of the semi crystalline polymers. First investigations of crystallization kinetics with the combined method on different semi crystalline polymers are presented.

CPP 8.21 Mon 16:00 Poster B

Distribution function of a wormlike chain with a fixed orientation of — ●SEMJON STEPANOW and FEDOR SEMERIYANOV — Universität Halle, Institut für Physik, 06099 Halle

We study the distribution function of the three dimensional wormlike chain with a fixed orientation of one chain end using the exact representation of the distribution function in terms of the Green's function of the quantum rigid rotator in a homogeneous external field. The transverse 1d distribution function of the free chain end displays a bimodal shape in the intermediate range of the chain lengths ($L_p, \dots, 3.5 L_p$). We present also analytical results for short and long chains, which are in complete agreement with the results of previous studies obtained using different methods.

CPP 8.22 Mon 16:00 Poster B

Thermomechanical Investigations of Filled Rubbers — ●WILLIBALD HENGL, GERALD JOHANNES SCHNEIDER, and DIETMAR GÖRITZ — Institut für Physik, Universität Regensburg, 93040 Regensburg

The reinforcing mechanism of rubber fillers is still an interesting topic. We made investigations of uniaxial elongation of filled rubbers by deformation calorimetry, whereby the change of internal energy can be calculated from the measured mechanical work and heat.

We present experiments mainly on silica-filled Polydimethylsiloxane (PDMS) with varying filler content and silica with and without a silane additive. As filled elastomers usually show strain-softening, the extensions have been repeated.

Although there are different stress-strain relations for each experiment, it is found, that the change of internal energy is predominantly controlled by the true stress acting on the specimen, independent of the composition and the history of the samples.

CPP 8.23 Mon 16:00 Poster B

In-situ-Beobachtung und statistische Auswertung der Struk-

turbildung in dünnen Blockcopolymer-Filmen — ●MARCUS BÖHME, SABINE SCHERDEL, NICOLAUS REHSE and ROBERT MAGERLE — Chemische Physik, TU Chemnitz, D - 09107 Chemnitz

Wir untersuchen mittels Tapping Mode Rasterkraftmikroskopie *in situ* die Strukturbildung in dünnen Filmen eines zylinderbildenden Polystyrol-*block*-Polybutadien-Blockcopolymeren in einer definierten Chloroformdampf-Atmosphäre. Dabei beobachten wir die Entstehung und Ausheilung von Einzeldefekten sowie Reorientierungen vorgeordneter Strukturen in der Nähe struktureller Phasenübergänge, deren Lage im Phasendiagramm durch den Lösungsmittelgehalt und die Dicke des Filmes bestimmt werden. Die statistische Auswertung zeigt enge zeitliche Zusammenhänge zwischen den beobachteten Erscheinungen und Änderungen im Lösungsmittelgehalt des flüssigen Filmes.

CPP 8.24 Mon 16:00 Poster B

Pulling on Single Siloxane Molecules — ●PETER SCHWADERER¹, CHRISTOPH BRÄUCHLE¹, ENNO FUNK², FRANK ACHENBACH², JOHANN WEIS³, and JENS MICHAELIS¹ — ¹Department Chemie und Biochemie, Ludwig-Maximilians-Universität München, Butenandtstraße 5-13, D-81377 München — ²Wacker Chemie AG, Johannes-Hess-Strasse 24, D-84489 Burghausen — ³Consortium für elektrochemische Industrie GmbH, Zielstattstr. 20, D-81379 München

Siliconelastomers are high-performance materials, used in a wide field of applications. Among their remarkable qualities are low temperature dependence of the mechanoelastic properties, high resilience against thermooxidation, high flexibility at low temperatures, adhesive behavior and physiological harmlessness. On the other hand siliconelastomers also have some disadvantages like low ultimate mechanical strength, vulnerability to hydrolytic reagents and moisture expansion in unipolar environment. Single molecule force spectroscopy using an AFM offers a unique possibility to investigate the mechanical performance of single siloxane polymer chains and their fixation in thin polymer networks. Both theoretical as well as experimental single molecule measurements can help to gain insights into the properties of the Si-O bond.

CPP 8.25 Mon 16:00 Poster B

Temperature Dependence of the Payne Effect — ●ANDREAS MICHAEL SCHMIDT¹, ANTJE BERGMANN², GERALD JOHANNES SCHNEIDER¹, and DIETMAR GÖRITZ¹ — ¹Institut für Physik, Universität Regensburg, 93040 Regensburg — ²Institut für Theoretische Festkörperphysik, Abteilung für Didaktik der Physik, Universität Karlsruhe, 76128 Karlsruhe

The "Payne-Effect" is an interesting phenomenon which can be observed in filled elastomers. It is characterised by a decline in the dynamical shear modulus with increasing deformation.

Instead of performing a conventional shear experiment we measured the shear force using a needle that could penetrate the sample periodically.

With our experimental setup we are able to vary the penetration depth, the deformation amplitude and the frequency of the needle oscillation.

We investigated SBR systems filled with VN3 silica, in which the filler content was varied. Furthermore, we performed annealing treatments on the samples and studied the filler rearrangement in the rubber matrix.

CPP 8.26 Mon 16:00 Poster B

Temperature resolved investigation of grating formation on azobenzene polymer films. — ●PADMANABH VEER¹, ULLRICH PIETSCH¹, and PAUL ROCHON² — ¹Dept. of Solid State Physics, University of Siegen, ENC, Siegen, 57068, Germany. — ²Dept. of Physics, Royal Military College, Kingston, Ontario, Canada, k7l3ng.

It was discovered 10 years ago that the exposure of an initially flat surface layer of an azobenzene-containing polymer to a holographic light pattern leads to the formation of surface relief structures (SRG) accompanied by a mass transfer over several micrometer. Many authors have investigated the process of SRG formation [1,2]. However, the nature of the driving force of this process is still unclear. We performed temperature resolved inspections of the SRG formation. The experiment was performed in a vacuum chamber to avoid the hot air turbulence. The sample is illuminated with circularly polarised light of wavelength 514nm and probed with He-Ne laser of wavelength 633nm. Inspecting the first order diffraction peak of a He-Ne laser, it has been seen that the grating inscription rate as well as the grating efficiency decrease with increasing sample temperature. No SRG formation is possible

approaching the glass transition temperature 'T_g' of the polymer film. A simple model considering two competitive processes can explain the data, the light induced alignment of chromophores along the valleys of the SRG and the thermally induced disorder of chromophores. [1] Rochon, P. et. al. Appl. Phys. Lett. 1998,72,2096. [2] Barrett, C. et. al. J. Phys. Chem. 1996,100,8836

CPP 8.27 Mon 16:00 Poster B

Crystallization behavior of pure iPS and iPS filled with nanoparticles — ●MOHAMED ISMAIL, ANDREAS WURM, and CHRISTOPH SCHICK — University of Rostock, Inst. of Physics, Polymerphysics,

In this contribution we demonstrate the crystallization behavior of pure iPS and iPS filled with nanoparticles by using DSC instrument. - We measured the heat capacity of pure iPS samples and iPS nanocomposites - The samples were prepared with different contributions of nano particles by solving iPS in a toluol and addition of the nanoparticles as well as applied the ultra sonic on the samples to distribute the nanoparticles through the polymer matrix. Finally, we dried the samples. - From the heat capacity data we obtained informations about the crystalline fraction, C, the rigid amorphous fraction, RAF, and the mobile amorphous fraction.

CPP 8.28 Mon 16:00 Poster B

The effect of matrix molecular weight on the interfacial morphology of iPP fiber/matrix single polymer composites — ●XIAOLI SUN, HUIHUI LI, and SHOUKE YAN — State Key Laboratory of Polymer Physics and Chemistry, Institute of Chemistry, The Chinese Academy of Sciences, Beijing 100080, P.R. China

To prepare samples of β -iPP, selective β -nucleants are commonly used. Moreover, crystallization of commercial iPP in temperature gradient, and forcing shearing in melt can also encourage the development of the β -phase.

In our previous studies, the interfacial structure of the iPP fiber/matrix polymer composites as a function of the fiber introduction temperature, fiber molecular weight as well as the subsequent crystallization temperature of the matrix was studied. It was found that partial melting of the iPP fiber is in favor of the formation of β -iPP crystals. In the present study, the influence of matrix molecular weight on the induced interfacial structure was studied. The matrix with lower molecular weight can be easily initiated to form β -iPP cylindrite by incomplete molten iPP fiber as researched previous. The matrix with higher molecular weight, however, cannot be induced to form β -iPP cylindrite when the isothermal crystallization is equal to 135 °C. But when using β -nucleating agent this matrix is able to effectively form β -spherulites when the isothermal temperature is under 140 °C. This can be explained in terms of different requirement for different matrix molecular weight chain to form β -iPP when iPP fiber was used to induce its matrix crystallization.

CPP 8.29 Mon 16:00 Poster B

Nanocalorimetric study of syndiotactic poly(propylene) (sPP) with different content of carbon nanotubes — ●SERGEY ADAMOVSKY¹, FELICE DE SANTIS², and CHRISTOPH SCHICK¹ — ¹Institute of Physics, University of Rostock, Universitaetsplatz 3, 18051 Rostock, Germany — ²Department of Chemical and Food Engineering, University of Salerno, 84084 Fisciano (SA), Italy

Polymer carbon nanotube composites attracted a great deal of attention in recent years. It is known, that electrical conductivity, shear viscosity, other mechanical and thermal properties of polymers are strongly influenced by the presence of small amounts (fractions of percent) of carbon nanotubes (CNT). Crystallization behaviour as well as crystal structure should be affected too.

A novel technique [1], based on a nanocalorimetric chip [2] was applied to study the crystallization of syndiotactic poly(propylene) (sPP) filled with different amount of carbon nanotubes. A pure sPP was measured as a reference. Sample mass of as small as about 100 ng allows us to use a heating/cooling rates of up to 500000 K/s which extends the rate range available in DSC dramatically. Together with DSC a range of cooling rates of 0.005 K/s to 500000 K/s was covered. A strong dependence of the crystallization temperature on cooling as well as of the crystallization half-time during isothermal crystallization on the CNT-content was observed.

1. S Adamovsky, C Schick. Thermochemica Acta, Vol. 415, Issue 1 (2004) Pages 1-7.

2. Sensor Integration, www.sensor.nl

CPP 8.30 Mon 16:00 Poster B

Rheo-FTIR studies on spider silk — ●JAN SÖLTER, PERIKLIS PADOPOULOS, and FRIEDRICH KREMER — Institut für Experimentelle Physik I, Universität Leipzig, Linnéstr. 5, 04103, Leipzig

Spider silk has unique mechanical properties which are currently not met by man-made materials. To study the interrelationship between (microscopic) molecular structure and the (macroscopic) mechanical response a polarized time-resolved FTIR-spectrometer is combined with a custom-made setup to measure the complex mechanical modulus. For that a dense wire grid of single parallel arranged spider threads of *Araneus diadematus* is prepared and a step-like increase of the strain is applied while measuring the resulting stress. The specificity of the IR spectral range enables one to trace in detail the microscopic response of the different molecular moieties, i.e. the reorientation and the order parameter, the phase relation within the molecular system with respect to the mechanical excitations and possible memory effects.

CPP 8.31 Mon 16:00 Poster B

Isothermal crystallization of PVDF using ultra-fast nanocalorimetry — ●EVGENY ZHURAVLEV¹, ARKADIUSZ GRADYS², ALEXANDER MINAKOV^{1,3}, and CHRISTOPH SCHICK¹ — ¹Institute of Physics, University of Rostock, Germany — ²Institute of Fundamental Technological Research, Polish Academy of Sciences, Warsaw, Poland — ³General Physics Institute, Moscow, Russia

By means of ultra fast thin-film nano-calorimetry, we were able to perform non-isothermal crystallization of poly(vinylidene fluoride) at cooling rates up to 100000 K/s. The new technique allows us to study samples of about 12 ng mass. Sample mass was estimated from measured heat capacity. At rates 12000 K/s and higher we were able to produce amorphous PVDF. At successive heating we observe so called cold crystallization. Isothermal crystallization of PVDF was investigated. Crystallization kinetics was studied at millisecond time scale. Experiments were performed from melt and from amorphous state of PVDF.

CPP 8.32 Mon 16:00 Poster B

Analysis of the microdomain dynamics in thin films of block copolymers — ●SABINE SCHERDEL¹, KLAUS MECKE², CHRISTIAN FRANKE¹, MARCUS BÖHME¹, and ROBERT MAGERLE¹ — ¹Chemische Physik, TU Chemnitz, D-09107 Chemnitz — ²Institut für Theoretische Physik I, Universität Erlangen-Nürnberg, D-91058 Erlangen

We investigate the structure formation in thin films of polystyrene-*block*-polybutadiene copolymers. With modern atomic force microscopes we record series of images with high temporal and spatial resolution in a relatively short time. The manual analysis of these data, however, takes often months. To accelerate the quantitative analysis we use and compare different image processing methods. By computing local Minkowski measures we get important morphological information about the geometry of the observed structures and their evolution with time. Another way to characterize structures is to reduce them to their medial axis and to identify and count the branching points of the skeletonized structure. Their temporal evolution and characteristic time constants are analyzed with correlation functions.

CPP 8.33 Mon 16:00 Poster B

Development of Entanglements in a Polymer Melt — ●THOMAS VETTOREL, THOMAS A. VILGIS, and KURT KREMER — Max-Planck-Institut fuer Polymerforschung, 55128 Mainz, Germany

Recent work by Rastogi et al. has shown that it is possible to prepare a polymer melt in an initially disentangled state. This system then relaxes to the normal, entangled melt state but gives rise to a long-lived metastable "new melt" in which different parts of the chains exhibit different mobilities due to an unusual distribution of entanglements. This yields a material whose particular mechanical properties could be of interest for many purposes.

We study the mechanisms leading to the relaxation to the entangled state by means of computer simulations, using a normal bead-spring model, with and without explicit bending rigidity. A fully disentangled polymeric system is created as a collection of chains collapsed in a globular state, packed together at the melt density. We then monitor the relaxation of this strongly out-of-equilibrium system, looking more particularly at the evolution of the entanglements: The entanglement length N_e is measured using the Primitive Path Analysis.

The first results show that in the case of relatively short chains (up to $N \approx 20N_e$), the relaxation of the entanglement length is very fast, suggesting that the situation is better described by a scenario like de

Gennes' explosion upon melting, even if a slowing down is observed in the diffusion of chains' centers of mass before equilibrium is reached, indicating a confinement effect.

CPP 8.34 Mon 16:00 Poster B

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CPP 8.35 Mon 16:00 Poster B

Surface functionalization by ultrathin plasma polymer coatings: From partial coverage to closed films — JAKOB BARZ^{1,2}, MICHAEL HAUPT¹, CHRISTIAN OEHR¹, and ●ACHIM LUNK² — ¹Fraunhofer IGB, Nobelstr. 12, 70569 Stuttgart — ²Institut für Plasmaforschung, Universität Stuttgart, Pfaffenwaldring 31, 70569 Stuttgart

Plasma processes based on different monomer precursors are successfully applied to deposit ultrathin polymer films onto different substrate materials. The film thickness and the chemical composition of the polymer are greatly influenced by the choice of the precursor, the deposition time, the electric power, the pressure, and additional gases.

In order to study various deposits, plasma processes were performed in a trifluoromethane (CHF₃) discharge, diluted by argon.

By the variation of the above parameters, the coating thickness varied between 0.5 and 10 nm as determined by spectroscopic ellipsometry. The surface tension was determined according to the Owens-Wendt-Rabel-method; for coatings above 2.9 nm thickness, the surface energy remained constant, independent from the polymer thickness or the dis-

charge parameters, at values of 15 mN/m disperse and 0.2 mN/m polar surface tension. At lower thicknesses, differences between advancing contact angles (representing the low-energy parts) and receding contact angles (representing high energy surface contributions) were observed. In the examined coatings, this behavior is attributed to the partial inset of polymer growth for mild plasma conditions, and further correlated to data from AFM and XPS measurements.

CPP 8.36 Mon 16:00 Poster B

Photovoltaic Devices Based on Semiconducting Block-Copolymers — ●S HUETTNER¹, S LINDNER², A CHICHE¹, G KRAUSCH¹, and M THELAKKAT² — ¹Physikalische Chemie II, Universität Bayreuth, 95440 Bayreuth, Germany — ²Makromolekulare Chemie I, Universität Bayreuth, 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(erylene 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 [2]. 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, 8832 (2004) [2] S. Lindner, S. Hüttner, A. Chiche, M. Thelakkat, G. Krausch, *Angew. Chem. Int. Ed.* 45, 3364 (2006)

CPP 8.37 Mon 16:00 Poster B

Self assembly of a crystalline block copolymer in a selective solvent — ●A.M. MIHUT¹, A. CHICHE¹, H SCHMALZ², and G KRAUSCH¹ — ¹Physikalische Chemie II, Universität Bayreuth, 95440 Bayreuth, Germany — ²Makromolekulare Chemie I, Universität Bayreuth, 95440 Bayreuth, Germany

We investigate the formation and growth of complex supramolecular structures formed by a crystalline diblock copolymer (PEO-PB) in a selective solvent. The interaction between the crystalline block and the solvent can be controlled by the temperature. While cooling the system, the solvent (heptane) becomes a selective solvent for the amorphous block (PB). The resulting structure is related to the interplay between the phase separation and the crystallization of the PEO block. We study the effects of the experimental conditions (cooling rate and final temperature) as well as the molecular parameters on the morphology of the supramolecular objects by scattering techniques and electron microscopy.

CPP 9: POSTER: Colloids and Nanoparticles

Time: Monday 16:00–18:00

Location: Poster B

CPP 9.1 Mon 16:00 Poster B

Zinc oxide nanoparticles inside microgel — ●MUKESH AGRAWAL¹, ANDRIJ PICH², NICK ZAFEIROPOULOS¹, and MANFRED STAMM¹ — ¹Leibniz-Institut für Polymerforschung Dresden e.V., Hohe Straße 6, 01069 Dresden, Germany — ²Institut für Makromolekulare Chemie und Textilchemie, Technische Universität Dresden, Mommsenstr 4, 01062 Dresden, Germany

We investigate on the synthesis of temperature and pH-sensitive hybrid microgels containing ZnO nanoparticles. The synthesis of ZnO nanoparticles was carried out in the presence of poly(N-vinylcaprolactum-co-acetoacetoxyethylmethacrylate-co-N-[3-dimethylamino)propyl] methacryl amide)(VCL/AAEM/PDMAPMam) and it was observed that these microgels act as the container for deposition of ZnO nanoparticles, under the specific reaction conditions, leading to the formation of hybrid microgels. A close relationship between changes in properties of microgels and the loaded ZnO content was reported. Microscopic studies confirmed the inclusion of nanoparticles into microgels. It has been found that prepared microgels have tendency to form composite films on solid substrates after water evaporation, with

homogenous distribution of ZnO nanoparticles in polymer matrix.

CPP 9.2 Mon 16:00 Poster B

Fluctuation-induced interaction between anisotropic colloids at fluid interface — ●EHSAN NORUZIFAR and MARTIN OETTEL — Institut fuer Physik, WA 331, Johannes-Gutenberg-Universitaet Mainz, 55099 Mainz, Germany

The effective interaction between anisotropic particles trapped at fluid interface necessarily contains a long-ranged part caused by capillary wave fluctuations [1]. Due to the restrictions the colloids impose on the capillary waves, the interaction is of Casimir type which can be calculated by integrating on all possible interface configuration weighted by a simple capillary wave Hamiltonian. For the specific case of ellipsoids, we consider the resulting anisotropic interaction with regard to ordering phenomena on the interface [2].

[1] H. Lehle, M. Oettel, and S. Dietrich, *Eur. Phys. Lett.* 75 (2006) 174

[2] J. C. Loudet, A. M. Alsayed, J. Zhang, and A. G. Yodh, *Phys. Rev. Lett.* 94 (2005) 018301

CPP 9.3 Mon 16:00 Poster B

Front instabilities in evaporating films of nanoparticle suspensions - simulation results — ●IOAN VANCEA¹, CHRISTOPHER MARTIN², EMMANUELLE VAUJOUR², PHILIP MORIARTY², and UWE THIELE¹ — ¹Max-Planck-Institut für Physik komplexer Systeme, Noethnitzer Str. 38, D-01187 Dresden, Germany — ²School of Physics & Astronomy, The University of Nottingham, University Park, Nottingham, NG7 2RD, United Kingdom

Various experimental settings involving drying suspensions of nanoparticles have been used to produce patterned nanoparticle layers [1,2]. Beside polygonal networks and spinodal structures one finds branched structures.

Using a variant of a Monte Carlo model introduced by Rabani et al. [1], we study front instabilities of initially straight or circular fronts.

We discuss in detail the influences that lead to the fingered structures. We show that even with a simple model including evaporation as the only dynamic process it is possible to determine many properties of the finger patterns.

Especially, we present results for a straight dewetting front that becomes transversally unstable depending on driving force (chemical potential), nanoparticle concentration and mobility (inverse of an effective viscosity). The fingering becomes stronger with increasing chemical potential and decreasing mobility. Concepts of quantification of the fingering are also discussed.

[1] E. Rabani et al., *Nature* **426**, 271-274 (2003).

[2] C. P. Martin et al., *Nano Lett.* **4**, 2389-2392 (2004).

CPP 9.4 Mon 16:00 Poster B

Influence of a Limited q-range on the Results obtained from Scattering Experiments — ●GERALD JOHANNES SCHNEIDER and DIETMAR GÖRITZ — Institut für Physik, Universität Regensburg, 93040 Regensburg

Scattering methods are widely used for investigating the structure of colloidsized objects. However, considering hierarchical structures, like e. g. colloidal silica, objects at characteristic length scales ranging from a few Angstrom up to millimeters are involved. Thus, even by combining different scattering techniques, in particular X-ray, neutron, and light scattering methods, a complete information on the structure is not available.

In our contribution we investigate the influence of the limitation of the q-range available. For this purpose, scattering diagrams were calculated to show the influence of the range of the momentum transfer to the radius of the gyration of the object extracted from the scattering curves. We show, if the the minimum value for the momentum transfer is not small enough, the error for the radius of gyration will be very large.

CPP 9.5 Mon 16:00 Poster B

Microstructure studies of microemulsions for decontamination — ●STEFAN WELLERT¹, HENRIK IMHOF¹, ANDRE STEPPIN¹, THOMAS HELLEWEG¹, MICHAEL DOLLE², HANS-JUERGEN ALTMANN², and ANDRE RICHARDT² — ¹TU Berlin, Stranski-Labor, Strasse des 17. Juni 124, D-10623 Berlin — ²Armed Forces Scientific Institute, (NBC-Protection) P.O.Box 1142, D-29623 Munster

A growing field of interest is the use of microemulsions as new and more efficient decontamination media for a variety of toxic compounds, for example organophosphorous agents. Because of the large internal surface water-in-oil microemulsions and bicontinuous structures are of interest for the mentioned application. In order to form environmentally compatible and effective decontamination media we studied the phase behavior of quaternary systems consisting of water, surfactant (IHF, APG), cosurfactant (2-propanol, pentanol) and different oils. The identified stable one-phase regions were investigated with scattering methods. To gain insight in the phase structures SAXS, DLS and SANS measurements were performed as a function of surfactant, cosurfactant and water content. A large internal surface is essential for a fast and efficient decontamination process. This large contact area between the contaminants solubilized in the oil phase and the active agents in the water phase leads to a strong influence of the structure factor $S(q)$. Due to this SANS contrast variation experiments were performed to extract the influence of the structure factor on the form factor signal. The results of these measurements are related to the measured efficiencies of the decontamination process.

CPP 9.6 Mon 16:00 Poster B

Decontamination with sugar surfactant based microemulsions — ●STEFAN WELLERT¹, HENRIK IMHOF¹, ANDRE STEPPIN¹, THOMAS

HELLEWEG¹, MICHAEL DOLLE², HANS-JÜRGEN ALTMANN², and ANDRE RICHARDT² — ¹TU Berlin, Stranski-Lab., Strasse des 17. Juni 124, D-10623 Berlin — ²Armed Forces Scientific Institute (NBC-Protection), P.O.Box 1142, D-29623 Munster

Environmental compatibility is one of the most important features of modern decontamination media for a large variety of toxic compounds as warfare agents or pesticides. Different selection factors like capacity, effectiveness, universality and economy determine the formulation and development of such systems. We showed by a study of the phase behavior the possibility to replace an existing macroscopic system by microemulsions containing the same main components. Environmental non harmful and non corrosive organic solvents and the use of APG surfactants promise a simple and safe application. To meet these requirements we used technical sugar surfactants and beside PCE also less harmful solvents like xylene and Biodiesel fuel. We present results from studies of the phase behavior of quaternary systems and the influence of an additional active component is discussed. For the decontamination oxidizing agents and enzymes are promising active components. The decontamination efficiency of both systems is first estimated on the basis of the ability to wet typical non-chemical resistant coated steel sheets. Afterwards, promising samples are tested using real surfaces covered with nerve agent.

CPP 9.7 Mon 16:00 Poster B

Silica Particle Distribution in Styrol Butadiene Rubber — ●GERALD JOHANNES SCHNEIDER¹, DIETMAR GÖRITZ¹, Gerd WEIDEMANN², JÜRGEN GOEBBELS², and HEINRICH RIESEMEIER² — ¹Institut für Physik, Universität Regensburg, 93040 Regensburg — ²Federal Institute for Material Research and Testing (BAM), Berlin

Due to the widespread use, studying the structure of silica is of general interest for fundamental research and for applications. For example, it is well known that rubber filled with silica can be used to improve the mechanical properties of the composite material. The goal of many different material models is to describe this so called reinforcement effect. The models depend on reliable information about the structure of the filler. However, the length scales involved range from nanometers up to millimeters and thus a complete study does not exist. Using synchrotron X-ray tomography experiments we are able to study the structure of silica in rubber with a resolution of 600 nm. Thus, one can investigate the micro dispersion of silica in rubber.

CPP 9.8 Mon 16:00 Poster B

In-situ investigation of the interfaces of a block copolymer solution under shear stress with μ -focus GISAXS — ●ANDREAS TIMMANN¹, STEPHAN VOLKHER ROTH¹, STEFFEN FISCHER², and STEPHAN FÖRSTER² — ¹HASYLAB at DESY, Notkestr. 85, D-22603 Hamburg, Germany — ²University of Hamburg, Inst. f. Phys. Chem., Grindelallee 117, D-20145 Hamburg, Germany

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

The experiments were performed the beamline BW4 at HASYLAB, Hamburg [1] using the microfocus setup. We present the results of the investigation of an 14.1 wt.% solution of a poly-(isoprene-block-ethylene oxide) in water. The block degrees of polymerization of the Isopren and the polyethylene oxide were 107 and 343, respectively.[2] The shear stress was applied by a stress-controlled Bohlin CVO rheometer in a plate-plate-geometry with a diameter of 20 mm and a gap of 1 mm. We investigated the interface layers of the solution to air and to the metal plates of the geometry, respectively. We found a dependency of the layer thickness of the metal-solution interface on the application of shear.

References: [1] Roth et al., *Rev. Sci. Instrum.*, 2006, 77, 085106

[2] A. Timmann, Doctoral Thesis, University of Hamburg, 2005

CPP 9.9 Mon 16:00 Poster B

Interaction of magnetic colloids in periodic potentials — LARYSA BARABAN, ●ARTUR ERBE, and PAUL LEIDERER — Universität Konstanz, FB Physik, Germany

Magnetic colloids are widely used as model systems for a variety of processes in statistical physics. In this work we study the behavior of micron-sized particles exhibiting a permanent magnetic moment. This moment is generated by a magnetic cap, which enables us to observe

the direction of the magnetic moment with standard video microscopy. Thus interactions in large particle arrays can be observed. We demonstrate the creation of such arrays in square and triangular symmetry and investigate the particle-particle interactions as well as the interactions with the substrate. The magnetic moments of the particles are characterized using SQUID, MFM, and magneto-optic techniques.

CPP 9.10 Mon 16:00 Poster B

Layer and lane formation in driven magnetic colloidal particles — ●MARCIN ZIENTARA, MICHAEL KOPPL, ARTUR ERBE, and PAUL LEIDERER — Universität Konstanz, FB Physik, Germany

The process of lane formation is a nonequilibrium phase transition occurring in two-component systems under the action of external forces. It aims at an increase of transport or motion efficiency if particles are driven by forces acting in opposite directions. The simplest situation to imagine is a mixture of particles, half of which has a positive charge and half has a negative charge. Such particles can be moved in opposite directions, if an external electric field is applied. If the force exceeds a certain threshold, the motions will separate and ordered lanes will appear. This phenomenon has been studied theoretically in a wide range of systems. We show experimental results of paramagnetic particles confined in a narrow channel driven by gravity. In this system layering of the particles leads to a similar ordering phenomenon. In a mixture of magnetic and non-magnetic particles lane formation is expected, if the particles are driven in opposite directions by application of a gradient in the magnetic field in combination with gravity.

CPP 9.11 Mon 16:00 Poster B

Dependency of colloid overcharge on the salt concentration — ●OLAF LENZ¹, MARCIA BARBOSA², and CHRISTIAN HOLM¹ — ¹FIAS, Frankfurt am Main, Germany — ²Universidade Federal do Rio Grande do Sul, Porto Alegre, Brazil

We have performed coarse-grained MD simulations of a highly charged colloid in a solution of 3:1 and additional 1:1 salt. The dependency of the colloid's overcharge on the concentration of the additional 1:1 salt has been studied. Depending on the colloid's characteristics and the concentration of the multivalent ions, a non-monotonic behavior has been found.

We compare these results with the theoretical predictions from a density functional theory by M. Barbosa.

CPP 9.12 Mon 16:00 Poster B

Employing TIRM to measure critical casimir forces in a binary liquid — ●LAURENT HELDEN, CHRISTOPHER HERTLEIN, and CLEMENS BECHINGER — 2. Physikalisches Institut, Pfaffenwaldring 57, D-70550 Stuttgart

The technique of total internal reflection microscopy (TIRM) is capable to measure interactions of a spherical colloidal particle close to planar wall. Forces as small as 5 fN can be detected, thus TIRM can be employed to directly measure extremely weak interactions like critical casimir forces.

Due to concentration fluctuations a colloidal particle suspended in a binary liquid at the critical composition close to a substrate experiences a critical casimir force upon approaching the critical temperature of decomposition T_c . We have directly measured interaction potentials for a polystyrene particle suspended in a mixture of water and 2,6-lutidine approaching T_c . In agreement with theoretical predictions strongly temperature dependent forces were detected. The sign of the forces depends on the wetting properties of probe particle and substrate.

CPP 9.13 Mon 16:00 Poster B

An Investigation of Precipitated Silica using Transmission Electron Microscope Tomography — ●BENJAMIN GEORG GREINER, GERALD JOHANNES SCHNEIDER, and DIETMAR GÖRITZ — Institut für Physik, Universität Regensburg, 93040 Regensburg

In general the morphology of active fillers is investigated using transmission electron microscopy. However, only projections of the samples are accessible. Thus, one can not differentiate between a disc-like or a spherical structure. In order to obtain such information we investigated precipitated silica using different tilt angles between the sample and the wave vector of the incident electron beam and reconstructed a three dimensional volume of the object. This method, denoted as electron tomography, allows a detailed investigation of the structure of objects at a length scale of a few nanometers. In particular a detailed investigation of the shape is possible.

CPP 9.14 Mon 16:00 Poster B

Capillary interaction between ellipsoidal colloids at a fluid interface — ●HARTWIG LEHLE^{1,2} and MARTIN OETTEL^{1,3} — ¹Max-Planck-Institut für Metallforschung, Heisenbergstr. 3, 70569 Stuttgart — ²Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart — ³Institut für Physik, WA 331, Johannes-Gutenberg-Universität Mainz, 55099 Mainz

In two recent publications, Loudet *et al.* describe the behavior of μ -sized ellipsoidal colloids trapped at a water-oil interface [1,2]. They find a strong anisotropic attractive force between the colloids which leads to the formation of complex chain- or raftlike structures at the interface and which can be qualitatively explained by the capillary interaction due to a quadrupolar meniscus deformation caused by the particle's anisotropy. A thorough theoretical investigation of these phenomena is, however, missing so far.

In a systematic approach we derive a quadratic free energy functional of the interface and the colloids trapped at it. Upon minimizing the free energy we calculate the equilibrium meniscus profiles of both, a single ellipsoid and two ellipsoids in arbitrary orientation with respect to each other. Finally, from the interface profiles we determine the orientation dependent capillary force between the ellipsoidal particles and discuss the results in detail.

[1] J. C. Loudet, A. M. Alsayed, J. Zhang, and A. G. Yodh, *Phys. Rev. Lett.* **94**, 018301 (2005)

[2] J. C. Loudet, A. G. Yodh, and B. Pouligny, *Phys. Rev. Lett.* **97**, 018304 (2006)

CPP 9.15 Mon 16:00 Poster B

Soft X-ray Spectromicroscopy at the Swiss Light Source — ●GEORGE TZVETKOV^{1,2}, JÖRG RAABE², RAINER FINK¹, and CHRISTOPH QUITMANN² — ¹Physikalische Chemie II, Friedrich-Alexander Universität Erlangen-Nürnberg, D-91058 Erlangen, Germany — ²Paul Scherrer Institut, 5232 Villigen, Switzerland

A new X-ray scanning transmission microscope (STXM) located at the Paul Scherrer Institut, Villigen, is now available. The microscope is attached to the PoLLux beamline at the Swiss Light Source synchrotron laboratory. The central theme of the STXM is the ability to obtain morphological and chemically-specific information on a full range of materials (inorganic/organic) under real conditions thus providing a unique facility. The operating energy range (from 200 eV to 1 keV) encompasses a significant number of important K- and L-absorption edges, and relatively thick samples can be studied with absorption contrast technique (NEXAFS spectroscopy). The range of potential applications is truly interdisciplinary, including materials science, biological and bio-medical science, and environmental science (e.g., polymers, nanomaterials, magnetic materials, biological materials, aerosols, minerals).

Here, several examples of different systems under study are presented. The overview addresses topics ranging from fundamental environmental chemistry to phase-change microcapsules.

CPP 9.16 Mon 16:00 Poster B

Influence of Temperature, pH and Ionic Strength on the Swelling-Behavior of New Poly(N-isopropylacrylamide-co-allylacetic acid) Microgels — ●MATTHIAS KARG and THOMAS HELLWEG — TU Berlin, Stranski-Laboratorium für Physikalische und Theoretische Chemie, Strasse des 17. Juni 124, D-10623 Berlin, Germany

The volume phase transition of colloidal microgels made of N-isopropylacrylamide (NIPAM) is well-studied and it is known that the transition temperature can be affected by copolymerization. A series of poly(N-isopropylacrylamide-co-allylacetic acid) copolymers with different contents of allylacetic acid (AAA) has been prepared using simple surfactant-free emulsion polymerizations. The thermoresponsive behavior of these particles was studied by means of dynamic light scattering (DLS). Further characterization was done employing atomic force microscopy (AFM), transmission electron microscopy (TEM) and zeta potential-measurements. While the TEM and AFM observations manifest the spherical shape and low polydispersities of the copolymers, the zeta potential measurements provide information about the relative surface charge.

Since these copolymers are much more sensitive to external stimuli such as pH and ionic strength than their pure PNIPAM counterparts the swelling behavior was investigated at two different pH values and different salt concentrations.

CPP 9.17 Mon 16:00 Poster B

Molecular dynamics simulation of the formation of NaCl-nanoparticles in supercritical water — ●NORBERT LÜMMEN and BJØRN KVAMME — University in Bergen, Institute for Physics and Technology, Allégaten 55, N-5007 Bergen, Norway

The formation of salt particles in supercritical water happens in both natural hydrothermal environments and industrial processes. Whenever the ocean is deeper than 2800m and heat sources like intrusive basalts are present, water can attain the supercritical state and salt particle formation takes place. The plugging of reactor pipes due to salt formation is a known technological problem in the Supercritical Water Oxidation (SCWO), a proposed method to purify water contaminated with organic waste.

NaCl-nanoparticle formation in supercritical water was investigated by molecular dynamics simulations as a test case for further studies on metal salt formation. The rigid SPC/E water model was employed while the ionic interactions were treated by the model of Smith and Dang. Constant temperature was achieved by a Nosé-Hoover thermostat and the density was chosen to match a system pressure around 25 MPa at different system temperatures and sizes at constant water to ion ratio. Particle formation takes place within a few hundred picoseconds after the jump from ambient to supercritical conditions. After nucleation clusters first grow by adding monomers and later via cluster-cluster-collisions. We present results on the time development of distributions of cluster sizes, compositions, and temperatures, radial distribution functions and an estimate of nucleation rates.

CPP 9.18 Mon 16:00 Poster B

Modelling of Scattering Diagrams — ●ADRIAN MAIER, KLAUS NUSSER, GERALD JOHANNES SCHNEIDER, and DIETMAR GÖRITZ — Universität Regensburg, 93040 Regensburg

Scattering methods are most suitable for studying the structure of unknown systems. Especially colloidal objects are of interest for both fundamental and applied science. Therefore an enormous amount of work has been done to extract structure information of such systems out of scattering diagrams. In particular the correlation between the structure of colloidal systems and the scattering diagrams is not fully understood yet. To gain more insight into this topic we numerically calculated scattering diagrams of simple colloidal objects.

In general experimental samples exhibit a significant polydispersity. In models, however, one usually assumes monodisperse particles. Consequently, we investigated the influence of a polydisperse distribution of diameters on scattering diagrams to determine the validity of the analysis.

CPP 9.19 Mon 16:00 Poster B

Macroscopically Thick Silica-Rubber Systems Investigated using GISAXS — ●TOBIAS PÖPPERL¹, GERALD JOHANNES SCHNEIDER¹, PETER MÜLLER-BUSCHBAUM², and DIETMAR GÖRITZ¹ — ¹Institut für Physik, Universität Regensburg, 93040 Regensburg — ²Physik Department LS E13, TU München

The mechanical properties of filler-rubber systems, with fillers such as e.g. silica, are mainly determined by the filler. In general silica can be interpreted as a fractal object with a hierarchical structure - with structure sizes ranging from nanometers up to several micrometers.

Established methods like Small Angle X-ray Scattering (SAXS) and Ultra Small Angle X-ray Scattering (USAXS) techniques are highly useful for investigating such systems, but cover only structure sizes smaller than one micrometer. Therefore, it is of interest to apply additional methods to expand the accessible range. Originally developed to investigate surface structures of thin films, the powerful technique of Grazing Incidence Small Angle X-ray Scattering (GISAXS) is such a method. It covers the range of a few nanometers up to several micrometers. For the first time GISAXS was used to investigate the morphology of silica dispersed in macroscopically thick rubber and the results are presented.

CPP 9.20 Mon 16:00 Poster B

New well-defined Hybrid Materials with Thermoresponsive PNIPAM-Shells and Inorganic Nanoparticle-Cores — ●MATTHIAS KARG¹, ISABEL PASTORIZA-SANTOS², LUIS LIZ-MARZÁN², and THOMAS HELLWEG¹ — ¹TU Berlin, Stranski-Lab., Germany — ²Universidad de Vigo, Grupo de Química Física, Vigo, Spain

A simple, emulsion polymerization of N-isopropylacrylamide with the crosslinker N,N'-methylenebisacrylamide leads to spherical hydrogels. Such particles are usually in the submicron size range and are therefore called microgels. Since PNIPAM microgels are thermoresponsive

they can be classified as smart materials and have been the topic of several investigations. As these microgels react much faster on external stimuli such as temperature, pH and ionic strength than their macroscopic counterparts they are interesting for different applications including sensors, drug delivery and separation media. Nevertheless the optical properties of organic polymers are poor because of their rather low refractive index. Composite materials made of microgels and inorganic nanoparticles combine the temperature-dependent swelling-behavior of the microgel and the high refractive index of the nanoparticles. We present here the preparation of different types of hybrid systems made of PNIPAM and silica and silica-coated gold nanoparticles. Characterization has been done using dynamic light scattering (DLS), transmission electron microscopy (TEM), scanning electron microscopy (SEM), atomic force microscopy (AFM) as well as UV-VIS-spectroscopy. The results show that well-defined core-shell systems with just one nanoparticle-core can be synthesized.

CPP 9.21 Mon 16:00 Poster B

Downsizing of Silica — ●TOBIAS PÖPPERL¹, GERALD JOHANNES SCHNEIDER¹, MATTHIAS KELLERMEIER², REGINA KLEIN², and DIETMAR GÖRITZ¹ — ¹Institut für Physik, Universität Regensburg, 93040 Regensburg — ²Institut für Physikalische und Theoretische Chemie, Universität Regensburg, 93040 Regensburg

The mechanical properties of elastomers can be influenced to a large extent by introducing different additives - like the active filler silica. Due to the mixing procedure, changes in the filler morphology can occur - for example downsizing of silica clusters. On the other hand, some properties of the elastomer may be independent of the additive itself, but linked to specific properties of the polymer chains that are relevant for the restructuring process. However, it is not possible to examine both of these influences entirely independent of each other.

To learn more about changes in silica morphology, we studied grinded plain silica. For grinding we used a centrifugal force ball mill and repeatedly extracted samples with advancing grinding time. To investigate the structure development in the so obtained samples we used Small Angle X-ray Scattering (SAXS) and Ultra Small Angle X-ray Scattering (USAXS).

CPP 9.22 Mon 16:00 Poster B

Dependence of the Structure of Carbon Black on its Concentration — ●TOBIAS SONNLEITNER, TOBIAS PÖPPERL, GERALD JOHANNES SCHNEIDER, and DIETMAR GÖRITZ — Institut für Physik, Universität Regensburg, 93040 Regensburg

The properties of polymer carbon black compounds strongly depend on the nano scale structure of carbon black. Preliminary experiments showed that for the purpose of investigating the detailed surface structure of nanoparticles small angle x-ray scattering (SAXS) and ultra small angle X-ray scattering (USAXS) are very suitable. The accessible length scales ranges from $d_{min} = 5$ nm to $d_{max} = 650$ nm. In this work we investigated samples of furnace carbon black N356, dispersed in a SBR 1500 matrix. We used filler contents ranging from 9 to 22 percent in volume. The results prove that there are no changes in the overall surface structure due to the filler degree. In the regime of larger length scales one finds a correlation between the mass fractal dimension and the filler loading of N356: The mass fractal dimension of the aggregates is reduced if the filling degree is increased.

CPP 9.23 Mon 16:00 Poster B

Contribution of Carbon Black Features to Tunnel Current — ●TOBIAS SONNLEITNER and DIETMAR GÖRITZ — Institut für Physik, Universität Regensburg, 93040 Regensburg

To get information concerning conductor insulator compounds such as rubber, one possibility is the dielectric spectroscopy. By measuring the dielectric constant of a compound as a function of the frequency of the applied electrical field one gets various information about the sample. On the one hand dielectric experiments deliver information on the conductance of the sample, and on the other hand information on the static limit of the dielectric function. The static limit of the dielectric function in case of higher filling degrees is linked to the amount of polymer chains between the filler particles. And again, the contribution of tunnel currents to the conductance of the sample is linked to the amount of rubber in between the filler particles. We investigated different carbon blacks (N326, N330, N339, N356) in a SBR 1500 matrix. The results of the experiments show that the amount of rubber in between the filler particles and the influence of tunnel currents are linked to a well known carbon black characteristic, the specific surface of the carbon black: greater specific surfaces lead to greater amounts

of rubber in between the filler particles and hence a lower contribution of tunnel currents to the conductance of the sample.

CPP 9.24 Mon 16:00 Poster B

Ultra Small Angle X-Ray Scattering Investigation of Colloidal Crystals in Latex Films — ●RAINER GEHRKE and STEPHAN VOLKHER ROTH — HASYLAB at DESY, Notkestr. 85, D-22603 Hamburg, Germany

Films obtained from coagulated dispersions of core-shell particles with a rigid thermoplastic core (polystyrene) and a soft elastomeric shell (polymethyl methacrylate-polyethylacrylate) form partially ordered structures which behave like photonic crystals [1]. This behaviour depends on the size of the particles. Samples with different particle size ranging from 200 nm to 300 nm have been characterized by means of Ultra Small Angle X-ray Scattering using synchrotron radiation at HASYLAB beamline BW4. In a layer near the film surface the particles form a regular fcc lattice with the (111) netplanes parallel to the surface. This ordering causes Bragg-like reflections in the scattering pattern. The material in-between the layers shows a scattering contribution caused by strong distance correlation without orientational ordering. From the scattering patterns obtained for different angles between the incoming X-ray beam and the film surface information about the degree of orientational ordering can be derived.

[1] T. Ruhl, G.P. Hellmann, *Macromol. Chem. Phys.* 202, 3502 (2001)

CPP 9.25 Mon 16:00 Poster B

SAXS studies of choline carboxylate surfactants - soaps of physiological origin and outstanding solubility — ●REGINA KLEIN¹, DIDIER TOURAUD¹, GERALD SCHNEIDER², TOBIAS PÖPPERL², and WERNER KUNZ¹ — ¹Institut für Physikalische und Theoretische Chemie, Universität Regensburg, 93040 Regensburg — ²Institut für Physik, Universität Regensburg, 93040 Regensburg

Surfactants have been used for centuries in everyday life, e.g. for cleaning purposes or for the formulation of foods. The functionality of soaps derives from their amphiphilic molecular structure which is characterized by a polar head group providing water solubility, and a non-polar tail driving the formation of self-assembled aggregates in solution (micelles and liquid crystals). Common anionic soaps, such as alkali carboxylates, are restricted in their applicability due to their limited solubility in water. Important features such as the washing ability or the solubilising power can be improved by increasing the length of the hydrophobic chain. However, the longer the non-polar tail, the less soluble in water the corresponding surfactant is. A way to enhance the solubility of carboxylate surfactants in water and to ensure at the same time biocompatibility of the system is to replace the conventional alkali counter-ion by a quaternary ammonium ion of biological origin, such as choline ((2-Hydroxyethyl)trimethylammonium). Choline - formerly known as vitamin B4 - plays several key roles in the human body. In the present study, phase diagrams of choline carboxylates (C12-C18) have been established. Structural details such as the micellar shape and size were investigated by small-angle X-ray scattering.

CPP 10: INTERNAL SYMPOSIUM Scattering Experiments I

Time: Tuesday 9:30–12:30

Location: H37

Invited Talk

CPP 10.1 Tue 9:30 H37

Polymer dynamics: From Synthetic Polymers to Biopolymers — ●DIETER RICHTER — Forschungszentrum Jülich, Institut für Festkörperforschung, 52425 Jülich, Germany

In polymeric materials the structures, the macroscopic mechanical and rheological properties and the phase changes are determined to high degree by thermal motion of the atoms and molecules. Most of the relevant dynamics takes place on mesoscopic lengths and time scales in between the picosecond atomic scale and the macroscopic frame. Offering the proper space time observation window, neutron spin echo (NSE) spectroscopy uniquely addresses these motions. We briefly present some key experimental results on the mesoscopic dynamics of polymer systems. We address briefly the standard model of polymer motion, the Rouse model, the role of topological confinement as expressed in the reptation model and finally, processes limiting the confinement * we discuss contour length fluctuations and constraint release of entangled chains. Very recently it became also possible to directly identify large scale internal dynamics of proteins by neutron spin echo. We report the results of these pioneering studies, which most likely will initiate further experiments on the large scale motions of proteins and their relation to the function.

CPP 10.2 Tue 10:00 H37

Glass-Forming Microemulsions and Liquid Dynamics in Soft Confinement — ●THOMAS BLOCHOWICZ¹, TINKA SPEHR¹, ANNIKA FRICKE¹, MARTIN MÜLLER¹, BERNHARD FRICK², and BERND STÜHN¹ — ¹TU-Darmstadt, Germany — ²ILL, Grenoble, France

Recently glass forming liquids have been investigated subject to nanoscale geometrical confinements of various kinds, in order to access changes in the molecular dynamics when the confinement comes close to a characteristic lengthscale of cooperative motion. Most experiments were performed with glass formers confined in nanopores in case of which, however, actual finite size effects are superposed with pressure effects or interactions with the confining walls. A different situation can be found in microemulsions, where, droplets of a hydrophilic substance are stabilized by surfactant molecules in a hydrophobic environment. When the substances involved are chosen properly vitrification in a so-called "soft confinement" can be observed. In our particular case we study droplets of glycerol in a matrix of toluene and m-xylene stabilized by the ionic surfactant AOT. The temperature dependent structure of these systems is investigated by small-angle X-ray and neutron scattering, whereas for the dynamical behaviour

quasielastic neutron scattering techniques are particularly useful due to their nanoscale spatial resolution. We present time-of-flight and backscattering measurements to access the dynamics of glycerol inside the emulsion droplets. As compared to bulk glycerol pronounced acceleration of the dynamics is observed whereas comparison of core and shell dynamics of the micelles yields almost identical behaviour.

CPP 10.3 Tue 10:15 H37

Starlike dendrimers in solutions: Structural properties and internal dynamics — ●SILKE RATHGEBER¹, MICHAEL MOKENBUSCH², JAMES L. HEDRICK³, MIKAEL TROLLSAS³, and ALICE P. GAST⁴ — ¹Max-Planck Institut für Polymerforschung, Polymer Physik, D-55128 Mainz, Germany — ²Forschungszentrum Jülich GmbH, Institut für Festkörperforschung, D-52425 Jülich, Germany — ³IBM Almaden Research Center, San Jose, California 95120-609, USA — ⁴Department of Chemical Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts 0213, USA

We measured the shape and the internal dynamics of starlike dendrimers under good solvent conditions with small-angle neutron scattering and neutron spin-echo spectroscopy, respectively. [1] Architectural parameters such as the spacer length and generation were varied in a systematic manner. Structural changes occurring in the dendrimers as a function of these parameters are discussed. A first cumulant evaluation of the NSE spectra for each scattering vector q separately yields the length scale dependent relaxation rates $\Omega(q)$. We observe a local minimum in the normalized relaxation rates $\Omega(q)/q^3$ on length scales corresponding to the overall dendrimer dimension. The dynamics is discussed within a Rouse-Zimm approach generalized to the case of starlike dendrimers of arbitrary geometry. The model allows an identification of the modes contributing to the relaxation of the dendrimer. The local minimum is due to collective breathing motions of (parts of) the dendrons relative to each other. Shape fluctuations are not observed. [1] S. Rathgeber et. al., *J. Chem. Phys.* **125**, 204908 (2006)

CPP 10.4 Tue 10:30 H37

Neutron Spectroscopy on nono-confined polymers in comparison with dielectric and thermal results — ●ANDREAS SCHOENHALS¹, BERNHARD FRICK², MARIA MAYOROVA³, and REINER ZORN³ — ¹Federal Institute of Materials Research and Testing, Unter den Eichen 87, D-12205 Berlin — ²Institut Laue-Langevin, B.P. 156, F-38042 Grenoble — ³Research Center Jülich, Institute for Solid State

Research, D-52425 Jülich

The effect of a nanometre confinement on matter is an interesting problem of soft-matter physics. Neutron scattering (NS) is a 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 Boson peak the vibrations at lowest frequencies are depressed by the confinement. The mean square displacement msd was calculated from elastic scans. 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 $S(Q,t)=\text{FT}(S(Q,E))$ is a broadening of $S(Q,t)$ with increasing confinement. These results are discussed together with dielectric measurements. This comparison gives strong evidence that (1) the thermodynamic state in a nanometer confinement is different from that of the bulk and that (2) an inherent length scale might exist for the glass transition.

CPP 10.5 Tue 10:45 H37

The boson peak: Theory of scattering from vibrational excitations in disordered materials — ●WALTER SCHIRMACHER¹, BERNHARD SCHMID¹, GIANCARLO RUOCCO², and TULLIO SCOPIGNO² — ¹Physik-Dept. E13, TUMünchen, D-85747 Garching — ²Dipt. di Fisica, Univ. di Roma, I-00185 Roma

A theory of vibrational excitations in disordered materials¹ and their observation by inelastic light, neutron, X-ray² and nuclear γ -ray scattering³, based on a model with fluctuating shear moduli is presented. The enhancement of the vibrational density of states (DOS) $g(\omega)$ over Debye's $g(\omega) \propto \omega^2$ law ("boson peak") is shown to be a direct consequence of the disorder. The observed spectra in coherent scattering experiments do not in general reveal the DOS directly. Only in incoherent neutron experiments and in nuclear resonant scattering of synchrotron radiation the scattering law is proportional to $g(\omega)$. Raman spectra are shown to reveal the imaginary part $\Sigma''(\omega)$ of the disorder-induced self energy, which is only indirectly related to the DOS, namely to its enhancement over the Debye DOS. The high-frequency sound damping, observed as broadening of the Brillouin line, is also proportional to $\Sigma''(\omega)$. It is shown that the existing spectra can be consistently interpreted in the light of this theory.

- [1] W. Schirmacher, *Europhys. Lett.* **73**, 892 (2006)
- [2] W. Schirmacher, G. Ruocco, T. Scopigno, submitted to *Phys. Rev. Lett.*
- [3] A. I. Chumakov *et al.* *Phys. Rev. Lett.* **92**, 245508 (2004)

15 min. break

Invited Talk

CPP 10.6 Tue 11:15 H37

Time-resolved small-angle neutron scattering — ●ROLAND MAY — Institut Max von Laue - Paul Langevin, BP 156, F-38042 Grenoble Cedex 9, France

Small-angle neutron scattering has a history of about 40 years, but only with the advent of modern fast electronics has it become feasible to penetrate into time regimes that are compatible with reaction rates and process times of biomolecules, polymers and colloids at full detector resolution. Neutron sources cannot compete with the flux or brilliance of X-ray sources. Therefore they are limited as far as the observation of very fast processes is concerned, unless if they can be easily and often repeated, as in cyclic events. Of course, neutrons have the special advantage of neutron contrast variation, allowing one to highlight parts of a structure, and they do not produce any radiation damage. This contribution will address these technical issues and give a number of examples from the slow kinetics of oil droplet formation to the observation of the photocycle of photo-active yellow protein in the tens of milliseconds range, and also mention how one can reach even shorter times with sophisticated time-of-flight techniques.

CPP 10.7 Tue 11:45 H37

Protein Interactions in Aqueous Solution Studied by Small-Angle X-ray Scattering — ●FAJUN ZHANG¹, MAXIMILIAN SKODA^{1,2}, ROBERT JACOBS³, RICHARD MARTIN⁴, CHRISTOPHER MARTIN⁵, and FRANK SCHREIBER¹ — ¹Institut für Angewandte Physik, Universität

Tübingen, 72076 Tübingen, Germany — ²PTCL, University of Oxford, UK — ³CRL, University of Oxford, UK — ⁴Department of Physics, University of Bath, UK — ⁵SRS, Daresbury, Warrington, UK

We have studied protein interactions in two related systems by small-angle x-ray scattering: a series of pure protein solutions with various salt and protein concentrations, and mixtures of protein with oligo(ethylene glycol) (OEG) thiol decorated gold colloids. Structure factors derived from hard sphere potential, screened Coulomb potential, and square well potential, combined with an oblate ellipsoid form factor are used to fit the scattering intensities. An interaction phase diagram has been constructed as a function of ionic strength and protein concentration [1]. For the mixture of protein with functional gold colloid, we present evidence for an attractive interaction between OEG-decorated gold colloids and a repulsive interaction between gold colloid and protein. The attractive potential originates from a depletion force which strongly depends on the size of colloids and the concentration of protein, while the repulsive potential is due to the protein resistance of the OEG monolayer. Indeed, we observed the aggregation of gold colloids, when protein concentration is higher than a critical value.

[1] Zhang, F.; Skoda, M.W.A.; Jacobs, R.M.J.; Martin, R.A.; Martin, C.M.; Schreiber, F. *J. Phys. Chem. B* 2006, in press.

CPP 10.8 Tue 12:00 H37

Surfactant Phase Transitions: New Insights From Time-resolved Small-angle Scattering Experiments — ANNIINA SALONEN¹, JACQUES LENG², PETER SCHURTENBERGER³, and ●STEFAN EGELHAAF⁴ — ¹Institute of Chemistry, Karl Franzens University, 8010 Graz, Austria — ²LOF unité mixte CNRS/Rhodia/Bordeaux, 33608 Pessac, France — ³Department of Physics, University of Fribourg, 1700 Fribourg, Switzerland — ⁴Condensed Matter Physics Laboratory, Heinrich-Heine-University, 40225 Düsseldorf, Germany

Most early studies on surfactant systems have addressed their equilibrium behaviour. These remain a prerequisite for further progress, but attention is turning to nonequilibrium phenomena. I plan to present two recent projects in this area:

First, time-resolved small-angle neutron scattering is used to investigate the intermediate structures during the growth of mixed micelles. The growth of the micelles is induced by a reduction in total surfactant concentration, which is realized by rapid mixing of a surfactant solution with buffer. The subsequent structural changes are followed by time-resolved small-angle neutron scattering.

Second, structural changes during the dissolution of lamellar phase are studied with small-angle x-ray scattering. After contact with water, lamellar phase can form fascinating interface instabilities, so-called myelins. Using time and space resolved small-angle x-ray scattering we investigate the changes in the lamellar phase during the formation and growth of these structures.

CPP 10.9 Tue 12:15 H37

Mapping the local nanostructure inside a specimen by tomographic small-angle x-ray scattering — ●JAN M. FELDKAMP¹, CHRISTIAN G. SCHROER¹, MARION KUHLMANN², STEPHAN V. ROTH², RAINER GEHRKE², NORBERT STRIBECK³, ARMANDO ALMENDAREZ-CAMARILLO³, and BRUNO LENGELER⁴ — ¹Institute for Structural Physics, Dresden University, D-01062 Dresden, Germany — ²HASYLAB at DESY, Notkestr. 85, D-22607 Hamburg, Germany — ³Institute of Technical and Molecular Chemistry, Hamburg University, Bundesstrasse 45, D-20146 Hamburg, Germany — ⁴II. Physikalisches Institut, Aachen University, D-52056 Aachen, Germany

Small-angle x-ray scattering is combined with scanning microtomography to reconstruct the small-angle diffraction pattern in the direction of the tomographic rotation axis at each location on a virtual section through a specimen. These data yield information about the volume-resolved local nanoscale structure of the sample. With rotational symmetry present in the diffraction patterns, e.g., for isotropic or fiber-textured local nanostructure, the full reciprocal space information in the small-angle scattering regime can be reconstructed at each location inside the specimen. The resolution in real space is determined by the size of the x-ray beam. The experiments were performed with the microbeam option at HASYLAB beamline BW4.

Using this new method, we prove the existence of a skin-core structure in injection molded samples, which cannot be detected in classical tomography.

CPP 11: INTERNAL SYMPOSIUM Scattering Experiments II

Time: Tuesday 14:00–18:15

Location: H37

Invited Talk

CPP 11.1 Tue 14:00 H37

Surface sensitive neutron scattering — ●R. STEITZ — Hahn-Meitner-Institut, SF1, Glienicker Str. 100, D-14109 Berlin

Current problems in soft matter science often require insight on the nanometer scale. In this contribution we will show how neutron reflectivity (NR) and grazing incidence small angle neutron scattering (GISANS) can be utilized to reveal details on thin films at solid-liquid and solid-gas interfaces. The first chapter will investigate the structure of the boundary of a hydrophobic polymer film and its adjacent water phase [1]. Chapter two will demonstrate that NR is an excellent tool for monitoring water uptake and respective structural changes in hydrophilic polyelectrolyte films [2] and chapter three will illustrate that application of GISANS can help to clarify transient lateral structures in molecular surfactant layers that are not detectable otherwise[3].

[1] R. Steitz, T. Gutberlet, T. Hauß, B. Klösgen, R. Krastev, S. Schemmel, A. C. Simonsen and G. H. Findenegg, *Langmuir* 19; 2409-2418 (2003). [2] R. Steitz, V. Leiner, R. Siebrecht and R. v. Klitzing, *Colloids and Surfaces A*. 163, 63-70 (2000). [3] R. Steitz, P. Müller-Buschbaum, S. Schemmel, R. Cubitt, and G. H. Findenegg, *EPL* 67, 962-968 (2004).

CPP 11.2 Tue 14:30 H37

X-ray reflectivity study of the adsorption of azacrown ethers and palmitic acid at the hexane-water interface — ●GUTBERLET THOMAS¹, WOJCIECHOWSKI KAMIL², TIKHONOV ALEXEY³, SCHLOSSMAN MARK⁴, and BUFFLE JACQUES² — ¹Lab. f. Neutr. Scattering, ETHZ & PSI, 5232 Villigen PSI, Switzerland — ²CABE, Dept. of Anal., Inorg. and Appl. Chem., University of Geneva, 1211 Geneva 4, Switzerland — ³NLSL, Upton, NY, USA — ⁴Dept. of Phys. and Chem., University of Illinois, Chicago, IL, USA

Azacrown ethers substituted with different alkyl chain length (decyl, palmitoyl, tetracosanoyl) and palmitic acid have been investigated at the aqueous-organic hexane-water interface by means of x-ray reflectivity. These systems are of interest in Permeation Liquid Membrane techniques to separate aqueous solutions by a hydrophobic membrane to select chemical species. The x-ray reflectivity measurements reveal the presence of a dense interfacial layer at the hexane-water interface. The longer alkyl chain substituted azacrown ethers show a diminished interfacial roughness. Here, the experimental set-up and results will be presented in detail and discussed.

CPP 11.3 Tue 14:45 H37

Annexin binding to solid supported membranes: a neutron and synchrotron scattering study — KIRSTIN SEIDEL, JOACHIM RÄDLER, and ●BERT NICKEL — Dep. für Physik, Ludwig-Maximilians-Universität, München

We have developed a microfluidic setup which allows to prepare and observe solid supported membranes by fluorescence microscopy. Two variants exist, one allows for complementary x-ray reflectivity experiments [1], while the other allows for complementary synchrotron studies at 20 keV. The amount of liquid needed is about 2 ml. As a model system, we have chosen Annexin II, which binds in a Ca dependent way to negatively charged membranes. Here, we report neutron reflectivity experiments at Amor (PSI) and Refsans (FRM-2) and compare them with respective synchrotron studies performed at HASYLAB Hamburg and ESRF. The goal of these experiments is to find the configuration of the membrane and the Annexin from the diffraction experiments, while the microscopy experiments allow to determine membrane fluidity with and without Annexin present. Experiments were performed in collaboration with B. Windschiegel and C. Steinem (U. Göttingen). Experiments at Refsans were done in collaboration with GKSS (R. Kampmann et al.)

[1] C. Reich, M. Hochrein, B. Krause, B. Nickel, *Review of Scientific Instruments* 76, 095103 (2005)

CPP 11.4 Tue 15:00 H37

Influence of spacer length and density on the vertical structures of supported membranes studied by neutron reflectivity — ●PETER SEITZ¹, OLIVER PURRUCKER², ANTON FÖRTIG³, RAIMUND GLEIXNER⁴, GIOVANNA FRAGNETO⁵, RAINER JORDAN³, and MOTOMU TANAKA^{1,2} — ¹Physikalisch-Chemisches Institut, Universität Heidelberg, Germany — ²Physik-Department E22, Technische Universität

München, Germany — ³Institut für Technische Chemie, Technische Universität München, Germany — ⁴Max Planck Institute of Biochemistry, Martinsried, Germany — ⁵Institut Laue-Langevin, Grenoble, France

We studied the structure of a new class of polymer-supported membranes, which are separated from the solid substrate via poly(2-methyl-2-oxazoline) spacers of defined length, functionalized with a surface coupling group and hydrophobic membrane anchors. The proximal leaflet was deposited via Langmuir-Blodgett transfer, followed by vesicle fusion to deposit the distal layer. Precise control of the polymer chain length and its lateral density enables the quantitative adjustment of the thickness and the viscosity of the polymer interlayer. Previously, we measured the membrane-substrate distance with fluorescence interference contrast microscopy (FLIC). To gain a deeper insight to the vertical structure of the membrane, we conducted specular neutron reflectivity experiments under a systematic variation of the spacer length and density, and calculated the static roughness and the volume fraction of water in the polymer interlayer.

CPP 11.5 Tue 15:15 H37

Nanotemplate fabrication and macroscopic alignment of nanoscale domains using self-organized diblock copolymers — ●DENIS KOROLKOV, PETER BUSCH, EMMANUEL KENTZINGER, LUTZ WILLNER, and THOMAS BRUECKEL — Forschungszentrum Jülich GmbH, Institut für Festkörperforschung, D-52425, Jülich

Fabrication of macroscopic domains of periodic nanoscale structures using self-organizing systems promises to be a simple and low cost method with potential to produce high-density arrays of magnetic devices [1]. A block-copolymer can self-assemble into microphase separated domains with a spacing of 10-100 nm which strongly depends on molecular weight, segment size, and the strength of interaction between the blocks. Without further constraint, the domains have no preferred orientation and form a disordered "fingerprint" structure.

In this study self-organization of polystyrene-polybutadiene (dPS-PB) diblock copolymer with various thicknesses and molecular weights was investigated. Using pre-structured Si wafer with gratings[2] of 1 μ m period and depth of 60 nm we were able to achieve a macroscopic alignment of polymer domains.

Structural characterization, in particular the degree of long-range order was done by combining a surface-sensitive technique like atomic force microscope (AFM) with grazing incidence small angle scattering (GISAS).

[1] I. W. Hamley *Nanotechnology* 14 (2003) R39-R54

[2] D. Sundrani, S.B. Darling, S.J. Sibener *Nano Lett.*, Vol. 4, No. 2, 2004

15 min. break**Invited Talk**

CPP 11.6 Tue 15:45 H37

Coherent x-ray studies of polymer membrane fluctuations and colloidal dynamics near the glass transitions — ●SIMON MOCHRIE — Department of Physics and Applied Physics, Yale University, New Haven, CT 06520, USA

This talk will briefly review the emerging technique of x-ray photon correlation spectroscopy (XPCS). Then, it will describe XPCS measurements of the dynamics of self-assembled block copolymer membranes within a dilute vesicle (L4) phase and within in a sponge (L3) phase which occur in homopolymer-triblock copolymer blends. In the L4 phase, the results are consistent with predictions for the dynamics of isolated membranes. In the L3 phase, there is a crossover from stretched exponential relaxations to highly-unusual compressed exponential relaxations. In the third part of the talk, the results of very recent measurements will be presented of the dynamics within a dense colloidal suspension in a binary fluid mixture. These measurements reveal the existence of re-entrant glassy behavior in this system, and further highlight the promise of the XPCS method at the next generation of high-brightness x-ray sources, such as PETRA III.

This work was carried out at beamline 8-ID at the Advanced Photon Source at Argonne National Laboratory in collaboration with Xinhui Lui, Peter Falus (Yale), Matt Borthwick (MIT), Suresh Narayanan, Alec Sandy, and Michael Sprung (APS) and is supported by the US

NSF via DMR 0453856.

CPP 11.7 Tue 16:15 H37

Speckle echo-technique for diffusing-wave spectroscopy of soft solids — ●PAVEL ZAKHAROV and FRANK SCHEFFOLD — University of Fribourg, Fribourg, Switzerland

We present a detection scheme for diffusing-wave spectroscopy (DWS) based on a two-cell geometry that allows efficient multi-speckle averaging with a single-mode detection. This is achieved by placing a fast-rotating diffuser in the optical path between laser and sample. We show that the recorded (multispeckle) correlation echoes provide an ensemble averaged signal without lengthy time averaging. Furthermore, combined with traditional two-cell DWS, the full intensity autocorrelation function can be measured with a single experimental setup. The scheme provides access to a large range of correlation times thus opening an experimental window for the study of slowly relaxing and arrested systems, such as viscoelastic complex fluids, colloidal glasses, and gels. We also demonstrate how the technique can be used to monitor dynamic properties of samples that evolve in time

CPP 11.8 Tue 16:30 H37

Bending elasticity of DPPC vesicles with changing cholesterol content — LAURA RODRIGUEZ-ARRIAGA¹, GUILLERMO ORTSGIL², ●THOMAS HELLWEG², BELA FARAGO³, CARLOS MENDUINA¹, and FRANCISCO MONROY¹ — ¹Departamento de Química-Física I, Facultad de Ciencias Químicas, Universidad Complutense de Madrid, E-28040 Madrid, Spain — ²Stranski Laboratorium, TU Berlin, Strasse des 17. Juni 124, D-10623 Berlin, Germany — ³Institut Laue-Langevin, Grenoble, France

A combination of neutron spin-echo spectroscopy and photon correlation spectroscopy (PCS) can be used to determine motions in colloidal particles in the nanosecond time range [1] (e.g. film deformation modes). In the present study we used this approach to discriminate membrane shape fluctuations of DPPC vesicles with different cholesterol content from their translational diffusion. The relative amplitude of the translational contribution to the intermediate scattering functions is found to decrease as q increases and the vesicle deformation mode becomes the main contribution to the relaxation function at times short enough, like the ones probed by the NSE technique. We have performed experiments on vesicles with different lipid composition and we have gained some insight in the compositional grounds of the bending elasticity of these models of cellular membranes. The bending elastic constant κ is calculated using the Zilman-Granek approach.

[1] Th. Hellweg, D. Langevin; PRE, **57** (1998) 6825.

CPP 11.9 Tue 16:45 H37

Micellar hydrogels of poly(2-oxazoline) copolymers containing fluorophilic, hydrophilic and lipophilic blocks — ●RUZHA IVANOVA¹, TUNE BONNÉ¹, KELL MORTENSEN², PHILIPP PRANZAS³, THOMAS KOMENDA⁴, KARIN LÜDTKE⁴, RAINER JORDAN⁴, and CHRISTINE PAPADAKIS¹ — ¹Physikdepartment E13, TU München, 85 747 Garching — ²Risø National Laboratory, Roskilde, Denmark — ³GKSS, Geesthacht — ⁴Department Chemie, TU München, 85 747 Garching

The self-assembly of novel amphiphilic poly(2-oxazoline) di- and triblock copolymers containing hydrophilic and fluorophilic and/or lipophilic blocks in aqueous solutions was studied. Small-angle neutron scattering together with contrast matching was used to study the size and the shape of the micelles as well as the effect of the copolymer concentration and the length of the hydrophilic block on the structure. It was shown that lipophilic-hydrophilic and hydrophilic-fluorophilic diblock copolymers do not form common micelles. This result is an important prerequisite for the formation of multi-compartment micelles and hydrogels in aqueous poly(2-oxazoline) systems. The triblock copolymers aggregate into micelles, and at higher concentrations, hydrogels are formed. We could show that the scattering curves of the hydrogels can be described by a coexistence of spherical lipophilic and elongated fluorophilic micellar cores linked by the hydrophilic blocks. Thus the studied poly(2-oxazoline) copolymers have large practical potential as multi-compartment vehicle systems in e.g. medicine or cosmetics.

15 min. break

Invited Talk

CPP 11.10 Tue 17:15 H37

Microbeam Synchrotron Radiation Scattering Experiments in Soft Condensed Matter — ●CHRISTIAN RIEKEL — ESRF, B.P.220, F-38043 Grenoble Cedex France

The talk will review scientific applications of small- and wide-angle X-ray scattering (SAXS/WAXS) techniques with micron- and submicron-sized X-ray beams at the ESRF. The two complimentary techniques are scanning-SAXS/WAXS and single crystal diffraction. I will show a number of scanning applications for synthetic polymers and biopolymers, which allow the generation of "diffraction images" based on the extraction of specific parameters such as local orientation, strain or crystallinity from a series of diffraction patterns. Single crystal microdiffraction has found many applications in protein crystallography but can also be used for small unit-cell biopolymers. This has allowed in the case of A-amylose replacing the combination of fiber diffraction & molecular modeling by atomic scale structural refinement. Microbeams are also very convenient for in-vivo studies of biological processes like silk extrusion, for studying protein aggregation in microfluidic environments or for grazing-incidence scattering (GISAXS) studies on small sample areas. The examples discussed in the review will show the strong interdisciplinary character of synchrotron radiation research.

CPP 11.11 Tue 17:45 H37

Micro-focus GISAXS Investigations of Microcantilever Sensors — ●JOCHEN S. GUTMANN^{1,2}, YAJUN CHENG¹, MINE MEMESA¹, SEBASTIAN NETT¹, 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

Microcantilever sensors (MC) are a versatile class of sensors, with the potential for a high spatial integration of very different analyte sensitivity into a single sensor unit. Polymeric coatings on MC sensors allow for a facile variation in analyte detection due the ease of functional chemical modification of the polymer layer. While homopolymer coatings are easily applied to the MC surface, polymer brushes extend the use of MC sensor technology into liquid environments. [1,2] In order to investigate the lateral structures of the polymer layers 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 of the HASYLAB. [3] The structural information obtained from the grazing incidence scattering experiments is then used to separate the mechanical sensing response of the MC sensor to its changes in structure and surface energy.

[1] Bumbu G.-G., Kircher G., Wolkenhauer M., Berger R., Gutmann J.S., Macromol. Chem. Phys. 2004, 205 (13): 1713-1720 [2] J. Zhao, R. Berger, J. S. Gutmann, Applied Physics Letters, 89, 033110 (2006). [3] M. Wolkenhauer, G.-G. Bumbu, Y. Cheng, S. V. Roth, J. S. Gutmann, Applied Physics Letters, 89, 054101 (2006).

CPP 11.12 Tue 18:00 H37

Polymer-based nanocomposites investigated with micro-GISAXS — ●S.V. ROTH¹, A. VELIGZHANIN¹, H. WALTER², R. DOMNICK³, O. LEUPOLD¹, R. GEHRKE¹, and P. MÜLLER-BUSCHBAUM⁴ — ¹HASYLAB at DESY, Notkestr. 85, D-22607 Hamburg, Germany — ²CSEM SA, Badenerstrasse 569, CH-8048 Zürich, Switzerland — ³Ara-Coatings GmbH & Co. KG, Gundstr. 13, D-91056 Erlangen, Germany — ⁴TU München Physik Department LS E13, James-Frank-Str.1, D-85747 Garching, Germany

Polymer-based nanocomposites allow to combine the extraordinary features of the individual materials forming the nanocomposite. Especially the richness of polymer structures in blend as well as block-copolymer systems in thin film geometry gives rise to new classes of nanocomposite materials. Annealing as a second step in nanocomposite preparation allows for further nanostructuring the polymer film inducing e.g. a definite roughness or particle distribution. In our approach we combine the richness of the polymer structure with a metal coating [1,2]. Such polymer-based metal nanocomposites are widely used in many optical and biotechnological applications. As experimental method to study such nanocomposites, we used microbeam grazing incidence small-angle x-ray scattering at the beamline BW4 of HASYLAB (Hamburg). Our results reveal the dominating influence of the polymer layer in the structure of this nanocomposite.

[1] S.V. Roth et al., *Appl. Phys. Lett.* **82**, 1935 (2003)

[2] S.V. Roth et al., *Appl. Phys. Lett.* **88**, 021910 (2006)

CPP 12: Polymer Physics III: Interfaces

Time: Tuesday 10:00–12:30

Location: H40

CPP 12.1 Tue 10:00 H40

Monte Carlo simulations of tethered chains in contact with an adsorbing surface — ●RADU DESCAS¹, JENS-UWE SOMMER², and ALEXANDER BLUMEN¹ — ¹Albert-Ludwigs-University, Theoretical Polymer Physics, Freiburg — ²Technical University of Dresden, Institute for Theoretical Physics, Dresden

We use MC simulations combined with scaling arguments to study the adsorption of tethered polymer chains at flat surfaces [1]. In the two-dimensional semi-dilute surface regime we analyze the average extension of single chains in the direction parallel and perpendicular to the surface. Our simulation results agree well with previous scaling predictions [2], especially for the parallel extension of the chains and much below the saturation concentration of the adsorbed layer. Increasing the surface concentration, saturation effects influence the adsorption free energy. The investigation of the free energy function leads us to propose a new scaling parameter which controls the saturation behavior in polymer layers. The strong decrease of the fraction of adsorbed monomers per chain with increasing concentration confirms our assumptions. Based on our model we infer the existence of a crossover-scaling region between the semi-dilute and the saturated state. Our results for the chains' extension give further support to our scaling model. Furthermore, we investigate the over-saturated surface regime which can be understood as the coexistence of a brush-like layer formed on top of a saturated adsorption layer.

[1] R. Descas, J.-U Sommer, and A. Blumen, *J. Chem. Phys.* in press.

[2] E. Bouchaud and M. Daoud, *J. Physique* 48, 1991 (1987).

CPP 12.2 Tue 10:15 H40

Polymer rings on structured surfaces — ●PETRA GUTJAHR, REINHARD LIPOWSKY, and JAN KIERFELD — Max Planck Institute of Colloids and Interfaces, Science Park Golm, 14424 Potsdam, Germany

Semiflexible polymer rings such as circular DNA which are adsorbed onto chemically or topographically structured substrate surfaces, exhibit a variety of morphologies. A simple but instructive example is provided by a striped surface domain. Upon increasing the adhesive strength of the striped domain, we find a morphological transition from a round toroidal conformation dominated by bending energy to an elongated configuration, in which the polymer ring is confined to the adhesive stripe. We determine the complete bifurcation diagram of the polymer shapes as a function of their contour length and the ratio of adhesion contrast to bending rigidity. This diagram exhibits several metastable configurations of the semiflexible polymer rings. In addition, these rings can undergo an adhesion transition, at which they bind to the striped domain.

CPP 12.3 Tue 10:30 H40

Submonolayer coverage of long chain alkanes at SiO₂/air interfaces: Nucleation, and phase behaviour - Molecular transportation, and structure formation — ●RALF KÖHLER and HANS RIEGLER — MPI of Colloids and Interfaces, Dept. Interfaces, 14424 Potsdam-Golm, Germany

The ordering behavior of submonolayers of long chain alkanes at SiO₂/air interfaces is a surprisingly complex phenomenon with two-dimensional nucleation, surface flow and structure formation. On-line optical microscopy observations (1) show three growth scenarios depending on the overall alkane coverage. The observed fractal crystallites (2,3) can be related to a process analogous to diffusion-limited aggregation (4). At least two qualitatively and quantitatively different domain shapes can be distinguished which could also be reproduced by computer simulations. 2d-nucleation theory reveals reasonable values for line tension and activation energies. The 2d-geometry also allows the identification of active nucleation sites in comparison to quasi-homogenous nucleated domains. The system also shows the equilibrium coexistence of the solid domains and a fluid alkane film in between whose thickness depends on the temperature. The observed confinement-induced melting temperature shift is in agreement with thermodynamical calculations assuming an effective interface potential. (1) R.Köhler et al., *Appl.Phys.Lett.* 89, 241906 (2006); (2) A.Holzwarth et al., *Europhys.Lett.* 52, 653 (2000); (3) H.Schollmeyer et al., *Langmuir* 19, 5042 (2003); (4) L.Knüfing et al., *Langmuir* 21, 992 (2005)

15 min. break

CPP 12.4 Tue 11:00 H40

Amphiphilic Block Copolymers at the Liquid-Fluid Interface: Dynamics in Different Regimes — ●ANTONIO STOCOC¹, STERGIOS PISPAS², and REINHARD SIGEL¹ — ¹MPI of Colloids and Interfaces, D-14476 Golm — ²Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, Athens, Greece

Structure and dynamics of a block copolymer at the water-air (WA) and the water-dodecan (WD) interface are investigated. Because of its amphiphilic property, polyisoprene-block-polyethyleneoxide (PI-PEO) is attracted to such interfaces. By changes of the interface concentration, the overlap and the stretching of the blocks is varied from the mushroom to the brush regime. The extent of the interfacial polymer layer is followed by reflection ellipsometry. Complementary information is obtained from static and dynamic evanescent wave light scattering. For both types of interface, a 2D diffusion process is found which slows down with increasing interface concentration. The significantly slower diffusion at the WD interface compared to the WA interface is discussed.

CPP 12.5 Tue 11:15 H40

Smectic Layering at Surfactant-laden Isotropic Liquid Crystal/Water Interfaces — ●CHRISTIAN BAHR — Max Planck Institute for Dynamics and Self-Organization, D-37073 Göttingen

Thermotropic liquid crystals exhibit surface-induced order at temperatures where the bulk phase is disordered. Many smectic compounds show in their isotropic phase the formation of a smectic layer at interfaces to air or solid substrates; when the isotropic – smectic-A bulk transition is approached, the ordered surface phase grows in thickness via a series of individual layering transitions. Theoretical models [1] predict complex surface phase diagrams in which the individual layer transition lines end at critical points or collapse at triple points to multiple-layer transitions.

We present here the first study of smectic layering at surfactant-laden liquid crystal/water interfaces. Variation of the surfactant concentration c_s offers an easy way to tune the strength of the ordering surface field [2]. Whereas at higher c_s -values the usual series of single-layer transitions occurs, we observe at low c_s -values layering transitions at which the thickness of the surface phase jumps by a multiple number of single smectic layers. The multiple-layer transition lines split off at triple points into single-layer transition lines. This is the first experimental observation of this type of surface triple points.

[1] Z. Pawłowska, T. J. Sluckin, and G. F. Kventsel, *Phys. Rev. A* **38**, 5342 (1988); A. M. Somoza, L. Mederos, and D. E. Sullivan, *Phys. Rev. E* **52**, 5017 (1995).

[2] Ch. Bahr, *Phys. Rev. E* **73**, 030702(R) (2006).

CPP 12.6 Tue 11:30 H40

Preferred orientations and stability of medium length *n*-alkanes solidified in mesoporous silicon — ●ANKE HENSCHL, TOMMY HOFMANN, PATRICK HUBER, and KLAUS KNORR — Saarland University, Saarbruecken, Germany

The *n*-alkanes C₁₇H₃₆, C₁₉H₄₀, and C₂₅H₅₂ have been imbibed and solidified in mesoporous, crystalline silicon with a mean pore diameter of 10nm. The structures and phase sequences have been determined by x-ray diffractometry. Apart from a reduction and the hysteresis of the melting/freezing transition, we find a set of six discrete orientation states ("domains") of the confined alkane crystals with respect to the lattice of the silicon host. The growth process responsible for the domain selection is interpreted as a nano-version of the Bridgman technique known from single crystal growth. Oxidation of the pore walls leads to extrusion of the hydrocarbons upon crystallization, whereas the solidified *n*-alkanes investigated in non-oxidized, porous silicon are thermodynamically stable.

CPP 12.7 Tue 11:45 H40

C60 modified PPO Polymer Membranes: Free Volume by Positron Annihilation Lifetime Spectroscopy — ●JAN KRUSE¹, KLAUS RÄTZKE¹, FRANZ FAUPEL¹, DANA STERESCU², DIMITRIOS STAMATIALLIS², and MATTHIAS WESSLING² — ¹Universität

Kiel, Lehrstuhl für Materialverbunde, Kaiserstr. 2, 24143 Kiel —
 2University of Twente, Membrane Technology Group, P.O. Box 217,
 7500 AE, Enschede

PPO (poly(2,6-dimethyl-1,4-phenylene oxide)) is a well known membrane material showing good gas separation properties. Addition of nanoparticles can greatly enhance the performance of composite membranes. We have modified PPO polymer with C60 buckyballs up to a content of 2wt%. Permeability experiments show a strong dependence on whether the C60 is dispersed in the polymer or chemically bonded to the polymer chains. Free volume studies performed by positron annihilation lifetime spectroscopy (PALS) were performed on samples with different C60 concentrations. Spectra of all samples containing C60 exhibit an additional large positronium lifetime, indicating large local free volume elements. The orthopositronium intensity decreases with increasing C60 content, stronger for chemically bonded than for dispersed C60. As the inhibition of positronium formation can be attributed to the C60 molecules, this will be discussed with respect to the homogeneity of distribution.

CPP 12.8 Tue 12:00 H40

New observations during onset and final stages of capillary-breakup experiments on semidilute polymer solutions —
 •RAINER SÄTTLER and CHRISTIAN WAGNER — Universität des Saarlandes, Geb. E2 6 3.OG, Postfach 151150, 66041 Saarbrücken

We investigate the droplet-pinching and capillary-breakup of polymer solutions using high speed video microscopy. Recent experiments on semidilute solutions of Polyethylene Oxide were performed to examine the nature and prerequisites for the supposedly iterative formation of

beads on the thinning filament, which form as the extension of the polymers saturates.

There are clear indications for concentration enhancement during the formation of the different generations of beads not taken into consideration in existing models. Special emphasis is put on the discussion which mechanisms control the onset of the instability. We found indirect evidence showing that besides inertial effects modes of capillary waves at amplitudes below the resolution of optical microscopy cause dramatic deviations from expectations assuming a simple extensional flow during the thinning of the capillary bridge.

The presented experimental results can contribute to a better understanding of the growth of these instabilities and the behaviour of polymers in extensional flow relevant for technical and biological processes as well as giving reason for enhancements in theoretical description.

CPP 12.9 Tue 12:15 H40

Oscillating Phase Separation in Polymer Solutions — DORIS VOLLMEYER and •GÜNTER AUERNHAMMER — MPI für Polymerforschung, Ackermannweg 10, 55128 Mainz

The kinetics of phase separation of polymer solutions under slow cooling is discussed. For a broad range of compositions (about 1g/L until 20g/L) and cooling rates (cooling rates below about 5K/h) the mixtures show pronounced oscillations in the heat capacity and the turbidity. Whereas the oscillations in the heat capacity seem to be due to the gel phase, the oscillations in the turbidity are due to the sol phase. The period of the oscillation does not depend on composition within the investigated temperature interval. The oscillations are of thermodynamic origin.

CPP 13: Polymer Physics IV: Thin Films

Time: Tuesday 14:30–17:15

Location: H40

CPP 13.1 Tue 14:30 H40

Graphitizing polyimide surfaces — •IRINA LAZAREVA, YURI KOVAL, M. ALAM, STEFAN STRÖMSDÖRFER, SLAVA DREMOV, and PAUL MÜLLER — Physikalisches Institut III, Universität Erlangen-Nürnberg Erwin-Rommel Str. 1, 91058 Erlangen, Germany

Various polymers can be converted to conducting state by ion irradiation. Recently we demonstrated that irradiation with Ar⁺ ions of energies even as low as 150 eV is effective. In contrast to high-energy ion bombardment, low-energy ion irradiation transforms only a thin surface layer. Depending on the irradiation conditions, the conducting layer can be partly or completely graphitized. We present our experimental results of graphitization of polyimide by Ar⁺ ions with energies between 150 eV and 1000 eV. The surface of the irradiated polyimide was investigated by atomic force and scanning tunneling microscopy. The atomic structure of the irradiated polyimide surface confirms the graphitic nature of the conducting layer. Transport properties of the graphitized layers were studied in the temperature range between 4.2 and 300 K. For high resistive films, the conductivity is provided by variable-range hopping. At high electric fields, the conductivity of the graphitized polyimide can be described by a Poole-Frenkel model. At temperatures below 10 K, tunneling becomes the main process of ionization, and a crossover to Fowler-Nordheim emission was observed. For higher radiation fluencies and higher process temperatures, the conductivity increased significantly and we observed semi-metallic behavior.

CPP 13.2 Tue 14:45 H40

Reversible charge storage and modification of thin polymer films investigated by electrostatic force microscopy — •ANDREAS KLEINER¹, OTHMAR MARTI¹, ARMIN KNOLL², BERND GOTSCHMANN², and URS DÜRIG² — ¹Institute of Experimental Physics, Ulm University, 89069 Ulm, Germany — ²IBM Research GmbH, Zurich Research Laboratory, 8803 Rüschlikon, Switzerland

Atomic force microscope (AFM) modes like force curve measurements, Pulsed Force Mode or intermittent contact techniques apply certain amounts of normal and lateral forces to the sample. In most cases this creates surface charges, similar to the macroscopic contact electrification of insulators. These charges can be imaged by Kelvin Probe or Electric Force Microscopy (KPFM / EFM). The quantity of charge depends on parameters like contact time, applied force or scanning velocity. By adjusting the tip voltage during contact, the amount and

polarity can be controlled and charges can be erased and overwritten without change in the polymer structure. High voltages between tip and sample lead to raised topographic features due to the large non-uniform electric field. The height of these structures reaches several nanometers, depending on tip shape and applied voltage, and is reversible. Long-term measurements of these surface charges on different polymers at various temperatures will lead to a better understanding of charge storage and transport mechanisms on thin films.

CPP 13.3 Tue 15:00 H40

Assembly of diblock copolymers on patterned substrates: A “Single-Chain-in-Mean-Field-Simulation” study — •MARCUS MÜLLER and KOSTAS DAOULAS — Institut fuer Theoretische Physik, Georg-August Universitaet, Goettingen

The directed assembly of diblock copolymers on patterned substrates is a way to create nanoscopically structured materials. We study the structure and kinetics of diblock copolymers on patterned substrates by simulating a large ensemble of independent chains in an external field. This external field depends on the density created by the ensemble of molecules and it is frequently updated as to mimic the instantaneous interactions of a molecule with its neighbors. This approximate, particle-based self-consistent field method allows to (i) incorporate arbitrary chain architecture (ii) includes fluctuations and (iii) the explicit propagation of the chain conformations in time permits us to study the kinetics of structure formation. The factors that control the accuracy of the method are quantitatively discussed [1] and the reconstruction of the soft morphology at substrate patterns that deviate from the periodic morphology of the diblock in the bulk are illustrated [2].

[1] K. Ch. Daoulas and M. Muller, J. Chem. Phys. 125, 184904 (2006); [2] K. Ch. Daoulas et al, Phys. Rev. Lett. 96, 036104 (2006)

CPP 13.4 Tue 15:15 H40

Demixing and dewetting in films of binary mixtures — •SANTIAGO MADRUGA and UWE THIELE — Max Planck Institute for the Physics of Complex Systems, Noethnitzer Str. 38, 01187 Dresden

Thin polymer films are often used in advanced technological applications either as homogeneous coatings or as structured functional layers. Their stability and therefore potential usage is mostly determined by the wettability properties of the substrate and is rather well understood for single component liquids.

However, in various applications the film consists of a binary mix-

ture such as a polymer blend. Then the dynamics of the decomposition in the film and of dewetting of the film couple. This allows for new pathways of structuring like decomposition induced dewetting [1]. We complete the bulk description of the dynamics of a binary mixture (model-H) [2] with boundary conditions for the evolving free surface.

The model is used to analyse the spinodal decomposition of a film of a binary mixture. The composition gradients give rise to a solutal Marangoni effect that modifies the dynamics deeply. Linear results obtained with the full transport equations for (a) purely diffusive transport described by the Cahn-Hilliard equation and (b) diffusive and convective transport described by model-H between parallel plates are compared to the case of a free surface.

We acknowledge support by the EU under grant MRTN-CT-2004-005728. [1] R. Yeushalmi-Rozen, T. Kerle, and J. Klein. *Science*. 285, 1254-1256 (1999); [2] D.M. Anderson, G.B. McFadden, and A.A. Wheeler. *Ann. Rev. Fluid Mech.* 30, 139-165 (1998).

CPP 13.5 Tue 15:30 H40

Molecular-dynamics simulations of thin films with a free surface — ●SIMONE PETER, HENDRIK MEYER, and JOERG BASCHNAGEL — Institut Cahrles Sadron, Strasbourg, France

We present results [1,2] from molecular-dynamics simulations for a model of non-entangled short polymer chains in a free standing and a supported film geometry. We investigate the influence of confinement on static and dynamic properties of the melt. We find that the relaxation at the surfaces is faster in comparison to the bulk. We perform a layer-resolved analysis of the dynamics and show that it is possible to associate a gradient in critical temperatures $T_c(y)$ with the gradient in the relaxation dynamics. This finding is in qualitative agreement with experimental results on supported polystyrene (PS) films [Ellison et al, *Nat. Mater.* 2, 695 (2003)].

Furthermore we show that the y -dependence of $T_c(y)$ can be expressed in terms of the depression of $T_c(h)$, the global T_c for a film of thickness h , if we assume that $T_c(h)$ is the arithmetic mean of $T_c(y)$ and parameterize the depression of $T_c(h)$ by $T_c(h) = T_c / (1 + h_0/h)$, a formula suggested by Herminghaus et al [*Eur. Phys. J E* 5, 531 (2001)] for the reduction of the glass transition temperature in supported PS films. We demonstrate the validity of this formula by comparing our simulation results to results from other simulations and experiments.

[1] S. Peter, H. Meyer and J. Baschnagel, *J. Polym. Sci. B*, 44, 2951 (2006)

[2] S. Peter, H. Meyer, J. Baschnagel and R. Seemann, *J. Phys: Condens. Matter* (2007)

30 min. break

CPP 13.6 Tue 16:15 H40

Investigation of Polymer Surfaces by Dynamic Force Spectroscopy — ●JAN-ERIK SCHMUTZ^{1,2} and HENDRIK HÖLSCHER^{1,2} — ¹CeNTech, Heisenbergstr. 11, 48149 Münster — ²University of Münster, Wilhelm-Klemm-Str. 10, 48149 Münster

The atomic force microscope (AFM) is often used in dynamic modes to enhance the resolution compared to the conventional contact mode. The tapping mode where the cantilever is oscillating with a fixed frequency near the sample surface is the standard mode used in air and liquids. With a slight modification of the excitation it is possible to gain more information about the sample surface. This so-called constant-excitation mode (CE-mode) enables the direct and continuous determination of conservative and dissipative tip-sample interactions [1]. Recently, we demonstrated the application of this technique to self-organizing DPPC films [2] which are frequently used as model systems for biological membranes. Beside a comparable resolution to the tapping mode this technique also gives quantitative information about the material properties like adhesion force and contact stiffness. Here we apply this technique to the copolymers acrylonitrile butadiene styrene (ABS) and styrene butadiene styrene (SBS). The advantages of the CE-mode compared to the tapping mode will be discussed.

[1] H. Hölscher, B. Anczykowski, *Surf. Sci.* 579, 21 (2005)

[2] J.-E. Schmutz, M.M. Schäfer, H. Hölscher (submitted)

CPP 13.7 Tue 16:30 H40

Thin Films of Semifluorinated Liquid Crystalline Side Chain Block Copolymers — ●PETER BUSCH^{1,2,3}, SITARAMAN KRISHNAN², MARVIN PAIK², GILMAN TOOMBES⁴, SOL GRUNER^{3,4}, and CHRISTOPHER OBER² — ¹JCNS-FRMI, Lichtenbergstr. 1, TU München, 85747 Garching — ²Department of Materials Science and Engineering, Cornell University, USA — ³Cornell High Energy Synchrotron Source (CHESS), Cornell University, USA — ⁴Department of Physics, Cornell University, USA

Fluorinated materials are interesting as coatings because of their low surface free energies. One possible approach to increase processability is the incorporation of semifluorinated alkenes as side chains to a polymer backbone, which is part of a diblock copolymer. [1] The side chains arrange into liquid-crystalline, smectic layers, which increases the structural complexity compared to block copolymers with two amorphous blocks.

We present an X-ray study of a thin film of a diblock copolymer consisting of a polystyrene block and a semifluorinated, liquid-crystalline (LC) block. The focus will be the interplay between the self organization of the side chains into smectic layers and the mesoscopic arrangement of the polystyrene blocks with respect to the LC-block, which is strongly related to the surface properties of the films.

[1] S. Krishnan, Y.-J. Kwark and C. K. Ober, *The Chemical Record*, 2004, 4, 315.

CPP 13.8 Tue 16:45 H40

Manipulation of smectic layers thickness in smectic elastomers by means of uniaxial stretching — ●VICTOR AKSENOV¹, MARTIN RÖSSLE², RALF STANNARIUS¹, and RUDOLF ZENTEL² — ¹Otto-von-Guericke-Universität Magdeburg, Institut für Experimentelle Physik, Universitätsplatz 2, D-39106 Magdeburg — ²Universität Mainz, Institut für Organische Chemie, Duesbergweg 10-14, D-55099 Mainz

The deformations of thin oriented films of smectic liquid crystal elastomers (LCE) have been studied on macroscopic and microscopic levels by small angle x-ray scattering (SAXS), optical reflectometry and polarized Fourier transform infrared (FTIR) spectroscopy [1, 2, 3] The polymeric network couples the microscopic characteristics such as director orientation and order parameter to the macroscopic dimensions of LCEs. For the material investigated in this work, it has been found that during stretching of free standing films with smectic layers parallel to the film surface, the optical thickness of the sample changes [1]. Small angle X-ray scattering (SAXS) measurements revealed the compression of the smectic layers in the SmA and SmC* phases [1]. The deformation induced tilt measured by polarized FTIR spectroscopy [3] is too small to explain the compression of the smectic layers.

[1] V. Aksenov, J. Bläsing, R. Stannarius, M. Rössle, and R. Zentel, 2005, *Liquid Crystals*, 32, No. 7, 805-813. [2] R. Stannarius, V. Aksenov, J. Bläsing, A. Krost, M. Rössle and R. Zentel, *Phys. Chem. Chem. Phys.*, 2006, 8, 2293-2298. [3] V. Aksenov et al. 2008, *Liquid Crystals* (In press).

CPP 13.9 Tue 17:00 H40

Orientation and structural changes upon uni- and biaxial drawing of polyamide 6 — ●HUSSEIN SHANAK¹, KARL-HEINZ EHSE¹, JAN LION¹, PETER LEIBENGUTH², and ROLF PELSTER¹ — ¹FR 7.2, Experimentalphysik, Universität des Saarlandes, Postfach 151150, 66041 Saarbrücken — ²Lehrstuhl für Funktionswerkstoffe, Universität des Saarlandes, Postfach 151150, 66041 Saarbrücken, Germany

The influence of drawing on orientation, crystallinity, structural properties and anisotropy of polyamide 6 films was investigated. The samples were uniaxially and biaxially stretched. Their crystallinity as well as size and orientation of the crystallites were evaluated using X-ray diffraction. The orientation was analyzed using pole figures and hermans functions. In case of uniaxial drawing, the crystallinity increases and the films show strong orientation with increasing drawing ratio. The orientation of the biaxially drawn films is high and it is inhomogeneous, depending on the position on the film. The structural data is correlated with dielectric anisotropy that was measured at microwave frequencies.

CPP 14: Biological Systems

Time: Tuesday 10:00–12:30

Location: H47

CPP 14.1 Tue 10:00 H47

DFT studies for structure, energetics, dynamics and electronics of glycine, alanine, and cysteine — ●ROBERT MAUL¹, KARSTEN HANNEWALD², FRANK ORTMANN², MARTIN PREUSS², and FRIEDHELM BECHSTEDT² — ¹Institut fuer Nanotechnologie, Forschungszentrum Karlsruhe, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen — ²Institut fuer Festkoerpertheorie und -optik, Friedrich-Schiller-Universitaet, Max-Wien-Platz 1,07743 Jena, Germany

The gas-phase geometries of the most stable conformers of glycine, alanine, and cysteine were optimized using a plane-wave density functional theory implementation in the VASP code. Different approximations for the exchange-correlation functional like LDA, GGA-PW91, and the hybrid functional PBE0 allow for an estimation of the non-local contribution of the functional to several geometry parameters and relative energies. Furthermore we calculated dipole moments and infrared spectra of the three most stable conformers of glycine, alanine and cysteine in good agreement with experimental results. In addition the calculated ionisation- and two particle excitation energies deviate only by 3% from the experimental values. Therefore it can be concluded that DFT-GGA performs comparably well with respect to accuracy and the speed of calculation, which permits the investigation of more complicated systems.

CPP 14.2 Tue 10:15 H47

Dissipative single- and two-electron transfer via bridges — ●SABINE TORNOW¹, F. ANDERS², and R. BULLA¹ — ¹Theoretical Physics III, Center for Electronic Correlations and Magnetism, University of Augsburg — ²Institute of theoretical Physics, University of Bremen

Electron transfer (ET) reactions are common in chemical, physical and biological systems and are often performed via bridges. Dependent on the energy of the bridge and coupling to the environment the process can be an incoherent sequential ET or a coherent superexchange mediated ET. With the help of the time dependent Numerical Renormalization Group we investigate the coherent and incoherent dynamics in the nuclear tunnelling regime. Furthermore, we discuss the multi-electron dynamics when we include two excess electrons into the system at low as well as large temperatures.

CPP 14.3 Tue 10:30 H47

How finite (Ala)_n polypeptides are stabilized by H bond cooperativity: A numeric atom-centered orbital based first-principles study — ●VOLKER BLUM, JOEL IRETA, and MATTHIAS SCHEFFLER — Fritz-Haber-Institut, Faradayweg 4-6, D-14195 Berlin

An infinite alpha-helical polypeptide (Ala)_∞ is clearly stable over a fully extended conformation. This stabilization is brought about by hydrogen bonds. In finite polypeptide chains, the strength of these crucial bonds depends on the length and environment of the helix, so that, e.g., a short α -helical polypeptide segment (Ala)₄ is actually *less* stable than a fully extended conformation. We here use all-electron density functional calculations in the PBE generalized gradient approximation by a recently developed, computationally efficient numeric atom-centered orbital based code¹ to investigate this H-bond *cooperativity* that is *intrinsic* to Alanine-based polypeptides (Ala)_n ($n=1-20,\infty$). We compare finite and infinite prototypical helical conformations (α , π , 3_{10}) on equal footing, with both neutral and ionic termination for finite (Ala)_n peptides. Moderately sized NAO basis sets allow to capture E_{hb} with meV accuracy, revealing a jump in E_{hb} (cooperativity) when two H-bonds first appear in line, followed by slower and more continuous increase of E_{hb} towards $n \rightarrow \infty$. ¹ V. Blum, R. Gehrke, P. Havu, V. Havu, X. Ren, M. Scheffler, *The FHI Ab Initio Molecular Simulations (aims) Project*, Fritz-Haber-Institut, Berlin (2006).

15 min. break

CPP 14.4 Tue 11:00 H47

Single molecule fluorescence at microstructured nanopatterns — ●ALEX G F DE BEER¹, MARCO SCHWIEDER^{1,2}, EVA BOCK^{1,2}, GUENTER MAJER¹, and JOACHIM P SPATZ^{1,2} — ¹Max-Planck Institute for Metals Research, Dept. of New Materials and Biosystems,

Heisenbergstrasse 3, D-70569 Stuttgart, Germany — ²University of Heidelberg, Dept. of Biophysical Chemistry, Im Neuenheimer Feld 253, D-69120 Heidelberg, Germany

Nanopatterns created using self assembly of block copolymer micelles can be used as a negative resist for electron beam lithography. This allows the preparation of surfaces consisting of patches of gold nanodots [1].

We use TIRF single molecule microscopy to study thiol-modified Alexa 488 labelled streptavidin molecules attached to single gold dots. The stoichiometry of attachment is of interest, along with electrodynamic interactions between the dye molecules and the gold dots. The size of the streptavidin molecule (roughly 6 nm) is small enough so that it fully lies within the interaction range of a gold particle (about 16 nm) [2]. We show a clear influence of the nanopattern on the properties of the dye, with an increased photobleaching resistance and decreased dye intensity. Using this decreased fluorescence intensity and accompanying increased photostability, it is possible to generate a photobleaching contrast between bound and unbound molecules, thus allowing to selectively image bound molecules only.

[1] R. Glass et al., *Advanced Functional Materials* 13, 569-575 (2003)

[2] E. Dulkeith et al., *Nano Lett.* 5(4), 585-589 (2005)

CPP 14.5 Tue 11:15 H47

Mineral phase distribution in biological composite material of a crustacean model organism — ●SABINE HILD¹, OTHMAR MARTI², and ANDREAS ZIEGLER¹ — ¹Central Facility for Electron Microscopy; University of Ulm, Albert-Einstein-Allee 11, 89069 Ulm — ²Experimental Physics; University of Ulm, Albert-Einstein-Allee 11, 89069 Ulm

Mineralized biological composites have attracted increasing interest because of their outstanding mechanical properties that are well adapted to their function. The mineralized exoskeleton (cuticle) of crustaceans is an excellent model in this field. To learn more about the properties, function and formation of biomaterials, we studied the spatial distribution of minerals, elements, and organic compounds within the cuticle of the terrestrial isopod *Porcellio scaber* on the sub-micrometer scale using confocal micro-Raman microscopy, REM and SFM. In cross-sections of the cuticle we found calcite and amorphous calcium carbonate (ACC) as the main biominerals. For the first time, we show that minerals are arranged in distinct layers. Calcite is restricted to the outer area of the cuticle, whereas ACC is localized in the middle having only little overlap with the calcite layer. Since the cuticle is subjected to periodic molting it is periodically decalcified and shed. A new larger cuticle, synthesized before shedding, is mineralized after every molt. These processes cause spatial and temporal variations of the mineral distribution. We show that the protective outer calcite layer is shed away during each molt, while ACC is recycled to quickly re-establish the protective calcite layer in the new cuticle.

CPP 14.6 Tue 11:30 H47

Hydration of Oligo(ethylene glycol) Self-Assembled Monolayers: An in situ PMIRRAS study — ●MAXIMILIAN SKODA^{1,2}, ROBERT JACOBS³, and FRANK SCHREIBER² — ¹Physical and Theoretical Chemistry Laboratory, Oxford University, UK — ²Angewandte Physik, Universität Tübingen, Germany — ³Chemistry Research Laboratory, Oxford University, UK

The interaction with water of protein-resistant monolayers (SAMs), self-assembled from (triethylene glycol) terminated thiol HS(CH₂)₁₁(OCH₂CH₂)₃-OMe solutions, was studied using in and ex situ polarization-modulated Fourier transform infrared spectroscopy. In particular, shifts in the position of the characteristic C-O-C stretching vibration were observed after the monolayers had been exposed to water. The shift in frequency increased when the SAM was observed in direct contact with a thin layer of water. It was found that the magnitude of the shift also depended on the surface coverage of the SAM. These findings suggest a rather strong interaction of oligo(ethylene glycol) SAMs with water and indicate the penetration of water into the upper region of the monolayer. Since the complexity of this system requires careful consideration of experimental parameters, some theoretical aspects of the signal generation will be discussed.

CPP 14.7 Tue 11:45 H47

Mechanical Properties of Polypeptide by using Atom Force Microscopy — ●KAITIAN LI, JENS HENTSCHEL, HANS BÖRNER, and ANDREAS FERY — Max-Planck-Institut für Kolloid und Grenzflächen, Am Mühlenberg 14424 Potsdam

Helical, tube- or tape-like structures formed by peptide self aggregation are a common motive found in biological systems. In this work, we explore the mechanical properties of such tubular aggregates formed from well defined synthetic block-copolymers, which consist of a peptide block which triggers self aggregation and conventional polymeric blocks. The amino acid sequence of the peptide encodes a high tendency to adopt an antiparallel β -sheet motif, and thus programs the formation of tapelike microstructures. The helical superstructures undergo defined entanglement to form superhelices. A twisted two-dimensional core-shell tape is proposed as a structure model, in which the peptide segments form an antiparallel β -sheet with a polymer shell. [1] Here, we discovered that the resulting helical superstructures, when deposited on a substrate, are 2.9 nm high, 10 nm wide, and up to 2.3 μ m long. We also try to measure their mechanical properties, which we directly measured through indentation type experiments using atomic force microscopy. We find that these structures which on the silicon substrate are deucedly soft and flexible. They could easily be deformed even by soft cantilever ($K \sim 0.05$). From the averaged point we can have a correspondingly Young's modulus as calculated by finite element analysis. We also plan test their bending elasticity by using a novel AFM based approach.

CPP 14.8 Tue 12:00 H47

Looping charged elastic rods — ●ANDREY CHERSTVY and RALF EVERAERS — Max-Planck-Institut für Physik Komplexer Systeme, Nöthnitzer Straße 38, D-01187 Dresden, Germany

Finding optimal shape of a charged elastic rod under external torque and forces, as a minimum of rod elastic [1] and electrostatic (el) energy, is a complicated problem [2]. We calculate el energy of DNA loops and planar untwisted DNA rings [3]. We sum Debye-Hueckel el potentials between charges on bent/looped rod. Equilibrium loop shape [4] is unchanged by el interactions and loops have no self-contacts. DNA

charges are modeled as straight or helical arrays. For large loops the excess el energy of DNA bending is well described by OSF theory of rod el persistence length. For small loops (eg. DNA wrapped around histones or DNA bent by lac-repressor [2]) the OSF assumptions are violated and el energies obtained are larger. For large rings the actual el excess energy is larger than OSF prediction due to a final penalty of approaching two DNA ends into a contact upon cyclization. For small circles, as there are not so many charges to sum over, the OSF underestimates el energy, especially at low salt. Our results are relevant to description of tight DNA looping in DNA-proteins complexes [2,5] and to cyclization of short DNAs [6] as a function of added salt.

[1] A.E.H. Love, Dover, NY (1944). [2] D. Swigon, et al., PNAS 103 9879 (2006). [3] A.G. Cherstvy and R. Everaers, in preparation. [4] J. Coyne, IEEE J. Ocean. Ing., 15 72 (1990). [5] A.G. Cherstvy et al., JPCB, 109 2962 (2005). [6] L. Czapla, et al., J. Chem. Th. Comput. 2 685 (2006) and refs. therein.

CPP 14.9 Tue 12:15 H47

Non-affine rubber elasticity for stiff polymer networks — ●CLAUS HEUSSINGER and ERWIN FREY — Arnold-Sommerfeld-Center, Ludwig-Maximilians Universität, München

The elastic response of cross-linked stiff polymer networks is usually interpreted in terms of affine stretching models, adopted from the theory of rubber-elasticity valid for flexible polymer gels. Unlike flexible polymers, however, stiff polymers have a highly anisotropic elastic response, where the low-energy elastic excitations are actually of bending nature. As a consequence, similar to springs connected in series, one would expect the softer bending mode to dominate the elastic energy rather than the stiff stretching mode. We propose a theory that, unlike recent affine models, properly accounts for the soft bending response of stiff polymers. It allows calculating the macroscopic elastic moduli starting from a microscopic characterization of the (non-affine) deformation field. The calculated scaling properties for the shear modulus are in excellent agreement with the results of recent simulations obtained in simple two-dimensional model networks, and can also be applied to rationalize bulk rheological data in reconstituted actin networks.

CPP 15: Diffusion and Transport Processes

Time: Tuesday 14:30–16:45

Location: H47

CPP 15.1 Tue 14:30 H47

Effect of coarse-graining on the dynamics of fluid mixtures: how important is the structure? — ●JÖRG SILBERMANN, SABINE KLAPP, and MARTIN SCHOEN — Stranski-Laboratorium für Physikalische und Theoretische Chemie, Sekretariat C7, Technische Universität Berlin, Straße des 17. Juni 115, D-10623 Berlin, Germany

We consider a colloidal model suspension consisting of large solute (A) particles immersed in a bath of smaller (B) particles with all interactions being of the Lennard-Jones type. This (reference) system is systematically simplified (coarse-grained) by replacing the original B particles by a reduced number of larger and heavier ones such that the mass and volume fraction of B particles is kept constant. Using Boltzmann inversion we adjust the (effective) intermolecular interactions between A particles in the coarse-grained system such that the static A - A structure of the reference system is preserved. By means of this procedure a whole set of systems is generated all exhibiting the same static A - A structure regardless of the degree of coarse-graining. We take the mass ratio of A and B particles to vary between 64 (reference system) and 1. Based on molecular dynamics (MD) computer simulations we identify the effects that coarse-graining of the solvent imposes on typical microscopic time correlation functions characterizing the single-particle and collective dynamics of the solute. Our results [1] indicate that coarse-graining may have a pronounced effect on the dynamics of the solute depending on the total packing fraction of the binary mixture.

[1] J. R. Silbermann et al., *Mol. Phys.*, (2006) submitted.

CPP 15.2 Tue 14:45 H47

Temperature Dependence of Positron Lifetime in a Polymer of Intrinsic Microporosity — ●KLAUS RÄTZKE¹, RODRIGO LIMA DE MIRANDA¹, JAN KRUSE¹, FRANZ FAUPEL¹, DETLEV FRITSCH², VOLKER ABETZ², PETER BUDD³, JAMES SELBIE³, NEIL MCKEOWN⁴, and BADER

GHANEM⁴ — ¹Univ. Kiel, Materialverbunde, Kaiserstr. 2, 24143 Kiel — ²Institut für Polymerforschung, GKSS, Max-Planck-Strasse 1, 21502 Geesthacht — ³School of Chemistry, The University of Manchester, Manchester M13 9PL, UK. — ⁴School of Chemistry, Cardiff University, Cardiff CF10 3AT, UK.

The performance of polymeric membranes for gas separation is mainly determined by the free volume. Polymers of intrinsic microporosity are interesting candidates for state of the art gas separation membranes due to the high abundance of accessible free volume. Positron annihilation lifetime spectroscopy is a generally accepted technique for investigation of free volume in polymers where the orthopositronium lifetime is directly connected to the mean free volume size. We performed measurements of the temperature dependence of the positron lifetime in a polymer of intrinsic microporosity (PIM-7) in the range from 143 to 523 K. The mean value of the free volume calculated from the ortho-positronium life time (~ 5 ns) is in the range of typical values for high free volume membrane polymers ($V = 0,47 \text{ nm}^3$). However, the temperature dependence of the positronium-lifetime is non-monotonous. Comparison with thermal expansion measurements will be made and a possible explanation of this unexpected behavior given.

CPP 15.3 Tue 15:00 H47

Beitrag abgesagt — ●XXX XXX —

CPP 15.4 Tue 15:15 H47

Microscopic Protein Diffusion at High Concentration — ●SEBASTIAN BUSCH¹, WOLFGANG DOSTER¹, STÉPHANE LONGEVILLE², VICTORIA GARCÍA SAKAI^{3,4}, and TOBIAS UNRUH⁵ — ¹Physics-Department E13, Technische Universität München, James Franck Straße 1, D-85747 Garching, Germany — ²Laboratoire Léon Brillouin, CEA-CNRS, DSM-DRECAM, CEA Saclay, 91191 Gif-sur-

Yvette, France — ³NIST Center for Neutron Research, National Institute of Standards & Technology, Gaithersburg, MD 20899, U.S.A. — ⁴Department of Materials Science and Engineering, University of Maryland, College Park, MD 20742, U.S.A. — ⁵Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II), TU München, Lichtenbergstr. 1, D-85747 Garching, Germany

A characteristic of the interior of cells is the high total concentration of macromolecules, occupying up to 20-30% of the total volume. This affects protein diffusion and protein association equilibria (highly nonideal solutions). The goal of our project is to understand the effect of protein-protein interactions on molecular diffusion at high concentration. The self-diffusion of myoglobin in concentrated solutions was investigated by neutron back-scattering spectroscopy. The quasi-elastic spectrum can be decomposed into two Lorentz curves: one with a linewidth increasing with Q , which is assigned to translational diffusion, the other broad Q -independent, reflecting protein-internal motions. The apparent diffusion coefficient decreases with increasing concentration and wave-vector, suggesting that protein diffusion deviates at high Q (1.75 \AA^{-1}) from its long-time Brownian limit.

15 min. break

CPP 15.5 Tue 15:45 H47

Modelling polyelectrolyte dynamics: The importance of hydrodynamic interactions — ●KAI GRASS¹ and CHRISTIAN HOLM^{1,2} — ¹Frankfurt Institut 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

In this contribution, we investigate the dynamical properties of short strongly charged polyelectrolytes by means of coarse-grained molecular dynamics simulations. By comparing a purely implicit treatment of the solvent with a Lattice Boltzmann modelled fluid, we show that hydrodynamic interactions have to be included to model the experimentally observed behaviour.

We compare the obtained results to recent experimental studies and illustrate the decisive features, such as the non-monotonic behaviour of the electrophoretic mobility on short length scales and the well-known transition to the free-draining regime. Additionally, we use the obtained diffusion and mobility coefficients to calculate estimates for the effective charge and hereby check the validity of the available theories for charge condensation.

All transport coefficients were obtained at zero and low-field conditions, respectively, in order to not perturb the counter ion cloud, and thus match experimental conditions closely.

CPP 15.6 Tue 16:00 H47

Diffusion and local dynamics in polysiloxane-based polymer electrolytes — MIRIAM KUNZE¹, YUNUS KARATAS², HANS-DIETER WIEMHÖFER², HELLMUT ECKERT¹, and ●MONIKA SCHÖNHOF¹ — ¹Institut für Physikalische Chemie und SFB 458, WWU Münster, Germany — ²Institut für Anorganische und Analytische Chemie und SFB 458, WWU Münster, Germany

A new improved Li ion conducting salt-in-polymer electrolyte system consisting of a polysiloxane backbone with oligoether side chains and added LiCF_3SO_3 (Li triflate = LiTf) is studied concerning the mechanisms governing ion dynamics. Conductivity values at 30 °C reach up to $7.8 \times 10^{-5} \text{ S cm}^{-1}$ after crosslinking, which is employed to enhance mechanical stability. We characterize this system by a combination of pulsed field gradient (PFG)-NMR diffusion and spin relaxation (R_1

and R_2) of ^7Li , ^{19}F and ^1H in dependence on T and salt content. Comparing diffusion coefficients of Li and Tf with conductivity data by the Nernst-Einstein-equation reveals that transport is dominated by diffusion of neutral ion pairs and clusters, while only a low fraction of free ions exists. Evaluating activation energies from diffusion coefficients and relaxation rates, respectively, shows that the underlying activation processes governing ionic mobility can be discussed by their relevant length scale rather than by the ion involved: Activation energies of diffusion, a long range process, are much larger than those of R_2 , which describe local mobility. An important conclusion is that the relatively high ionic conductivity could even be increased, if salt dissociation can be enhanced further.

CPP 15.7 Tue 16:15 H47

Single molecule fluorescence correlation spectroscopy study of polymer-surfactant interactions — ●STANISLAUS JOHN BOSCO¹, HEIKO ZETTL¹, JÉRÔME CRASSOUS², MATTHIAS BALLAUFF², and GEORG KRAUSCH² — ¹Physikalische Chemie II, Universität Bayreuth, 95440, Bayreuth, Germany — ²Physikalische Chemie I, Universität Bayreuth, 95440, Bayreuth, Germany

The association between water soluble polymers and surfactants has drawn much attention to understand the fundamental properties in intermolecular interactions and hydrophobic aggregation phenomena. In order to understand the polymer/surfactant interactions in a single molecule level, we have used fluorescence correlation spectroscopy (FCS). As a model system we investigated complex formation between a hydrophobically modified nonionic polymer, methyl cellulose and the anionic surfactant sodium dodecyl sulfate (SDS) in water. FCS can follow the motion of individual SDS micelles and single MC/SDS aggregates via measurement of the diffusion time of single dye molecules attached to MC/SDS complexes [1]. Two possible aggregations (large and small) can be distinguished above the critical aggregation concentration (CAC). Rheology was used to follow the macroscopic properties of the polymer/surfactant systems. The dynamic behavior of the large aggregates found in FCS resembles the macroscopic properties. Moreover the influence of temperature on the aggregation behavior has also been studied.

[1] S. John Bosco, H. Zettl, J.J Crassous, M. Ballauff, G. Krausch, *Macromolecules*, 39, 8793-8798 (2006)

CPP 15.8 Tue 16:30 H47

PhoCS - Photothermal Correlation Spectroscopy — ●ROMY RADÜNZ and FRANK CICHOS — Molecular Nanophotonics, Universität Leipzig, Linnéstraße 5, 04103 Leipzig

Fluorescence correlation spectroscopy (FCS) is a versatile tool to explore molecular dynamics with single molecule sensitivity. It is widely used in exploring biophysical processes even in living cells. However, it is based on fluorescence and therefore suffers from photophysical weaknesses of the chromophores, such as photoblinking, photobleaching or weak signal to background contrast due to autofluorescence. We present results of a new experimental technique called photothermal correlation spectroscopy (PhoCS). PhoCS employs a photothermal contrast mechanism to detect non-fluorescent nanoparticles of only a few nanometers in size. Light, which is absorbed by the particle is released as heat and induces a local refractive index change around the nanoparticle, which is optically detected. This contrast mechanism is used to generate timetraces of nanoparticle diffusion in an equivalent way as it is done in FCS. Thus PhoCS opens new ways of local dynamic measurements with nanometer sized photostable tracers.

CPP 16: Colloids and Nanoparticles III

Time: Tuesday 17:00–18:30

Location: H47

CPP 16.1 Tue 17:00 H47

Direct measurement of the critical Casimir force in a binary liquid — ●CHRISTOPHER HERTLEIN, LAURENT HELDEN, and CLEMENS BECHINGER — 2. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart

A colloidal particle suspended in a binary liquid at the critical composition close to a substrate experiences a critical Casimir force upon approaching the critical temperature of decomposition T_c . We have measured interaction potentials for a single polystyrene particle sus-

pending in a mixture of water and 2,6-lutidine approaching T_c using Total Internal Reflection Microscopy (TIRM). TIRM is a technique for precise measurements of colloid-wall interaction potentials based on single particle evanescent wave light scattering. The measured interaction potentials display a clear contribution of the critical Casimir force which becomes stronger upon approaching T_c and is either attractive or repulsive depending on the preference for water or lutidine of substrate and/or particle.

CPP 16.2 Tue 17:15 H47

Influence of the preparation and processing on thermal and mechanical properties of metal/poly(methyl methacrylate) nanocomposites — ●CHRISTIAN HUB¹, SHANE HARTON², MARCUS HUNT³, RAINER FINK¹, and HARALD ADE⁴ — ¹Universität Erlangen, Lehrstuhl für Physikalische Chemie II, Erlangen, Germany — ²Columbia University, Department of Chemical Engineering, New York, USA — ³North Carolina State University, Department of Fiber & Polymer Science, Raleigh, USA — ⁴North Carolina State University, Department of Physics, Raleigh, USA

The inclusion of nanoparticles into polymeric materials is well-known to increase mechanical strength, provide tunable optical and electrical properties, or improve thermal resistance of the host polymer matrix. Because of the technologically relevant applications of nanocomposites, numerous investigations showing significant, and sometimes anomalous, changes in the observed properties have been done in recent years. In the current study the influence of the sample preparation and processing on thermal and mechanical properties of silica/PMMA nanocomposites were investigated. The changes in mechanical and impact strength of the obtained nanocomposites have been probed by dynamic mechanical analysis. Thermal properties have been investigated by differential scanning calorimetry. We will demonstrate that equilibrium inclusion of nanoparticles within polymer matrices can have a significant impact on mechanical properties of the host polymer, even though it may not be accompanied by changes in other properties such as the glass transition temperature (funded by DAAD).

CPP 16.3 Tue 17:30 H47

High-resolution photoemission study of II-VI semiconductor nanoparticles — ●TINA GRABER, FRANZISKA NIEDERDRAENK, CHRISTIAN KUMPF, ACHIM SCHÖLL, and EBERHARD UMBACH — Universität Würzburg, Experimentelle Physik II, Am Hubland, 97074 Würzburg

Semiconductor nanoparticles are of rapidly increasing interest due to their various actual and potential applications, such as, e.g., active components in LEDs or solar cells. Very small (1-5 nm) particles are also of particular interest in fundamental research since they represent a size scale which is in between the well-established descriptions of solid state and molecular physics.

We report on high resolution X-ray photoemission data of ZnO, CdSe and CdSe/ZnS core-shell nanoparticles in the range of 1-5 nm diameter. The particles were produced by a wet-chemical preparation method with organic stabilizers and drop-deposited on H-passivated silicon and polycrystalline Au substrates. A detailed analysis was performed to identify the various contributions from the core, shell, interface, and surface to the total signal in order to understand the influences of different synthesis routes on the particle composition. Influences of different solvents as well as beam damage and aging processes are discussed.

CPP 16.4 Tue 17:45 H47

Raman intensity profiles of individual single-walled carbon nanotubes — ●MARTIN FOUQUET¹, HAGEN TELG¹, JANINA MAULTZSCH², CHRISTIAN THOMSEN¹, JAMES HONE³, and TONY HEINZ² — ¹Institut für Festkörperphysik, Technische Universität Berlin, Germany — ²Departments of Physics and Electrical Engineering, Columbia University, USA — ³Department of Mechanical Engineering, Columbia University, USA

We performed resonant Raman measurements on individual single-walled carbon nanotubes grown across a 100 micrometer wide slit. We collected intensity profiles of the radial breathing mode (RBM) and the high energy modes (HEM) by varying the excitation energy between 1.85 eV and 2.2 eV. In metallic nanotubes, the characteristic Fano-lineshape of the HEM is found, confirming that it is intrinsic to individual metallic tubes. We observe that the lineshape and peak positions depend on the resonance Raman condition, and their dependence on excitation energy is discussed.

CPP 16.5 Tue 18:00 H47

Schwingungseigenschaften von (3,3) Kohlenstoffpicotubes — ●NILS ROSENKRANZ¹, MARÍA MACHÓN¹, RAINER HERGES² und CHRISTIAN THOMSEN¹ — ¹Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — ²Institut für Organische Chemie, Universität Kiel, Otto-Hahn-Platz 4, 24098 Kiel, Germany

Als Picotubes bezeichnet man hochsymmetrische Kohlenwasserstoffmoleküle, die strukturell eng verwandt mit den kleinsten Nanotubes sind. Als zentraler Ausgangspunkt einer gezielten Synthese von Nanotubes sind Picotubes von fundamentaler Bedeutung. Die hier vorgestellten Semitrimere ähneln einem Ausschnitt eines (3,3) Nanotubes. Wir stellen erstmalig die Schwingungseigenschaften dieses Moleküls vor. Mittels winkelabhängiger Ramanspektroskopie an Semitrimerkristallen konnten die Symmetrien der einzelnen Moden bestimmt werden. Unsere Ergebnisse zeigen Analogien zu den Schwingungseigenschaften von Nanotubes. Insbesondere konnten wir eine Mode identifizieren, die große Ähnlichkeit zu der für Nanotubes sehr charakteristischen Atmungsmoden aufweist.

CPP 16.6 Tue 18:15 H47

Photoactivation of Quantum Dots Controlled Embedded into Silica colloids — ●CHRISTINA GRAF^{1,2}, SOFIA DEMBSKI², ANNE BOCK², TIM KRÜGER³, and ECKART RÜHL^{1,2} — ¹Institut für Chemie und Biochemie, Freie Universität Berlin, Takustr. 3, 14195 Berlin — ²Institut für Physikalische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, — ³Theodor-Boveri-Institut für Biowissenschaften, Universität Würzburg, Am Hubland, 97074 Würzburg

Quantum dots (QD) are nowadays widely used as markers in life science. However, after the transfer into biological systems their fluorescence quantum yield (QY) is often reduced. Photoactivation with UV or visible light is a powerful tool to increase the photoluminescence (PL) of QD. Here, we present a study on the influence of the local environment on the photoactivation of QD. CdSe/ZnS QD embedded in silica colloids were studied in various liquids. Under continuous photoactivation with UV or visible light the PL of the embedded QD can be stably up to ten times enhanced and strongly depends on the local environment. Hereby, the thickness-dependent permeability of the silica shell controls the influence of the outer media on the QD. If foreign ions are present the activation can be fully retained after termination of the activation, while in their absence the process is partially reversible. Considering the present results, a new model for the photoactivation of QD in various environments is developed. It comprises photopassivation and a subsequent oxidation processes. The embedded QD also retain their QY inside living cells. Moreover, they can be long-time photoactivated in living cells.

CPP 17: Micro and Nano Fluidics I: Structured Substrates

Time: Wednesday 14:00–15:45

Location: H37

Invited Talk

CPP 17.1 Wed 14:00 H37

Liquid distribution in a granular pile — MARIO SCHEEL, MARTIN BRINKMANN, ●STEPHAN HERMINGHAUS, and RALF SEEMANN — MPI for Dynamics and Self-Organization

The addition of small amounts of liquid to a granulate dramatically changes the mechanical properties of the latter. This is due to capillary bridges forming between mutually adjacent grains in the pile, which exert an attractive force by virtue of the surface tension of the liquid. However, within a wide range of liquid content the mechanical properties of a wet granulate are surprisingly independent. This peculiar behavior is explored experimentally and theoretically by means of the liquid distribution within the granulate. The liquid distribution within

a model granulate consisting of glass beads is analyzed experimentally by x-ray tomography as function of wettability and packing density. Liquid morphologies and the resulting capillary forces are calculated numerically by a minimization of the surface energy of the liquid. The constant mechanical properties of wet granulates for a large range of liquid contents is a result of one particular type of liquid morphology, which dominates over all other possible morphologies in case of a wetting liquid.

CPP 17.2 Wed 14:30 H37

Anisotropic self-diffusion in nanofluidic structures — ●MARTIN SCHOEN¹, KEITH GUBBINS², and HENRY BOCK³ — ¹Stranski-

Laboratorium für Physikalische und Theoretische Chemie, Fakultät für Mathematik und Naturwissenschaften, Technische Universität Berlin, Straße des 17. Juni 135, 10623 Berlin, Germany — ²Department of Chemical and Biomolecular Engineering, 911 Partners Way, North Carolina State University, Raleigh, NC 27695-7905, U.S.A. — ³Department of Chemical Engineering, Heriot-Watt University, Edinburgh EH14 4AS, United Kingdom

By means of equilibrium molecular dynamics simulations we investigate self-diffusion in a "simple" fluid confined to nanoscopic slit-pores. The pore walls are decorated with wettable and nonwettable chemical "stripes" that alternate in the x-direction and are assumed infinitely long in the y-direction. We consider the impact of pore width as well as variations of the width of the wettable stripes. Depending on these model parameters and the thermodynamic conditions the confined fluid may exist as one of three morphologically distinct phases: a thin fluid film, a fluid bridge spanning the gap between the stripes, or a nanostructured liquid. By analyzing mean square displacements, velocity autocorrelation functions and in particular their power spectra a detailed picture of mass transport and its relation to the dimensions of the chemical patterns on the substrates emerges. In particular, we find that the axial symmetry of the diffusion tensor preserved in the liquidlike phases is disrupted in both the film and the bridge phases.

CPP 17.3 Wed 14:45 H37

Manipulation of wetting morphologies in triangular grooves — ●KRISHNACHARYA KHARE¹, MARTIN BRINKMANN¹, BRUCE M. LAW², STEPHAN HERMINGHAUS¹, and RALF SEEMANN¹ — ¹Max Planck Institute for Dynamics and Self-Organization, D-37073 Göttingen — ²Department of Physics, Kansas State University, USA

Wetting behavior of liquids in triangular grooves is studied experimentally and theoretically. For contact angles smaller than 90 degree minus half the opening angle of the groove, the liquid forms filaments with negative mean curvature extended along the entire length of the groove. For larger contact angles, liquid either forms elongated filaments of finite length and positive mean curvature or drop-like morphologies. Electrowetting is used to vary the contact angle and to switch between these morphologies. In this way, liquid filaments can be pulled out of a large feeding drop forming elongated filaments in prefabricated grooves. When being quenched from the filling to the non-filling regime the liquid filaments undergo dynamic instability and break up into isolated droplets with a preferred distance. This preferred droplet distance compares favorably with a straight forward theoretical model assuming the instability to be driven by the local variation of the Laplace pressure with filament width. This instability may be viewed as a generalization of the Rayleigh-Plateau instability and resembles the spinodal instability of thin films.

CPP 17.4 Wed 15:00 H37

Motion of nanodroplets near edges and wedges — A.

MOOSAVI^{1,2}, ●M. RAUSCHER^{1,2}, and S. DIETRICH^{1,2} — ¹Max-Planck-Institut für Metallforschung, Heisenbergstr. 3, 70569 Stuttgart — ²Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart

Nanodroplets residing near wedges or edges of solid substrates exhibit a disjoining pressure induced dynamics. Our nanoscale hydrodynamic calculations reveal that non-volatile droplets are attracted or repelled from edges or wedges depending on details of the corresponding laterally varying disjoining pressure generated, e.g., by a possible surface coating. [A. Moosavi et al., Phys. Rev. Lett. 97, 236101 (2006)]

CPP 17.5 Wed 15:15 H37

Line tension effects for liquid droplets on circular surface domains — ●PEDRO BLECUA, JAN KIERFELD, and REINHARD LIPOWSKY — Max Planck Institute of Colloids and Interfaces, Science Park Golm, 14424 Potsdam, Germany

We study the morphologies of single liquid droplets wetting a substrate in the presence of a line tension of the three phase contact line. On a homogeneous substrate the line tension leads to a discontinuous unbinding of the droplet if its volume is decreased below a critical value. For a droplet wetting a structured surface with a circular domain, a *line tension contrast* gives rise to discontinuous depinning transitions of the contact line at the domain boundary as a function of the droplet volume, which can be studied analytically for axisymmetric droplet shapes. We calculate the corresponding free energy bifurcation diagram. Numerical minimization of the droplet free energy shows that line tension contrasts can stabilize non-axisymmetric droplet shapes thus modifying the bifurcation diagram.

CPP 17.6 Wed 15:30 H37

Nanobubbles in Solid-State Nanopores — ●U. F. KEYSER^{1,2}, R. M. M. SMEETS¹, M. Y. WU¹, N. H. DEKKER¹, and C. DEKKER¹ — ¹Kavli Institute of Nanoscience, Delft University of Technology, The Netherlands — ²Institut für Experimentelle Physik I, Universität Leipzig, Germany

From conductance and noise studies, we infer that nanometer-sized gaseous bubbles (nanobubbles) are the dominant noise source in solid-state nanopores[1]. We study the ionic conductance through solid-state nanopores as they are moved through the focus of an infrared laser beam. The resulting conductance profiles show strong variations in both the magnitude of the conductance and in the low-frequency noise when a single nanopore is measured multiple times. Differences up to 5 orders of magnitude are found in the current power spectral density. In addition, we measure an unexpected double-peak ionic conductance profile. A simple model of a cylindrical nanopore that contains a nanobubble explains the measured profile and accounts for the observed variations in the magnitude of the conductance.

[1] R. M. M. Smeets, U. F. Keyser et al., Phys. Rev. Lett. 97, 088101 (2006)

CPP 18: Light-Induced Phenomena

Time: Wednesday 14:30–15:45

Location: H40

CPP 18.1 Wed 14:30 H40

Tuning phonon spectra of two-dimensional colloidal crystals — ●JÖRG BAUMGARTL¹, MARIA ZVYAGOLSKAYA¹, HANS HENNING VON GRÜNBERG², and CLEMENS BECHINGER¹ — ¹Universität Stuttgart, 2.Physikalisches Institut, Pfaffenwaldring 57, D-70569 Stuttgart, Germany — ²Karl-Franzens-Universität, Institut für Chemie, Heinrichstraße 28, A-8010 Graz, Austria

By exposing two-dimensional (2D) colloidal crystals to tunable substrate potentials one can selectively manipulate the corresponding phonon band-structure. We explore this idea theoretically and experimentally by studying the overdamped lattice dynamics of colloidal crystals subjected to one- and two-dimensional periodic substrate potentials which are created by interfering laser beams. Experimentally, the phonon spectrum is obtained from the particle dynamics observed by videomicroscopy whereas the theoretical analysis is based on a calculation of the elastic energy of a 2D crystal in the presence of a substrate potential using the harmonic approximation. Depending on the geometry and the strength of the underlying lattice potential, the phonon spectra can be substantially changed which is in agreement with our theoretical calculations.

CPP 18.2 Wed 14:45 H40

Laser-induced phonon-phonon interactions in bismuth — ●EEUWE SIEDS ZIJLSTRA and MARTIN GARCIA — Theoretische Physik, Fachbereich Naturwissenschaften, Universität Kassel, Heinrich-Plett-Str. 40, 34132 Kassel, Germany

We compute laser-induced interactions between coherent phonons in bismuth and demonstrate that they are key to understanding important experiments performed with intense femtosecond laser pulses. In particular, we find mixing signals and higher harmonics arising from the coupling between phonons of different and the same symmetries, respectively. We show that the phonon-phonon interaction is strongly dependent on the laser fluence and is for that reason only observable when sufficiently strong laser pulses are used. Our results offer a unified description of the different experimental observations performed so far on bismuth.

CPP 18.3 Wed 15:00 H40

Reversible and Irreversible Photobleaching of Organic Dyes in Polymers — ●JÖRG SCHUSTER, JÖRG BRABANDT, and CHRISTIAN VON BORCZYKOWSKI — Center for nanostructured materials and an-

alytics, TU Chemnitz, 09107 Chemnitz

The photoinduced decay of fluorescence of organic dyes (photobleaching) is usually discussed in terms of irreversible photochemical modifications of the dye molecules (often photooxidation). We can show now, that the fluorescence decay from a number of dyes is mostly reversible in the initial part. The reversible decay is due to fluorescence intermittency with power law distributed on- and off- intervals (blinking) [1,2].

By measuring the recovery of the initially bleached luminescence after a given waiting time as a function of the bleaching time we are able to discriminate the reversible and irreversible fraction of the luminescence decay. The finding, that an intermittency induced photophysical bleaching process dominates the initial stages of photobleaching may shine new light on the puzzling variety of data on nonexponential photobleaching kinetics which has been published in the literature on photobleaching during the past decades. Once deconvoluted, the irreversible photochemical bleaching kinetics follows a simple single exponential decay. The photophysical bleaching is assigned to the photoejection of charges into the polymer. This reversible photoionisation process takes place on time scales from milliseconds to minutes.

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

[2] Schuster et al., J. Luminescence, in press

CPP 18.4 Wed 15:15 H40

Molecular tracer diffusion in thin azobenzene polymer layers — ●NORMAN MECHAU^{1,3}, MARINA SAPHIANNIKOVA², and DIETER NEHER¹ — ¹Institute of Physics, University of Potsdam, Am Neuen Palais 10, 14469 Potsdam, Germany — ²Leibniz Institute of Polymer Research, Hohe Straße 6, 01069 Dresden, Germany — ³Forschungszentrum Karlsruhe, Institut of Nanotechnology, 76021, Karlsruhe, Germany

Translational diffusion of fluorescent tracer molecules in azobenzene polymer layers is studied at different temperatures and under illumina-

tion using the method of fluorescence recovery after photo-bleaching. Diffusion is clearly observed in the dark above the glass transition temperature, while homogenous illumination at 488 nm and 100 mW/cm² does not cause any detectable diffusion of the dye molecules within azobenzene layers. This implies that the viscosity of azobenzene layers remains nearly unchanged under illumination with visible light in absence of internal or external forces.

CPP 18.5 Wed 15:30 H40

Ortsaufgelöste Messung der thermischen Leitfähigkeit in Flüssigkeiten* — ●JUDITH SCHWESYG, HELGE EGGERT, DIRK APITZ und KARSTEN BUSE — Physikalisches Institut, Universität Bonn, We-gelerstr. 8, 53115 Bonn

Bildgebende Verfahren sind in vielen Bereichen der Wissenschaft und Technik von fundamentaler Bedeutung. Hierbei werden verschiedenste Kontrastmechanismen benutzt, z. B. Absorptions-, Brechungsindex- und Temperaturunterschiede. Ein neuer Ansatz ist, als Kontrast Inhomogenitäten der Wärmeleitfähigkeit in Flüssigkeiten oder Festkörpern zu messen und bildlich darzustellen. In diesem Vortrag wird ein pulsholographisches Verfahren vorgestellt, mit dem es gelingt, die thermische Leitfähigkeit in Flüssigkeiten ortsaufgelöst zu messen. Es basiert auf der Tatsache, dass vom Zerfall thermischer Gitter, die durch Beleuchtung mit zwei interferierenden Nanosekundenlichtpulsen erzeugt wurden, auf die thermische Leitfähigkeit geschlossen werden kann. Als Beispielsystem dient das Zweikomponentensystem Toluol-Wasser. Es werden Messergebnisse sowie die aus diesen erstellten zweidimensionalen Bilder präsentiert. Des Weiteren tritt durch die Pulsbeleuchtung ein Grenzflächeneffekt auf: Von der Grenzschicht gehen aufgrund unterschiedlicher Material-Kompressibilitäten Schallwellen aus, die durch Beugung nachgewiesen werden. Dieser Effekt kann ebenfalls zur Bildgebung genutzt werden.

*Wir danken der Deutschen Forschungsgemeinschaft (BU 913/17), der Deutschen Telekom AG und der Deutschen Telekom Stiftung für die finanzielle Unterstützung.

CPP 19: POSTER: Micro and Nano Fluidics

Time: Wednesday 16:00–18:30

Location: Poster B

CPP 19.1 Wed 16:00 Poster B

Cantilever micro rheometer for measurement of sugar solutions — ●MARC HENNEMEYER and ROBERT STARK — Dept. Geo und Umwelt, Ludwig-Maximilians-Universität, Theresienstr. 41, 80333 München

Measurement of rheological properties of liquids is of high interest in many areas like medicine and biology. As traditional measurement techniques require relatively big amounts of sample fluid, the last years have seen an increased interest in the miniaturization of measurement tools. Micro mechanical sensors as used in atomic force microscopy are ideally suited as sensors in micro fluidic devices. Although the vibration of cantilevers does not respond to viscosity changes of fluids on macroscopic scales, micrometer scaled plates are affected by the viscous properties of the surrounding fluids. In this work a simple measurement tool for the rheological measurements on arbitrary Newtonian liquids is presented which is based on the analysis of stochastic cantilever oscillations. The system can be operated with standard consumer computer hardware, which dramatically reduces the costs for the system. The system presented in this work is a very cost effective set up that can be used for a wide range of experiments in cost sensitive environments. It could be shown, that for viscosity measurements on basis of the method introduced by Sader, standard computer hardware can be used to substitute expensive data acquisition hardware. The measurements on sugar solutions could evaluate the viscosity and density of the solutions to an accuracy of about 10%.

CPP 19.2 Wed 16:00 Poster B

Dewetting dynamics of thin polymer films on topographic and elastic substrates — ●KONSTANTINA KOSTOIROU, KRISHNACHARYA KHARE, MARTIN BRINKMANN, STEPHAN HERMINGHAUS, and RALF SEEMANN — Max Planck Institute for Dynamics and Self-Organization, D-37073 Göttingen, Germany

Dewetting dynamics of polymer films in triangular grooves and on elastic substrates are studied experimentally and theoretically. Liquid filaments, in triangular grooves, with convex liquid-vapor inter-

face are unstable and undergo dynamic instability resulting in equally spaced individual droplets with a preferred distance. This instability is driven by the local variation of the Laplace pressure with filament width and resembles a generalized Rayleigh-Plateau instability. From the time scale of the dynamic instability we extract slip properties of the polymer/substrate interface. Additionally we study the dewetting dynamics of thin polymer films on rubber elastic substrates. Here, the dynamics are additionally determined by the dissipative properties of the elastic substrate. We compare the flow behavior of liquid polymer films on substrates of different visco-elasticity and constant wettability. Our experiments show that dewetting is faster on substrates with larger elastic modulus.

CPP 19.3 Wed 16:00 Poster B

Raman spectroscopy on periodic mesoporous organosilica with different pore sizes — ●MARTIN ANDREAS SCHREIBER¹, MARTIN GÜNGERICH¹, WOLFRAM HEIMBRODT¹, TORSTEN HENNING², PETER JENS KLAR², VIVIAN REBBIN³, MICHAEL FRÖBA³, LUTZ EICHHORN⁴, JÜRGEN BRANDNER⁴, and KLAUS SCHUBERT⁴ — ¹Dept. Physics and WZMW, Philipps University of Marburg, Germany — ²1. Physics Institute, Justus-Liebig-University of Gießen, Germany — ³Institute of Inorganic and Analytical Chemistry, Justus-Liebig-University of Gießen, Germany — ⁴Forschungszentrum Karlsruhe, IMVT, Eggenstein-Leopoldshafen, Germany

Periodic mesoporous organosilica (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. Two-point attached organic units within the silica matrix in the pore walls are a genuine part of the 3D pore wall framework. These organic functionalisations is very versatile making these hybrids interesting for applications in catalysis and micro-reactor technology.

Here we study the adsorption and desorption behavior in dependence of the pore-size of benzene-functionalized and ethane-functionalized PMOs in the temperature range between 20 and 140°C by Raman spectroscopy. We find significant differences in the adsorption-desorption

behaviour for the solvents ethanol and benzene suggesting that PMOs make a selective separation of solvent vapours possible.

CPP 19.4 Wed 16:00 Poster B

Mechanical properties of wet granular matter — ●MARIO SCHEEL, MARTIN BRINKMANN, STEPHAN HERMINGHAUS, and RALF SEEMANN — MPI for Dynamics and Self-Organization

The macroscopic mechanical properties of a dry granulate change dramatically when small amounts of liquid are added. This is due to capillary bridges forming between mutually adjacent grains in the pile, which exert an attractive force by virtue of the surface tension of the liquid. The mechanical properties of a wet model granulate consisting of glass spheres with a narrow size distribution are studied. We determine the critical fluidization acceleration for vertical agitation, the tensile strength, and the yield stress of the granulate for various liquid contents. We compare the results from these different methods with each other and discuss them in the framework of structural information extracted from x-ray tomography images of granulates, i.e. the packing density and the liquid distribution. In-situ x-ray tomography experiments reveal furthermore insights into the redistribution of the liquid within a sheared granulate and the redistribution of liquid within a formerly fluidized granulate.

CPP 19.5 Wed 16:00 Poster B

A Study on the Permeability of Nanoporous Vycor — ●SIMON GRÜNER¹, STEFANIE GREULICH¹, DIRK WALLACHER², and PATRICK HUBER¹ — ¹Saarland University, Saarbrücken, Germany — ²Hahn-Meitner Institute, Berlin, Germany

We have designed and built a membrane flow apparatus (MFA) to measure the liquid permeability K of porous monoliths such as nanoporous Vycor as a function of applied pressure difference ΔP ($0 < \Delta P < 70\text{bar}$), temperature T and pore wall chemistry (silanization). The pore structure of the matrix (mean pore diameter $d \approx 8\text{nm}$, porosity $\phi \approx 30\%$) is characterized by nitrogen sorption isotherms at $T = 77\text{K}$.

First measurements of the volume flow rate \dot{V} of n-hexane through Vycor at $T = 18^\circ\text{C}$ nicely confirm Darcy's law, that is $\dot{V} \propto \Delta P$. Nonetheless the derived permeability K is somewhat smaller than expected from calculations assuming the above mentioned values for ϕ and d . We rather obtain a best agreement between experiment and theory with a pore radius 0.4nm smaller than that derived from the sorption isotherm. This reduction corresponds to about one immobile monolayer (boundary layer) of lying hexane molecules at the wall.

This work has been supported by the DFG within the priority program 1164 (HU850/2-1).

CPP 19.6 Wed 16:00 Poster B

Discrete Microfluidics: Combinatorial Chemistry with Emulsions — ●VENKATACHALAM CHOKKALINGAM, CRAIG PRIEST, STEPHAN HERMINGHAUS, and RALF SEEMANN — Max Planck Institute for Dynamics and Self-Organization, D-37073 Göttingen, Germany

Microfluidics usually involves single phase liquids transported through microchannel networks. Instead of single phase flow we explore a droplet based discrete microfluidics for possible applications in combinatorial chemistry. The online generation of highly monodisperse emulsions in a single step is studied to compartment liquids within microchannels. Furthermore, we explore the manipulation of monodisperse emulsions using the distinct interaction of the internal length scale of the liquid (drop diameter) with the external provided geometry of the microchannels for positioning, sorting, dividing and exchanging droplets in 'lab-on-chip' style processing. Coalescence between adjacent compartments can be induced applying an electrical potential of a few volts across their lamella. As a first approach towards combinatorial chemistry we study all possible volumetric combinations of two chemicals. Adjusting the temporal concentration of the two chemicals accordingly to the channel geometry down stream when injecting them into the microfluidic channel leads to a 2D reaction library where the two concentration gradients vary along the x- and y-axis, respectively.

CPP 19.7 Wed 16:00 Poster B

Thermally Excited Capillary Waves on a Surface Frozen Liquid: A GIXPCS Study — P. HUBER¹, ●M. WOLFF¹, V. SCHOEN¹, M. DEUTSCH², E. SLOUTSKIN², B. OCKO³, J. BAUMERT³, A. MADSEN⁴, and M. SPRUNG⁵ — ¹Universitaet des Saarlandes, Saarbruecken, Germany — ²Bar-Ilan University, Ramat-Gan, Israel — ³Brookhaven National Laboratory, NY, United States — ⁴European Synchrotron Radiation Facility, Grenoble, France — ⁵Advanced Photon Source, Argonne National Laboratory, United States

We present results of grazing incidence x-ray photon correlation spectroscopy (GIXPCS) measurements on thermally-excited capillary waves at the free surface of a tetracosane ($\text{C}_{24}\text{H}_{50}$) melt as a function of temperature. The measurements have been carried out at the ESRF, Grenoble, France and APS, Argonne National Laboratory, USA.

Upon surface freezing - the formation of a single crystalline monolayer at the melt's surface, close to, but above the bulk solidification temperature - we find a change both in the damping and in the dispersion relation of the capillary waves.

Our findings on the behavior of *microscopic* capillary waves, presented here, corroborate earlier results regarding the changes in the dynamics of *macroscopic* capillary waves upon surface freezing [1].

[1] P.Huber et al., Physical Review Letters **94**, 184504 (2005)

CPP 19.8 Wed 16:00 Poster B

Rheological and structural phase diagrams of salted solutions of the tri-block copolymer EO₂₀-PO₇₀-EO₂₀ — ●NICOLE VOSS¹, MARCO WALZ¹, MAX WOLFF², and ANDREAS MAGERL¹ — ¹Chair for Crystallography and Structural Physics, University of Erlangen-Nürnberg, Staudtstr. 3, 91058 Erlangen — ²Chair for Condensed Matter Physics, Ruhr-University Bochum, Universitätsstr. 150, 44780 Bochum

Aqueous solutions of tri-block copolymers have well known rich phase diagrams of ordered structures which can also be identified through rheometry. We have studied the influence of adding electron-rich salts with concentrations up to 1.5 mol/dm^3 on the phase diagram of the tri-block copolymer Pluronic[®] P123 (central block of 70 propylene oxide units terminated by two end groups of 20 ethylene oxide units). While the morphology of the phase diagram is preserved, a linear shift of -12°C per 1 mol/dm^3 CsCl is observed for the phase boundary of the cubic phase with high viscosity. The results are interpreted by the modification of the water structure, i. e. the ions of CsCl surround themselves with hydration shells and also dehydrate the PPO block. This mechanism decreases the solubility of the polymer and favours micellization at lower temperatures.

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

CPP 19.9 Wed 16:00 Poster B

Shear flow pumping in open microfluidic systems — ●MARKUS RAUSCHER^{1,2}, SIEGFRIED DIETRICH^{1,2}, and JOEL KOPLIK³ — ¹Max-Planck-Institut für Metallforschung, Heisenbergstr. 3, 70569 Stuttgart — ²Institut für Theoretische und Angewandte Physik, Universität Stuttgart, 70569 Stuttgart — ³Benjamin Levich Institute and Department of Physics, City College of the City University of New York, New York, NY 10031, USA

We propose to drive open microfluidic systems by shear in a covering fluid layer, e.g., oil covering water-filled chemical channels. The advantages as compared to other means of pumping are simpler forcing and prevention of evaporation of volatile components. We calculate the expected throughput for straight channels and show that devices can be built with off-the-shelf technology. Molecular dynamics simulations suggest that this concept is scalable down to the nanoscale.

CPP 19.10 Wed 16:00 Poster B

Dynamics of droplets on open microfluidic Y-junctions — ●FABIAN DÖRFLER^{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, Universität Stuttgart, 70569 Stuttgart

We investigate the dynamics of droplets on chemical channels with Y-junctions driven by body forces. Chemical channels are wetting stripes on otherwise non-wetting surfaces in which liquids can be guided.

We analyse the energy of a droplet in the vicinity of a junction in a capillary model in quasistationary approximation. We investigate the pinning of the droplets in the junction and from the local contact angle we determine thresholds for the spilling of droplets onto the non-wetting substrate.

CPP 19.11 Wed 16:00 Poster B

Correlating macroscopic viscosity and microscopic structure of the tri-block copolymer EO₂₀-PO₇₀-EO₂₀ — ●MARCO WALZ¹, MAX WOLFF², NICOLE VOSS¹, ANDREAS MAGERL¹, and HARTMUT ZABEL² — ¹Chair for Crystallography and Structural Physics, University of Erlangen-Nürnberg, Staudtstr. 3, 91058 Erlangen, — ²Chair for

Condensed Matter Physics, Ruhr-University Bochum, Universitätsstr. 150, 44780 Bochum

A neutron scattering study on the structure of the tri-block copolymer Pluronic® P123 (EO₂₀-PO₇₀-EO₂₀) in aqueous solution near a solid boundary is presented. An initially unexpected hysteresis found in the macroscopic viscosity is correlated with solid state orderings observed by near surface diffraction. The alignment of the structures is sensitive to the surface and its chemical termination. With temperature, the fcc lattice constant varies between 218 Å and 231 Å for 18°C and 32°C, respectively. The rocking curves, also with hysteresis, have a clear two-component profile giving information about long range correlations and short range disorder of the micelles.

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

CPP 19.12 Wed 16:00 Poster B

Thinning Dynamics of Foam Films from Dodecyl Maltoside (C12G2) — ●SILKE STÖCKLE, RUMEN KRASTEV, and HELMUTH MÖHWALD — Max-Planck Institute of Colloids and Interfaces, Potsdam/Golm, Germany

The surface dimensions of foam films range between micrometers and meters while their thickness is in the range of nanometers. These dimensions make the films a valuable system to study the behaviour of liquids in confined geometries. Foam films are liquid films which separate two gas phases. Thin foam films are stabilised by surfactants and consist of two surfactant monolayers in contact with an aqueous core. In order to understand time dependant changes in colloidal systems like the formation of aggregates, or the flow of colloids through micro-channels, the dynamics of film thinning is a crucial aspect to investigate. During the process of thinning, the distance between the film surfaces becomes substantially smaller than the interfacial zone around the surfaces. The interaction of the film surfaces changes not only the diffusion of the molecules adsorbed at the film surface but as well the viscous-elastic properties of the bulk. The contribution shows results on the thinning dynamics of films stabilised by C12G2. The experiments were performed using the *dynamic method* technique. Up-to-date analysis was used to obtain the influence of the film surface dynamic properties on the film thinning. The results show the influence of the surfactant density on the film thinning process.

CPP 19.13 Wed 16:00 Poster B

Wet Chemical and Dry Plasma Surface Hydrophilisation of epoxy-based Polymers (SU-8) — ●FERDINAND WALTHER¹, POLINA DAVIDOVSKAYA¹, STEFAN ZÜRCHER², MICHAEL KAISER³, HELMUT HERBERG³, ALEXANDER M. GIGLER¹, and ROBERT W. STARK¹ — ¹CeNS and Crystallography, LMU München, Germany — ²Laboratory for Surface Science and Technology, ETH Zurich, Switzerland — ³University of Applied Sciences, FB06, Munich, Germany

The effect of oxygen plasma treatment on surface energy, topography and surface chemistry of the negative photoresist epoxy novolak SU-8 was investigated by contact angle goniometry, atomic force microscopy (AFM) and X-ray photoelectron spectroscopy (XPS). Directly after plasma treatment, the surfaces were completely wetted by water with a contact angle between water and the SU-8 surface below five degrees. The surface free energy can be increased significantly depending on the plasma dose. The surfaces remained hydrophilic for several months showing a moderate hydrophobic recovery. The surface topography of the plasma treated SU-8 showed a formation of nanoscale aggregates. The rms-roughness of the topography was correlated with the plasma dose. An increased plasma dose induced aggregates of up to 200 nm in size. XPS measurements revealed changes in surface chemistry due to the plasma process and an increased antimony concentration on the surface.

CPP 19.14 Wed 16:00 Poster B

Characterization of Colloids, Polymer Solutions and Nanoparticles Suspensions Flow by Surface Sensitive Scattering — ●J.-F. MOULIN¹, V. KÖRSTGENS¹, E. METWALLI¹, W. WANG¹, S.V. ROTH², and P. MÜLLER-BUSCHBAUM¹ — ¹TUMünchen, Physik-Department E13, James-Frank-Str. 1, D-85747 Garching, Germany — ²HASYLAB@DESY, Notkestr. 85, D-22603 Hamburg, Germany

We will present the results of microbeam grazing incidence x-ray scattering (GISAXS) performed on fluidic channels. GISAXS enables to characterize the in plane ordering at the substrate surface and has proven a valuable technique for the characterisation of thin films and

interfaces. Combining these strengths with fluidics opens a new field of potential studies: the formation of thin films from solutions can be followed as a function of the relevant parameters (e.g. flow, nature of the solvent), phenomena such as size sorting of colloids, influence of shear on polymers at interfaces (slippage) can also be investigated. The design of the experiment as well as experimental results demonstrating the feasibility of such measurements will be presented.

Funding of this work by the DFG priority program SPP 1164, project Mu 1487/2 on Nano and Microfluidics is gratefully acknowledged.

CPP 19.15 Wed 16:00 Poster B

Fingering instability in entangled polymer films — ●JULIA MAINKA¹, CHIARA NETO², OLIVER BÄUMCHEN¹, and KARIN JACOBS¹ — ¹Saarland University, Experimental Physics, D-66041 Saarbrücken, Germany — ²Department of Applied Mathematics, Research School of Physical Sciences and Engineering, Australian National University, 0200 Canberra A.C.T., Australia

Viscous fingering is a prevalent phenomenon in dewetting polymer melts that arises at the interface between the moving liquid and the solid substrate. In our investigations we consider the fingering instability that occurs at the linear three phase contact line of a liquid polystyrene film. The film retracts from a highly non-wettable solid substrate only under the action of capillary driving forces. The investigations are realized by means of optical and atomic force microscopy under different external conditions. When dewetting starts, the material removed from the dewetted area forms a rim at the front of the receding film. The rim grows in size, and after a certain time, begins fluctuating in height and with. With increasing undulations, and further retracting of the contact line, material in the shape of fingers is left behind. The fingering is a consequence of an analogon of the Rayleigh-Plateau instability. The aim of our investigations is to show how parameters like molecular weight of the polymers, film thickness and slippage influence the dynamics and the morphology of the emerging finger structures. In particular, slippage and entanglement of the polymer seem to contribute to the understanding of the observed fingering instabilities.

CPP 19.16 Wed 16:00 Poster B

Semiflexible and sheared: actin filaments in microflow — ●DAGMAR STEINHAUSER, HOLGER STARK, and THOMAS PFOHL — Max-Planck-Institut für Dynamik und Selbstorganisation, Bunsenstr. 10, 37073 Göttingen

Actin filaments, aside from their biological renown as providing the 'skeleton' of cells, also proffer an ideal platform from which to study - more generally - the properties of semi-flexible polymers. Microfluidic devices made using soft-lithography are easily adapted in dimension and geometry to create well-defined flow environments. Actin filaments inside microfluidic channels are visualized by stroboscopic laser light illumination. Single filaments are considered in a symmetric channel with Poiseuille velocity profile, and the stochastic and deterministic behaviors of the filaments are analyzed for different flow rates. A detailed analysis of the center-of-mass probability distribution along a cross-section of the channel is reported, and a spatial varying orientation and conformation of the filaments are found. This work is supported by the DFG within the priority program SPP 1164.

CPP 19.17 Wed 16:00 Poster B

Free Standing Filaments Formed by Bent-shaped Molecules — ●ALEXANDRU NEMES, ALEXEY EREMIN, and RALF STANNARIUS — Institute of Experimental Physics, University of Magdeburg, Universitätsplatz 2, D-39106 Magdeburg, Germany

In few mesophases of bent-shaped liquid crystals, stable free standing filaments can be prepared with slenderness ratio (length to diameter ratio) of more than 1000 (Jákli et al. 2003). Their bundle-like structure was found with help of X-Ray, AFM, SEM and optical measurements [1]. In previous experiments it has been observed that the filaments respond with a lateral deflection to a strong DC electric field applied perpendicular to the filament axis. This technique was used as an excitation method to pluck the filaments and forced them, when the DC field was removed, to damped oscillations. The model we used to describe these free oscillations helps us to understand which forces are dominant in such liquid chords [2]. To understand the nature of the electric forces on the filaments, AC electric fields are applied perpendicular to the filament axis. The analysis of the Fourier transformed response of the filament oscillations reveals the functional interactions of the electric field with the material.

[1] A.Nemes, A.Eremin, R.Stannarius, M.Schulz, H.Nádasi,

W. Weissflog, Phys. Chem. Chem. Phys., 2006, 8, 469

[2] R. Stannarius, A. Nemes, A. Eremin, Phys. Rev. E, 2005, 72, 020702

CPP 19.18 Wed 16:00 Poster B

Flow NMR of complex systems — •ULRICH SCHELER and FRANK BAGUSAT — Leibniz-Institut für Polymerforschung Dresden e.V., Hohe Str. 6, D-01069 Dresden

A combination of NMR imaging and pulsed field gradient (PFG) NMR is applied to investigate flow. NMR longitudinal relaxation is used to generate contrast in a binary system of oil and water. The spatial distribution of each component and its flow pattern are measured separately. As a model a Couette cell with an additional area of high shear is used as model geometry. While a flat smooth interface is found at rest, the interface become bent under rotation, finally emulgation starts because of the velocity differences between the components. Flow from a submillimeter tube into a wide box and out of the box is investigated as well to understand shear-induced mixing and demixing.

CPP 19.19 Wed 16:00 Poster B

Towards a microscopic understanding of slip — •DOROTHEE MEIER¹, MAX WOLFF¹, MARCO WALZ², NICOLE VOSS², RENATE FETZER³, KARIN JACOBS³, ANDREAS MAGERL², and HARTMUT ZABEL¹ — ¹Lehrstuhl für Festkörperphysik, Ruhr-Universität Bochum, 44780 Bochum, Germany — ²Lehrstuhl für Kristallographie und Strukturphysik, Universität Erlangen-Nürnberg, 91058 Erlangen, Germany — ³Lehrstuhl für Weiche Kondensierte Materie, Universität des Saarlandes, 66041 Saarbrücken, Germany

In recent years, the increasing interest in flow in confined geometries has raised the need for a deeper understanding of the microscopic origin of boundary slip.

Neutrons are exceptionally well suited for the investigation of soft matter systems. This is related to their high transmittance through many kinds of materials as well as to the high scattering length density of deuterium in comparison to the x-ray cross section of hydrogen.

Furthermore, sample properties can be tuned via isotopic substitution.

We have investigated the density in the near surface region in systems which undergo boundary slip via neutron and x-ray reflectometry. Our model systems are stationary and flowing liquids in contact with polystyrene coated silicon crystals as well as polystyrene films on OTS and DTS grafted to a silicon wafer. The reflectivities show differences in the density profiles of systems which are known to undergo slip in comparison to non-slipping samples. This could be related to different interdiffusion properties of the distinct substances used.

This work is supported by the DFG Priority Program SPP 1164.

CPP 19.20 Wed 16:00 Poster B

Thin liquid polymer films: Preparation parameters impact polymer dynamics — •LUDOVIC MARQUANT, DANIEL PODZIMEK, RENATE FETZER, and KARIN JACOBS — Saarland University, Experimental Physics, D-66041 Saarbrücken, Germany

The dynamics of polymer films dewetting from hydrophobic substrates can be influenced by several phenomena. First the impact of the boundary conditions can be developed. When we observe the profile of a growing rim of polystyrene film dewetting either from octadecyltrichlorosilane or dodecyltrichlorosilane (respectively OTS and DTS) bounded to a silicon wafer, we can observe that the slip length is varying in both cases and the dewetting process is significantly faster on DTS than on OTS brushes [1]. One other important phenomenon we focus on is the polymer chain dynamics. The influence of different conformations of the macromolecules within the solvent used for spin-coating is investigated by acting on the polymer / solvent interaction. In other words the use of a range from good to theta solvents allows us to analyse the properties of the polymer coating. The films are prepared with a thickness in a range of several tens up to several hundreds of nanometres. The methodologies developed are scanning probe microscopy, ellipsometry and optical microscopy.

[1] R. Fetzer, M. Rauscher, A. Münch, B. A. Wagner and K. Jacobs, Europhysics Letters 75 (2006) 638

CPP 20: POSTER: Biological Systems + New Materials

Time: Wednesday 16:00–18:30

Location: Poster B

CPP 20.1 Wed 16:00 Poster B

High Frequency Quartz Crystal Microbalance Flow Cell with Enhanced Accuracy for Liquid and Biochemical Sensing — •PAULA SAGMEISTER, INGRID GRAZ, and REINHARD SCHWÖDIAUER — Soft Matter Physics, J. Kepler Universität, Altenbergerstraße 69, 4040 Linz, Österreich

Throughout the last twenty years, acoustic wave sensors have been proven as extremely sensitive and accurate devices for a wide variety of physical, chemical and biochemical sensing applications. Systems based on thickness shear mode (TSM) quartz resonators, working in a liquid environment with resonance frequencies between 5 and 15 MHz, are already established (and commercially available) for real-time measurements of biochemical interactions. The utilisation of high frequency fundamental (HFF) quartz resonators, with resonance frequencies up to 150 MHz (and beyond), could further improve the sensitivity of such systems by orders of magnitude. We present a fully biocompatible flow cell, designed for HFF quartz resonators which, in spite of their small size, can be removed and exchanged quickly and with ease. The system performance is evaluated and quantified by a number of experiments including various viscosity measurement of diluted sugar solutions, the detection of a bovine serum albumin (BSA) monolayer and other biochemical reactions. We further address some specific problems especially related to reusability and cleaning procedures.

CPP 20.2 Wed 16:00 Poster B

Kinetics, intermediates, and mechanisms of the aggregation of amyloid protein systems — •GUDRUN LOTZE¹, ANDREAS BÖGEHOLD², BERND ABEL², and HAUKE SCHOLLMAYER¹ — ¹Georg-August Universität Göttingen, Institut für Röntgenphysik, Friedrich-Hund-Platz 1, 37077 Göttingen — ²Georg-August Universität Göttingen, Institut für Physikalische Chemie, Tammannstraße 6, 37077 Göttingen

Neurodegenerative diseases such as Alzheimer's, Parkinson's and the

transmissible spongiform encephalopathies are characterized by abnormal protein aggregates, often in form of highly symmetric amyloid fibrils. Amyloid fibrils are polypeptide aggregates in which the polypeptide backbone is arranged in a specific cross- β sheet quaternary structure. However, the molecular mechanisms and timescales of the formation of intermediates and fibrils are still not fully understood and currently subject of intense research.

Insulin is a well suited model system to analyze the kinetics of fibril formation. We use x-ray scattering and transmission x-ray microscopy to investigate different states (intermediates and fully grown fibrils) of molecular structure and topology of the model system insulin.

CPP 20.3 Wed 16:00 Poster B

Protein Dynamics in the Light of Single-Molecule Spectroscopy — •JÜRGEN BAIER¹, MARTIN RICHTER¹, SILKE OELLERICH¹, RICHARD COGDELL², and JÜRGEN KÖHLER¹ — ¹Experimental Physics IV and BIMF, University of Bayreuth — ²Division of Biochemistry and Molecular Biology, University of Glasgow, United Kingdom

Proteins are supramolecular machines that perform a variety of tasks in living organisms. However, a protein is not a rigid structure and due to the relatively weak interactions that stabilise its 3-dimensional structure the lowest energy state of a protein is not unique. The potential energy hypersurface features a multitude of barriers and is commonly described by a rugged energy landscape where each minimum represents a different conformational substate. Since conformational fluctuations of the protein are equivalent to rearrangements of its atoms, chromophores embedded in the protein experience those changes as fluctuations in the local interactions. As a consequence the pigments react on conformational changes of the protein with changes of their electronic transition energies. Here we focus on the B800 BChl *a* molecules of the peripheral light-harvesting complex (LH2) from photosynthetic purple bacteria as local probes to study the conformational dynamics. We have recorded long sequences of fluorescence-excitation spectra from individual LH2 complexes and performed a statistical

analysis of the spectral fluctuations of the B800 absorptions. The results are compared with predictions of the standard TLS model for spectral diffusion in glasses. We find a fundamental difference between the relaxation behaviour of our test protein and glasses.

CPP 20.4 Wed 16:00 Poster B

The electronic structure of core complexes from *Rps. palustris* — ●THOMAS PREM¹, MARTIN RICHTER¹, JÜRGEN BAIER¹, SILKE OELLERICH¹, FRANCESCO FRANCA^{2,3}, GIOVANNI VENTUROLI², DIETER OESTERHELT³, JUNE SOUTHALL⁴, RICHARD COGDELL⁴, and JÜRGEN KÖHLER¹ — ¹Experimental Physics IV and BIMF, University of Bayreuth — ²Department of Biology, University of Bologna and INFN, Italy — ³Department for Membrane Biochemistry, MPI for Biochemistry, Martinsried — ⁴Division of Biochemistry and Molecular Biology, University of Glasgow, United Kingdom

The primary reactions of purple bacterial photosynthesis occur within two pigment-protein complexes, the core RC-LH1 complex and the peripheral LH2 complexes. In the RC the reduction of a ubiquinone (UQ) to ubiquinol (UQH₂) takes place. In order to make contact with the cytochrome b/c1 complex as part of the cyclic electron pathway, the UQH₂ has to leave the RC. Hence, either the LH1 ring is not complete, i.e. there is a gap, or the LH1 structure is inherently flexible enough to allow UQH₂ to diffuse through it. A recent rather low resolution X-ray crystal structure of the RC-LH1 core complex from *Rps. palustris* showed the presence of a gap in the LH1 ring. This presence, though functionally critical, has become very controversial. We recorded single-molecule fluorescence-excitation spectra for individual RC-LH1 complexes of *Rps. palustris* and describe how the presence of a narrow spectral feature at the low-energy end of the spectrum unequivocally establishes the presence of a gap in the electronic structure consistent with the presence of the physical gap.

CPP 20.5 Wed 16:00 Poster B

Adhesion and wetting: from monolayer to capillary bridges — ●RALF KAMINKE and KLAUS MECKE — Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen

Nanomechanical AFM measurements of adhesion forces revealed a strong dependence on humidity for Geckos spatula on various hydrophobic substrates [G. Huber et al, PNAS 102, 16293 (2005)]. Whereas capillary condensed water bridges are unlikely to form between hydrophobic substrates, adsorbed particles may build molecular bridges which seems to be sufficient to explain the increase of adhesion with humidity - even at sub-monolayer coverage. Adsorption isotherms as well as adhesion forces changes qualitatively at the crossover from nanometer thickness of liquid films to monolayers where the details of the substrate potential are relevant. Most density functionals use a hard sphere fluid as a reference system for an expansion of the attractive dispersion forces and model substrates by plane walls. However, close to a solid substrate the entropy of a fluid is dominated by the occupation probability of discrete adsorption sites formed by the corrugated substrate surface. We propose a density functional which captures accurately the monolayer adsorption properties but covers also the growth of mesoscopic films and capillary condensation at hydrophilic conditions. We discuss the dependence of wetting and adhesion on humidity and substrate strength, in particular at the crossover from single particle to capillary condensed bridges.

CPP 20.6 Wed 16:00 Poster B

Biological Calcium Carbonate Precipitation — ●SIGRID HENNIG, CHRISTIAN SOOR, SABINE HILD, and ANDREAS ZIEGLER — Central Facility for Electron Microscopy; University of Ulm, Albert-Einstein-Allee 11, 89069 Ulm

Biomaterials have unique structures and morphologies, which acquire much better performance than geological minerals. Calcium carbonate is the most common mineral found in living organisms occurring as calcite, aragonite, and, to a lesser extent, vaterite and hydroxy calcite. Interestingly many organisms form amorphous calcium carbonate (ACC) that would be unstable in-vitro. ACC is thought to be a precursor phase for crystalline modifications and, because of its high solubility, occurs in transient calcium carbonate reservoirs. The terrestrial crustacean *Porcellio scaber* develops large ACC reservoirs that are used for the mineralization of the new cuticle synthesized before the old cuticle is shed in a process called moulting. In order to investigate the formation and stabilization of biogenic ACC under physiological conditions we analysed the cation composition in the region of ACC formation, isolated the proteins of the organic matrix and tested their effects on mineral precipitation. We show that under

these conditions the physiological Mg concentration (13 mM, Ca:Mg about 1:1) has a large effect on crystal morphology. Matrix proteins prevent crystal precipitation and lead to formation of 50 nm large colloidal particles. Depending on matrix concentration these particles are arranged in hollow sphere super structures resembling ACC spherules in *P. scaber* during natural degradation.

CPP 20.7 Wed 16:00 Poster B

Stimuli-responsive networks containing superparamagnetic nano-particles — XUENA ZOU¹, ●SILKE RATHGEBER¹, and PATRICK THEATO² — ¹Max-Planck Institute for Polymer Research, Polymer Physics, D-55128 Mainz — ²Johannes Gutenberg-University, Institute of Organic Chemistry, D-55099 Mainz

We report the synthesis and characterization of poly(N-isopropylacrylamide) (PNiPAM) hydrogels containing superparamagnetic nano-particles which are i.a. chemically bonded to the network. Changing magnetization by swelling (humidity), pH, temperature and stress will lead to new stable stimuli-responsive materials for sensor applications but also to materials which show, in response to an external magnetic field gradient, actuatoric properties. The synthesis of the PNiPAM gel is performed via a reactive poly(pentafluorophenylacrylate) (PPFPA) precursor gel. The advantage of the presented synthesis lies in the fact that the properties, e.g. the lower critical solution temperature, of the final hydrogels can be tuned by the degree of conversion from PPFPA to PNiPAM and/or incorporation of various functional groups, e.g. pH-dependent groups. Beside standard physicochemical characterization methods we report results from cryo-transmission electron microscopy to characterize the magnetic nano-particles and their distribution in the gels. Magnetic properties of the magnetic nano-particles and the loaded hydrogels were studied using a superconducting quantum interference device. The density of the magnetic nano-particles in the hydrogels was calculated according to the response of the gels to the external field.

CPP 20.8 Wed 16:00 Poster B

Thin polymer blend films of conducting homopolymers — ●M. RUDERER, J.-F. MOULIN, and P. MÜLLER-BUSCHBAUM — TU München, Physik-Department E13, James-Franck-Str. 1, D-85747 Garching, Germany

Two conduction homopolymers, MEH-PPV Poly(1-methoxy-4-(2-ethylhexyloxy)-p-phenylenevinylene) and P3BT (poly(3-butylthiophene-2,5-diyl)), are blended with different ratios. Thin films are prepared via spin-coating on glass slides. The resulting surface structures are characterized by optical microscopy and atomic force microscopy (AFM). With optical spectroscopy (UV/Vis) in reflection and transmission geometry the absorbed part of the optical spectrum is detected. The resulting parameters are correlated with the bulk phase diagram of the components.

CPP 20.9 Wed 16:00 Poster B

Azo-dye/ polymer composite - a novel class of materials for optical coatings — SVEN MACKO, ●RAFAEL MEINHARDT, ANSGAR DRAUDE, and HILMAR FRANKE — Department of applied physics, university of Duisburg-Essen, Lotharstr.1, 47057 Duisburg, Germany

Polymer films of dipolar and nondipolar materials with a thickness up to 1-2 microns have been prepared on glass substrates. Vapor deposition of azo-dyes (< 500 nm) and subsequent annealing leads to composite layers which are different from usual solution prepared guest-host systems. These composite layers can be prepared with high dye concentrations. Absorption spectra and metal film enhanced leaky mode spectroscopy have been applied prior and after the deposition of the dye layers. A strong interdiffusion has been observed. The obtained composite material is quite different from the well known guest-host systems.

Regarding their optical properties the composites behave more like organic glasses than guest-host systems. In comparison with the pure polycrystalline layers the scattering can be reduced with the composites and smooth surfaces may be obtained. Stable and efficient holographic gratings could be recorded in these layers.

CPP 20.10 Wed 16:00 Poster B

Structure of polymer coatings established for advanced quantum efficiency of photomultiplier tubes — ●V. KÖRSTGENS¹, C.-C. HSU², D. PANEQUE³, E. LORENZ², and P. MÜLLER-BUSCHBAUM¹ — ¹TU München, Physikdepartment E13, James-Franck-Str. 1, D-85748 Garching — ²Max-Planck-Institut für Physik, Föhringer Ring 6, D-

80508 München — ³Stanford Linear Accelerator Center, Menlo Park, CA

Coatings consisting of a polyacrylate and para-terphenyl as wavelength shifter are established from solutions in chlorinated organic solvents via a spin-coating process. The coatings are milky in appearance and the coated photomultiplier tubes show an advanced quantum efficiency. Preparation conditions were varied with controlled humidity and the exposition of the sample to a flow of humid nitrogen while spin-coating and evaporation of the solvent. Optical microscopy revealed structures originated from crystallization of para-terphenyl and a superposed porous structure of the polymer matrix. Surface structures established on flat substrates under same conditions were also investigated by atomic force microscopy (AFM). The origin of the obtained structures is discussed in context to well-known structures referred to as breath figures. The relation between the surface structures of the polymer coating and the observed advanced quantum efficiency of photomultiplier tubes is addressed.

CPP 20.11 Wed 16:00 Poster B

IR to VIS ellipsometric studies of self assembled monolayers on metal and metal oxide surfaces — P. ANGELOVA¹, ●K. HINRICHS², E. JÄHNE³, M. GNAUCK³, K.-J. EICHHORN⁴, K. KOSTOVA¹, and D. TSANKOV^{1,2} — ¹Institute of Organic Chemistry, Bulgarian Academy of Sciences, 1113 Sofia, Bulgaria — ²ISAS, Institute for Analytical Sciences, Department Berlin, 12489 Berlin, Germany — ³Institute of Macromolecular Chemistry, Dresden University of Technology, 01062 Dresden — ⁴Institute of Polymer Research, 01062 Dresden, Germany

Self assembled monolayers (SAM) were formed from terminally aryl-functionalized alkanethiols on Ag and Au surfaces and from long-chain alkylphosphonic acids and alkylphosphoric acid esters on aluminium oxide. The thiol compounds were synthesized from para-substituted benzyl esters of 16-mercaptohexadecanoic acid containing Cl, NO₂, CN and OCH₃ as substituents. The monolayers were characterized by IR and VIS ellipsometry, X-ray photoelectron spectroscopy and contact angle measurements. The different properties of the end groups affected the organizational order within the monolayer yielding different degree of orientation and tilt angles. For the bidentate or tridentate chemisorbed monolayers on the aluminum oxide surface formed from alkylphosphonic acid and alkylphosphoric acid ester a high degree of conformational order is found.

CPP 20.12 Wed 16:00 Poster B

Rigid amorphous fraction in polymer nano-composites — ●ALBERT SARGSYAN^{1,2}, ANAHIT TONOVAN², SEVAN DAVTYAN², and CHRISTOPH SCHICK¹ — ¹Institute of Physics, University of Rostock, Germany — ²State Engineering University of Armenia, Yerevan, Armenia

It is frequently reported that semicrystalline polymers show 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 contributes neither to the heat of fusion or X-ray crystallinity nor to the relaxation strength at glass transition, see [1] for a review. The RAF is assumed to be in a glassy state above the common glass transition temperature. From heat capacity the temperature and time dependence of the RAF can be obtained. Polymer nano-composites can be used as such a model structure if they exhibit a RAF. If the polymer nano-particle interaction is strong enough there may be a significant RAF because of the large surface area of the nano-particles. The main advantage lies in the fact that the part causing the immobilization of the polymer molecules, i.e. the nano-additive, does not melt or crystallize in the relevant temperature range. So the essential disturbing factor for a direct observation of the devitrification is excluded. This may allow determining the devitrification of the RAF in polymer nano-composites by using calorimetric methods. The most recent data on this work is presented

CPP 20.13 Wed 16:00 Poster B

Nanoconfinement - A new strategy to manipulate the crystalline state of pharmaceuticals — ●G.T. RENGARAJAN, S. PANKAJ, D. ENKE, and M. BEINER — Martin-Luther-Universität Halle-Wittenberg, Naturwissenschaftliche Fakultät II, D-06099 Halle (Saale), Germany

The manipulation of the crystalline state of substances existing in different polymorphic forms is an important issue in many fields of appli-

cation. In case of pharmaceuticals the stabilization of unstable forms is interesting since solubility and bioavailability are usually improved. We will show that it is possible to manipulate the crystallization behavior of pharmaceuticals and to stabilize unstable crystalline forms by confining the substance in pores with diameters in the range 20-400 nanometers [G.T. Rengarajan et al., J. Am. Chem. Soc., to be published.]. The crystallization behavior of a pharmaceutical model system in two different types of nanostructured inorganic host systems is studied by DSC and x-ray scattering. The results clearly show that the most unstable crystalline form of this pharmaceutical melts and is stable for long times under confinement which was never observed for bulk samples. This allows to extract the thermodynamic parameters of this crystalline form which have not been reported so far and shows that this is an interesting field of application for nanostructured host-guest systems. The influences of pore geometry and surface interaction are studied and possible explanations for the differences between the crystallization behavior in the bulk and under confinement are discussed.

CPP 20.14 Wed 16:00 Poster B

Towards multifunctional composites: preparation and characterization of polymer-dispersed liquid crystals — ●LAKSHMI MEENA GANESAN, AXEL MELLINGER, MICHAEL WEGENER, WERNER WIRGES, and REIMUND GERHARD — Universität Potsdam, Institut für Physik, 14469 Potsdam, Germany

Micrometer-sized liquid-crystal droplets embedded in a polymer matrix induce optical switching behavior in the composite film through the alignment of the director along an external electric field. When a ferroelectric polymer is used as matrix material, the electric field generated by the piezo- or pyro-electric effect of the matrix material could potentially be used to switch the director of the LC. Employing a solvent-induced phase separation (SIPS) method, polymer-dispersed liquid crystal (PDLC) films were prepared from poly(vinylidene fluoride - trifluoroethylene) and a nematic liquid crystal. The films were sandwiched between two glass plates coated with transparent indium tin oxide (ITO) electrodes, and the field-dependent optical transmission of the charged PDLC films was measured. The phase-transition behavior of the liquid crystal was studied by means of infrared spectroscopy.

CPP 20.15 Wed 16:00 Poster B

Optimization of Alginate-Based Isocapillary Matrices for their Application in Biomedicine — ●MATTHIAS KELLERMEIER, RAINER MÜLLER, and WERNER KUNZ — Institut für Physikalische und Theoretische Chemie, Universität Regensburg, 93040 Regensburg

Unidirectional diffusion of divalent cations such as Cu²⁺ or Ca²⁺ into sols of sodium alginate provokes the formation of a hydrogel pervaded by capillaries which are aligned parallel to the direction of the cation flow showing hexagonal arrangement in cross-section. Gelation occurs due to the complexation and dehydration of the polysaccharide chains by the cations, leading to the release of water into the free lumen of the forming capillaries and the fixation of the polymer in the walls around them. Typical pore diameters vary in the range of 5-100 μm. The formation of highly ordered capillaries in alginate gels can be interpreted as a dissipative process similar to Rayleigh-Bénard convection, resulting from opposing diffusion gradients and friction. With respect to biomedical applications, these isocapillary gels can be modified either by incorporating inorganic particles into the gel matrix followed by densification and ceramization, or by stabilization of the alginate framework via covalent cross-linking of the chains, resulting in scaffolds useable as bone implants and for the regeneration of nerves. The aim of the present study is to optimize the pore structure of alginate gels in view of these applications. We focus on the effect of a series of additives in the sol, such as salts, sugars and surfactants. Furthermore, we have studied the variability of the pore structure of alginate gels by employing both different cations and counter-ions.

CPP 20.16 Wed 16:00 Poster B

In-situ measurement of the inverse piezoelectric coefficient in ferroelectrets — ●XUNLIN QIU, AXEL MELLINGER, MICHAEL WEGENER, WERNER WIRGES, GUGGI KOFOD, and REIMUND GERHARD — Universität Potsdam, Institut für Physik, 14469 Potsdam, Germany

A number of cellular polymer-ferroelectret materials were discovered to exhibit a strong piezoelectric response after proper charging [1]. The effective polarization (i.e., the density of macroscopic dipoles) in ferroelectrets originates from barrier discharges within the voids which are initiated when the charging voltage exceeds a threshold value. In

the present work, the build-up of the effective polarization of ferroelectrets under suitable voltage waveforms was studied by acoustic measurements of the inverse piezoelectric effect. The radiated sound signal has a contribution not only from the effective charge density, but also from the Maxwell stress. Therefore, a “butterfly” curve for the sound signal was obtained during charging under linearly increasing or decreasing voltages. The absolute piezoelectric d_{33} coefficients were determined by dielectric resonance spectroscopy immediately after charging. By comparing these d_{33} values with the zero-field sound signals, all other sound-signal measurements were converted to piezoelectric coefficients. A polarization-voltage (P-V) hysteresis loop was obtained by analyzing the data in light of an existing model for the piezoelectric d_{33} coefficient of ferroelectrets [2].

[1] S. Bauer, R. Gerhard-Mulhaupt, G. M. Sessler, *Phys. Today* **57**, 37 (2004).

[2] M. Paaanen, J. Lekkala, H. Välimäki, *IEEE-TDEI* **8**, 629 (2001).

CPP 20.17 Wed 16:00 Poster B

Surface science investigations of cellulose, lignin and polymer compounds based on them for applications in fuel cells — STEFAN KRISCHOK¹, SYED IMAD-UDDIN AHMED¹, ●ANDREAS COMOUTH¹, MARCEL HIMMERLICH¹, ROSINA STANEVA¹, AXEL KAUFFMANN², JÜRGEN PFITZER³, M. HUBER⁴, WOLFGANG BENDEL⁵, and JUERGEN A. SCHAEFER¹ — ¹Institute für Physik und Institut für Mikro- und Nanotechnologien, Technische Universität Ilmenau, P.O. Box 100565, 98684 Ilmenau, Germany — ²Fraunhofer Institut für Chemische Technologie (ICT), Joseph-von-Fraunhofer-Straße 7, 76327 Pfinztal, Germany — ³TECNARO GmbH, Burgweg 5, 74360 Ilsfeld-Auenstein, Germany — ⁴SFC Smart Fuel Cell AG, Eugen-Sänger-Ring 4, 85649 Brunnthal-Nord, Germany — ⁵Biomasseprojekt GmbH, Fritz-Reichle-Ring 4, 78351 Radolfzell, Germany

Research in fuel cells has intensified due to their potential in various fields. One of the main fuel cell components - the bipolar plate, is currently based on metals or graphite. A pyrolyzed cellulose- and lignin-based polymer compound shows excellent potential. However, various critical issues still need to be addressed, such as impurity poisoning in Direct Methanol Fuel Cells (DMFC). In this context, X-ray photoelectron spectroscopy (XPS), X-ray Diffraction (XRD) and thermal desorption provide important indications about the presence of impurities, degree of pyrolysis and desorption processes occurring during pyrolysis. Such knowledge enables an optimization of the material composition and pyrolysis parameters, thus making it suitable for fuel cell applications.

CPP 20.18 Wed 16:00 Poster B

AFM Studies of Defect-induced Surface Modulations in Smectic Liquid Crystals — ●WEI GUO and CHRISTIAN BAHR — Max Planck Institute for Dynamics and Self-Organization, D-37073 Göttingen

Smectic-A liquid crystals show a common defect structure, focal conic defects, which consist of a complex arrangement of curved equidistant molecular smectic layers. In thin smectic films between a substrate and an air interface, focal conics cause depressions at the air interface which can be imaged by AFM microscopy [1].

We present here an AFM study of the defect-induced surface modulations in smectic films on various substrates and at various phase transitions. Whereas substrates causing a random planar alignment (the liquid-crystal director is oriented parallel to the substrate surface but there is no preferred in-plane orientation) lead to a pattern of circular surface depressions, we observe for substrates with an unidirectional planar alignment (the director possesses one or more preferred in-plane orientations) linear groove-like surface modulations of the air interface. In thicker films on these substrates, a complex structure is observed, in which the grooves seem to be decorated by rows of interdigitating circular focal conics.

We study also the behavior of the surface modulations at different liquid-crystal phase transitions like smectic-A – nematic, smectic-A – isotropic, or smectic-A – smectic-C.

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

CPP 20.19 Wed 16:00 Poster B

DC Electrical Transport through Metallic Nanostructures — ●RADIM KRĚNEK¹, VĚRA CIMROVÁ², and MANFRED STAMM¹ — ¹Leibniz Institute of Polymer Research Dresden, Germany — ²Institute of Macromolecular Chemistry AS CR, Prague, Czech Republic

Diblock copolymer nanotemplates provide a prospective way for development of ordered patterns of nanoobjects with e.g. magnetic (hard disks) or optoelectronic (LEDs, photovoltaic cells) functionality. Thin films of diblock copolymer enriched by a low molar mass additive are casted on conductive surfaces in order to ensure good electrical contact for electroplating of magnetic materials or optoelectronic devices. Extraction of the additive results in a porous nanostructure, but quality (depth) of the pores is very sensitive to the substrate roughness. As well, appearance of the top electrode depends on the applied material, technique and ambient conditions. We demonstrate various electrical transport regimes in relation with the roughness of the bottom electrode and the cluster size, loading rate, etc. of the sputtered metal applied for the top electrode. These transport regimes (injection limited currents, space charge limited currents, tunneling) are discussed regarding vertical profiles of the films.

CPP 20.20 Wed 16:00 Poster B

Spontaneous onion formation from planar lamellar nuclei — ●YASUTAKA IWASHITA¹ and HAJIME TANAKA² — ¹Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — ²Institute of Industrial Science, University of Tokyo, Tokyo, Japan

Onion phase, which is composed of multilamellar vesicle (MLV, or onion) structures in lyotropic liquid crystals, has been studied in its formation under shear flow since the discovery by Roux *et al.* in 1993. However it has been also reported that onion phase can be formed spontaneously via sponge (isotropic)-to-lamellar phase transition without shear when lamellar phase nucleates as onions. In this study we report a new interesting step of the lamellar ordering (nucleation) from the sponge phase observed directly with optical microscopy: Initially lens-shaped nuclei (planar lamella) nucleate, and then they spontaneously transform into onion nuclei. We also reveal that the origin of this shape transformation is the competition between curvature elastic and interfacial energy. This means a remarkable fact that the initial most stable bulk structure (planar lamella) spontaneously changes into the metastable higher-energy bulk structure (onion). Finally we mention the aspect as a novel ordering step peculiar to a system of low-dimensional internal order (layered structure): The fate of nuclei can be seriously affected by the competition between interfacial and elastic deformation energy in general.

CPP 20.21 Wed 16:00 Poster B

Self organization and light induced patterning of azo-dye layers — RAFAEL MEINHARDT, VLADIMIR MURADOV, ●ANSGAR DRAUDE, and HILMAR FRANKE — Department of applied physics, university of Duisburg-Essen, Lotharstr.1, 47057 Duisburg, Germany

Thin layers of azo-dyes have been prepared from the vapour phase on pure glass, metal/ glass and ITO/ glass substrates. The films have been patterned using light or electrostatic charging of the substrate. As characterization methods plasmon spectroscopy, AFM investigations, X-ray scattering and holographic recording have been used.

A strong tendency for the formation of crystals is found especially in the range of 20-70 nm thick depositions. The crystallization depends on the roughness of the substrate and the presence of deposited electrostatic charges. Oriented transparent regions may be prepared as well as scattering unoriented areas. Both types of layers are sensitive for an optical reorientation via the Cis-Trans isomerization.

CPP 20.22 Wed 16:00 Poster B

Self-assembled treelike patterns from an evaporating binary solution — ●LEONID GOVOR, GOTTFRIED BAUER, and JÜRGEN PARISI — Institute of Physics, University of Oldenburg, Carl-von-Ossietzky Str. 9-11, D-26129 Oldenburg, Germany

Spontaneous formation of treelike patterns which developed during evaporation of the solvent from a phase-separated bilayer resulting from a binary polymer solution spin-coated onto a solid substrate has been studied. The initial bilayer consists of a poly(isobutyl methacrylate) (BMA) layer on top of a nitrocellulose (NC) solution layer. During evaporation, the top BMA layer becomes unstable and transforms into short ridges. Finally, the inhomogeneous evaporation of the solvent from the NC solution layer connects the BMA ridges to treelike patterns. To support our model, we present results of a complementary experiment based on casting of the BMA solution on an inclined glass substrate.

CPP 20.23 Wed 16:00 Poster B

Anregungstransfer in molekularen Aggregaten — ●GEORG SCHULZ, JAN RODEN, ALEXANDER EIFELD und JOHN S. BRIGGS

— Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg

Molekulare Aggregate, die aus Dipol-Dipol-gekoppelten Farbstoffmolekülen bestehen, sind nach wie vor reger Gegenstand der Forschung. Bei der Aggregation bilden sich delokalisierte Zustände, die sowohl eine (oft) drastische Änderung des Aggregatabsorptionsspektrums bewirken und auch für effizienten Energietransfer entlang des Aggregats sorgen. Beispiele solcher Aggregate sind J-Aggregate, bei denen ein sehr schmales, rotverschobenes Absorptionsband entsteht, oder die Lichtsammeleneinheiten bei der Photosynthese. Ein Problem bei der Beschreibung molekularer Aggregate ist die Berücksichtigung intramolekularer Vibrationen. Mit Hilfe der CES-Näherung konnten wir die Absorptionsspektren und optische Rotation solcher Quantenaggregate unter Einbeziehung ihrer Vibrationen [1] und Unordnung [2] hervorragend beschreiben. Wir betrachten nun den Energietransfer im Rahmen der CES-Näherung.

[1] A. Eisfeld, J. S. Briggs, Chem. Phys. 281, 61, Chem. Phys. 324, 376

[2] A. Eisfeld, J. S. Briggs, Phys. Rev. Lett. 96, 113003

CPP 20.24 Wed 16:00 Poster B

Growth of metal nanoparticles on tubular J-aggregates by photo-induced electron transfer processes — DÖRTHE MELITTA EISELE¹, ●OMAR AL-KHATIB¹, ANNA BURMISTROVA¹, HANS VON BERLEPSCH², CHRISTOPH BÖTTCHER², and STEFAN KIRSTEIN¹ — ¹Humboldt-Universität zu Berlin — ²Freie Universität Berlin

In this contribution it is shown that an electron transfer reaction from cyanine dyes to noble metal ions can be utilized to grow metallic nanoparticles at the surface of respective molecular aggregates. Therefore tubular J-aggregates with typical diameters of 20 nm and length exceeding 10 μm are formed in aqueous solutions using amphiphilic tetrachloro-benzimidazocarbocyanine dyes. The aggregates are characterized by means of cryogenic electron transmission microscopy (cryo-TEM) and by scanning force microscopy (AFM). Upon addition of noble metal salts (Na_2PdCl_4 or AgNO_3) to the aggregate solution metallic nanoparticles that are rather uniform in size with a mean diameter of a few nanometers are growing on the surface of the aggregates as observed by cryo-TEM. In case of Pd salt the aggregates are destroyed upon particle formation, while in case of Ag salt the aggregates are unaffected by the formation of silver particles. 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 optical spectra with varying silver ion concentration allows to investigate the influence of the particle growth on aggregate structure and morphology.

CPP 20.25 Wed 16:00 Poster B

Nanotemplates from monolayers of electron donors and acceptors self-assembled at solid-liquid interfaces — ●MIN AI¹, FRANK JÄCKEL^{1,2}, XINLIANG FENG³, WEI ZHUANG¹, KLAUS MÜLLEN³, and JÜRGEN RABE¹ — ¹Humboldt University Berlin, Department of Physics, Newtonstr. 15, 12489 Berlin, Germany — ²present address: Stanford University, Department of Chemistry, 333 Campus Drive, CA 94305-5080, Stanford, USA — ³Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

We studied a potential nanotemplate for molecular and organic electronics consisting of an electron-withdrawing acceptor, an alkylated coronenebis(dicarboximide) derivative, and an electron-pushing donor, benzo[*o*]bistriphenylene[2,1,12,11-efghi:2*,1*,12*,11*-uvabc] ovalene. Self-assembled monolayers of the neat donor and acceptor and their mixture respectively were investigated by scanning tunneling microscopy (STM) at the interface between an organic solution and highly oriented pyrolytic graphite (HOPG). The pure electron acceptor forms two highly ordered crystalline phases with either one molecule ("oblique cell") or four molecules ("zigzag cell") per unit cell respectively. The neat electron donors could not be visualized. In the electron donor/acceptor mixtures, two distinct types of crystal structures are revealed, one with four donors and one acceptor, and the other with two donors and two acceptors in the unit cell. Molecular packing models are presented according to the STM images. The packing is attributed to the interactions between the molecules and between molecules and HOPG.

CPP 20.26 Wed 16:00 Poster B

Nanostructuring and nanoaggregates on functionalized surfaces — ●THOMAS BAUMGÄRTEL¹, HARALD GRAAF¹, MAIK VIELUF¹, and CHRISTIAN VON BORCZYKOWSKI — Centre for nanostructured mate-

rials and analytics, TU Chemnitz, 09107 Chemnitz

We investigated the nano-structuring of silicon covered with an alkene monolayer. This was achieved by local anodic oxidation by an atomic force microscope (AFM). The monolayers are formed by a self assembling process through a heat induced chemical reaction. The molecules of these monolayers are highly ordered featuring relative physical and chemical stability. Thus they represent a way to passivate the surface. Furthermore the surface properties could be tuned easily by variation of the head groups of the alkenes.

Local anodic oxidation degrades the monolayer partially and the underneath silicon surface is oxidized resulting in a silicon oxide nanostructure. The organic monolayer influences the oxidation process naturally. A clear dependence of the oxidation time on the strength of the electric field was found.

The nanometer-sized siliconoxide structures were used for selective binding of optical active materials. Non-covalent interactions (e.g. ionic and hydrophobic) proved to be an elegant way for a selective modification of the structures as well as the surrounding surface. The in this manner modified surfaces have been examined both by atomic force microscopy and optical widefield microscopy.

CPP 20.27 Wed 16:00 Poster B

Tuning surface chemistry of thin PEO films by control of morphology — ●EVELYN MEYER and HANS-GEORG BRAUN — Leibniz Institut für Polymerforschung Dresden, Max Bergmann Center of Biomaterials, D-01069 Dresden, Hohe Strasse 6

Ultrathin polyethyleneoxide (PEO) layers are of great importance as protein resistant coatings to avoid nonspecific protein adsorption. The controlled introduction of chemical groups (NH_2) into PEO layers allows a specific immobilization of proteins. Depending on the solution concentration PEO films, prepared by dip-coating, crystallize in unilamella or multilamellae morphologies. Chain length of PEO molecules and interaction of the amino-terminated PEO with the surface influence growth morphologies and distribution of amino groups on the lamella surface and consequently the grafting density of biomolecules attached to the lamella surface. The water soluble morphological PEO units can be immobilized at the surface by electron beam lithography. The arrangement of reactive amino groups within the morphological entities can be checked by selective fluorescence staining and fluorescence microscopy.

CPP 20.28 Wed 16:00 Poster B

Aligned Polyelectrolyte Chains Adsorbed onto an Oppositely Charged Lipid Monolayer — ●JENS-UWE GÜNTHER, OLAF SOLTWEDEL, HEIKO AHRENS, and CHRISTIANE A. HELM — Institut für Physik, Ernst-Moritz-Arndt Universität, F.-L.-Jahn-Str. 16, D-17487 Greifswald, Germany

The negatively charged polyelectrolyte PSS (Poly styrene sulfonate) is adsorbed onto positively charged TAP or DOAB monolayers (1,2-Dipalmitoyl-3-Trimethylammonium-Propane, dioctadecylammonium bromide, respectively) at the water surface. The structure of the supramolecular complex is investigated with synchrotron grazing incidence diffraction. In-plane diffraction peaks at small angles measure the separation of the aligned polyelectrolyte chains, while those at large angles measure the quasi-crystalline structure of the alkyl chains within the lipid monolayer. Depending on the polyelectrolyte concentration in solution, the lipid charge is partially neutralized by the PSS and partially by anions, or complete charge compensation occurs. The influence of the ion concentration in the aqueous polyelectrolyte solution is discussed. The two peaks of the rod-scan at small angles indicate that the lipid monolayer buckles directly above the aligned PSS chains.

CPP 20.29 Wed 16:00 Poster B

Lattice dynamics of a two-dimensional colloidal crystal subjected to a substrate potential — ●MARIA ZVYAGOLSKAYA¹, JÖRG BAUMGARTL¹, HANS HENNING VON GRÜNBERG², and CLEMENS BECHINGER¹ — ¹Universität Stuttgart, 2.Physikalisches Institut, Pfaffenwaldring 57, D-70569 Stuttgart, Germany — ²Karl-Franzens-Universität, Institut für Chemie, Heinrichstrasse 28, A-8010 Graz, Austria

In the presence of a substrate potential the phonon band-structure of a two-dimensional (2D) crystal can be tuned by varying the strength or the shape of the substrate potential. Here we study this idea by subjecting a 2D colloidal crystal to a commensurate one-dimensional (1D) substrate potential with sinusoidal modulations in one or two spatial

directions. Experimental realization of such potentials is achieved by interfering laser beams. We record the trajectories of colloidal particles by means of video-microscopy and then calculate the 1D and 2D phonon band-structure and the phonon spectrum. The 1D band-structure and the phonon spectrum allow for studying how the shape of the band structure is altered by the substrate potential. The 2D band structure displays the breaking of the 6-fold symmetry of the intrinsic colloidal crystal down to a 2-fold symmetry caused by the substrate potential.

CPP 20.30 Wed 16:00 Poster B
Temperature-Dependent Holographic Studies of Azobenzene-Containing Diblock Copolymers — ●HUBERT AUDORFF¹, LOTHAR KADOR¹, CARSTEN FRENZ², and HANS-WERNER SCHMIDT² — ¹Universität Bayreuth, Physikalisches Institut und Bayreuther Institut für Makromolekülforschung (BIMF), 95440 Bayreuth — ²Universität Bayreuth, Makromolekulare Chemie I, 95440 Bayreuth

The light-induced reorientation of azobenzene and mesogenic side groups in the minority phase of diblock copolymers has been investigated with holographic methods at different temperatures. The materials consist of a matrix of polystyrene and minority phases which contain chromophores and mesogens in different ratios. Plane gratings were inscribed at temperatures between 20 °C and 90 °C. The influence of the temperature on the achievable refractive-index modulation, writing time, sensitivity, short-term relaxation, and long-term stability of the gratings was measured. With increasing temperature, the achievable refractive-index modulation becomes smaller, whereas the sensitivity is roughly constant. The stability drops strongly, when the glass transition temperature is approached.

CPP 20.31 Wed 16:00 Poster B
Single-laser-pulse-induced switching of molecular spin states — ●SÉBASTIEN BONHOMMEAU¹, NIKO PONTIUS¹, HERMANN DÜRR¹, WOLFGANG EBERHARDT¹, SAIOA COBO², GABOR MOLNÁR², and AZZEDINE BOUSSEKSOU² — ¹Berliner Elektronenspeicherring-Gesellschaft für Synchrotronstrahlung m.b.H (BESSY), Albert-Einstein-Straße 15, 12489 Berlin, Germany — ²Laboratoire de Chimie de Coordination,

CNRS UPR-8241, Route de Narbonne 205, 31077 Toulouse, France

Light-induced phenomena in spin crossover complexes have aroused a lot of interest since the discovery of the LIESST (Light-Induced Excited Spin State Trapping) effect in solid state. Here, we demonstrate by means of Raman spectroscopy that a bi-directional spin transition can be obtained at room temperature when applying a nanosecond laser pulse in the hysteresis loop of the spin crossover complex Fe(pyrazine)[Pt(CN)₄]. This phenomenon is interpreted as a photo-induced phase transition exhibiting a threshold energy density. In order to provide a deeper insight on the electronic properties of such polymeric materials, X-ray photoemission and absorption experiments have also been performed on a multilayer assembly of thin films of Fe(azopyridine)[Pt(CN)₄] that display spin crossover. This information is of paramount importance to shed new light on the photo-induced dynamics, in the subpicosecond time scale, which will be investigated using the femtoslicing facility now available at BESSY GmbH.

CPP 20.32 Wed 16:00 Poster B
Simultaneous scanning tunneling and atomic force microscopy at ambient conditions using quartz tuning fork sensors — ●STEFAN STRÖMSDÖRFER, VIATCHESLAV DREMOV, IRINA LAZAREVA, YURI KOVAL, and PAUL MÜLLER — Physikalisches Institut 3, Universität Erlangen-Nürnberg, Germany

We demonstrate the operation of a tuning fork based AFM in non-contact mode with simultaneous acquisition of both the tunneling current and the frequency shift of a vibrating conducting cantilever.

We were able to show atomic resolution of the graphite lattice of HOPG at ambient conditions. Whereas STM shows the well known mapping of every second carbon atom, in AFM the complementary subset of carbon atoms was visualized. These results agree qualitatively with previous measurements performed in UHV.

As the frequency shift, i.e. the force gradient determines the control, there is no restriction on the conductivity of the samples. The technique enables measurements of the tunneling current even if the sample surface contains insulating regions. We applied this method in the measurement of the conductivity along nanowires deposited onto an insulating substrate.

CPP 21: POSTER: Dynamics and Diffusion

Time: Wednesday 16:00–18:30

Location: Poster B

CPP 21.1 Wed 16:00 Poster B
A new way of implementing partial slip boundary conditions — ●JENS SMIAITEK¹, FRIEDERIKE SCHMID¹, and MICHAEL ALLEN² — ¹Condensed matter theory, Faculty of physics, University of Bielefeld, 33615 Bielefeld, Germany — ²Department of Physics and Centre for Scientific Computing, University of Warwick, Coventry CV4 7A1, United Kingdom

Partial slip boundary conditions determine the flow profile in the micrometer scale of modern separation devices where evidence is found that the famous macroscopic no slip boundary conditions are no longer applicable.

We present a new approach to implement partial slip boundary conditions for the study of flow profiles in Dissipative particle dynamics. An extension of the Langevin equation is used to create a viscous layer that exerts friction on the fluid particles in the vicinity of the boundaries. The method is both applicable for particle-based as well as lattice-based algorithms and can be used to generate shear flows like Couette or Poiseuille flow profiles. Crucial parameter for those boundary conditions are the slip length and the position of the hydrodynamic boundaries. Combinations of the above mentioned flow profiles are used to determine both parameters exactly.

The presented method allows to tune the slip length systematically and an analytic equation for the calculation of the slip length as a function of the model parameters can be given.

CPP 21.2 Wed 16:00 Poster B
²H-NMR-Untersuchungen der modifizierten Defektdynamik in dotiertem Eis — ●DANIEL SCHRAFT¹, BURKHARD GEIL², MARCO SCHEUERMANN¹ und FLORIAN LÖW¹ — ¹Institut für Festkörperphysik, TU Darmstadt, Hochschulstr. 6, D-64289 Darmstadt — ²Lehrstuhl für Experimentelle Physik III, Universität Dortmund, Otto-Hahn-Str. 4,

D-44221 Dortmund

In einer früheren Studie¹ wurde mittels ²H-NMR der Mechanismus des Protonentransports in hexagonalem Eis untersucht. Die Resultate belegen einen Zwischengittertransport intakter Wassermoleküle. Aufbauend auf der zitierten Arbeit dient dieser Beitrag nun dazu, den Einfluss zusätzlich eingebrachter ionischer Defekte auf die Zeitskala und den Mechanismus des Protonentransports zu untersuchen. Dazu wird an mit HCl, NH₃ und KOH dotierten Proben Spin-Gitter-Relaxationszeiten, stimulierte Echos und Spektren gemessen.

¹B.Geil et al. Phys. Rev. B 72, 014304 (2005)

CPP 21.3 Wed 16:00 Poster B
Molecular dynamics in a glass-forming liquid crystal as studied by broadband dielectric and thermal spectroscopy — ANA BRÁS¹, MADALENA DIONÍSIO¹, HEIKO HUTH², CHRISTOPH SCHICK², and ●ANDREAS SCHOENHALS³ — ¹REQUIMTE, Departamento de Química, Faculdade de Ciências e Tecnologia da Universidade Nova de Lisboa, P-2829-516 Caparica — ²University of Rostock, Department of Physics, Universitätsplatz 3, D-18051 Rostock — ³Federal Institute of Materials Research and Testing, Unter den Eichen 87, D-12205 Berlin

Broadband dielectric (10 mHz to 1GHz) and thermal spectroscopy (1 mHz to 10 kHz) was employed to study the molecular dynamics of the nematic liquid crystalline mixture E7. In agreement with theoretical considerations the dielectric spectra shows two relaxation processes. The process at lower frequencies is due to hindered rotational fluctuations about the short molecular axis (delta-relaxation) of the molecules. The process at higher frequencies is related to librational fluctuations around the long molecular axis (tumbling modes). The temperature dependence of the relaxation rate for the delta-process and the tumbling in the nematic phase obey the empirical Vogel-Fulcher-Tamman behavior which is typical for glass-forming systems.

For the first time it was shown that the temperature dependence of the relaxation rates for the delta-process and the tumbling modes is essential different using a derivative technique. The comparison of the dielectric with the thermal data gives the result that the glass transition in this system corresponds to the tumbling mode.

CPP 21.4 Wed 16:00 Poster B

Experimentelle Untersuchung der Dynamik im Tetrahydrofuran-Hydrat-Clathrat mit Hilfe der 2H-NMR — ●ANDRE NOWACZYK, BURKHARD GEIL und ROLAND BÖHMER — Experimentelle Physik III, Universität Dortmund, 44221 Dortmund, Germany

Hydrat-Clathrate können als Speicher- bzw. Transportmedium niedermolekularer Gase von großem Nutzen sein. Für eine effiziente Ausnutzung dieser Möglichkeiten ist es nötig, die Dynamik, sowohl des durch Wasserstoffbrücken gebundenen H₂O-Gitters, als auch der eingeschlossenen Gastmoleküle zu studieren. Als Modellsystem dient in unserem Fall das besonders stabile Tetrahydrofuran-Hydrat-Clathrat. Durch gezielte Isotopenmarkierungen am Clathrat lassen sich mit der 2H-NMR die Bewegungen von Gitter und Gastmolekül getrennt untersuchen. Dazu werden neben Relaxationsmessungen und eindimensionalen Festkörperspektren auch Messungen von Zwei-Zeiten-Autokorrelationsfunktionen verwendet. Letztere erlauben neben der Bestimmung der Zeitskalen auch Erkenntnisse über die Geometrien der dynamischen Prozesse zu gewinnen.

CPP 21.5 Wed 16:00 Poster B

Dielectric response of polar liquids in narrow slit pores — VLADIMIR FROLTSOV¹ and ●SABINE KLAPP^{1,2} — ¹Stranski-Laboratorium, Technische Universität Berlin, Strasse des 17. Juni 115, 10623 Berlin — ²Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin

Based on molecular dynamics (MD) simulations and a simple (Stockmayer) model we investigate the static and dynamic dielectric response of polar liquids confined to narrow slit pores. The MD simulations are used to calculate the time-dependent polarization fluctuations along directions parallel and perpendicular to the walls, from which the components of the frequency-dependent dielectric tensor can be derived via linear response theory. Our numerical results reveal that the system's response is strongly anisotropic. The parallel dielectric function, $\epsilon_{\parallel}(\omega)$, has Debye-like character very similar to the corresponding isotropic bulk function, $\epsilon_{\text{bulk}}(\omega)$, at the same chemical potential. Indeed, the main confinement effect on $\epsilon_{\parallel}(\omega)$ consists in a shift towards smaller values relative to the bulk function. On the other hand, in perpendicular direction we observe a characteristic peak in the absorption part of the dielectric function, $\epsilon_{\perp}(\omega)$. This peak is absent in the bulk system and reflects strongly pronounced, damped oscillations in the polarization fluctuations normal to the walls.

V. A. Froltsov and S. H. L. Klapp, J. Chem. Phys. **124**, 134701 (2006).

V. A. Froltsov and S. H. L. Klapp, submitted

CPP 21.6 Wed 16:00 Poster B

Determination of microscopic interaction constants with unprecedented accuracy — ●FELIX LEHMKÜHLER, MICHAEL PAULUS, SIMONE STREIT, and METIN TOLAN — Experimentelle Physik I/DELTA, Universität Dortmund, Otto-Hahn-Straße 4, 44221 Dortmund

The poly(propylene glycol) 4000 (PPG4000) - isobutane interface was studied by x-ray reflectivity measurements. The interface was investigated under different pressures between 1.0 bar and 2.6 bar which is close to the condensation pressure of isobutane at the temperature of 289K. While adsorption of molecular thin films of isobutane is expected for hydrophobic interacting systems like glycerol-isobutane or water-propane, the formation of isobutane films on PPG4000 surface is suppressed by the high miscibility of isobutane and PPG4000. Thus no evidence for the formation of isobutane films was found.

The surface roughness of the substrate was estimated to vary between 0.4 nm at 1 bar nitrogen and 0.8 nm at 2.6 bar isobutane pressure. This is explained by the change of surface tension of the PPG4000-isobutane mixture with isobutane pressure. Ideal solution of isobutane in PPG4000 regarding to Raoult's Law is assumed to describe the measurements. The surface tension is calculated with the capillary waves theory to confirm the ideal solution with theoretical models for surface tension behavior of binary liquid mixtures. The Parachor-method and gradient theory are applied. Furthermore, the

gradient theory allows to determine microscopic interaction constants qualitatively and quantitatively.

CPP 21.7 Wed 16:00 Poster B

Diffusion and spin relaxation in thin excited slices — ●ACHIM GÄDKE¹ and NIKOLAUS NESTLE^{1,2} — ¹TU Darmstadt, Institut für Festkörperphysik — ²BASF AG Ludwigshafen

NMR experiments involving thin excited slices are of interest both for conventional NMR microimaging and for mechanically detected magnetic resonance. Especially in the latter case, the thickness of the excited slices may be well below 1 μm . In samples containing fast-diffusing liquid components such as water, the diffusive exchange of spin magnetization between such a thin excited slice and its surrounding on the time scale of the NMR experiments plays a major role [1]. Using static field gradients of 170 T/m we investigate the effects of periodic excitation inside thin slices. Vertical positioning of the sample cells at μm precision relative to the magnetic field gradient and flat coil design for optimal signal filling factor are prerequisites to systematic studies. A novel experimental cell adapted to such a coil design will be presented and experimental options for manipulating diffusion and relaxation properties of the walls and the liquid in the cell while retaining the exact positioning with respect to the magnet will be discussed. Both simulation and experimental results on the slice's NMR response under periodic excitation will be presented and consequences for further development in micro-MRI and mechanically detected NMR will be discussed.

[1] A. Gädke, N. Nestle, Diffusion Fundamentals 3 (2005) 38.1 - 38.12

CPP 21.8 Wed 16:00 Poster B

Relaxation and transport properties of the macromolecules in solution: effects of the friction tensors — ●ALEXANDER UVAROV and STEPHAN FRITZSCHE — Institut für Physik, Universität Kassel, D-34132 Kassel, Germany; uvarov@physik.uni-kassel.de.

Many problems in bio- and chemical physics involve the transport and relaxation properties of macromolecules which immersed in solution. A few well-known examples refer to the dielectric and nuclear magnetic relaxation as well as to the depolarization of the fluorescence light. During the past decade, therefore, a large number of experiments and molecular dynamic simulations (MDS) have been carried out in order to describe the relaxation properties of the macromolecules.

In the present contribution, we explore the question of how the bead-bead and bead-solvent interaction affects the relaxation processes of macromolecules. The behaviour of the friction tensor parameters [1] are analyzed for N-bead chain and for quite different thermodynamical regimes of the solution. The results from our semi-phenomenological theory are found to compare very well with experiment [2] and MD simulations [3] over a wide range of of macromolecule-solvent mass as well as interaction strength ratios.

[1] A. Uvarov and S. Fritzsche, Phys. Rev. E73, 011111 (2006); Chem. Phys. Lett, 401, 296 (2005); Phys. Rev. Lett. submitted (2006).

[2] B. Chen, E. Sigmund and W. P. Halperin, Phys. Rev. Lett. 96, 145502 (2006).

[3] J. R. Schmidt and J. L. Skinner, J. Phys. Chem. B. 108, 6767 (2004); J. Chem. Phys. 19, 8062 (2003).

CPP 21.9 Wed 16:00 Poster B

Lattice Boltzmann simulation of electroosmotic flow — ●MARCELLO SEGA¹ and CHRISTIAN HOLM^{1,2} — ¹Frankfurt Institute for Advanced Studies, Frankfurt, Germany — ²Max Planck Institute for Polymer Research, Mainz, Germany

We report on simulation of electroosmotic flow in a slit pore by means of coupled Molecular Dynamics - Lattice Boltzmann techniques. Proper dielectric boundary conditions for the confining media are treated by the use of a recently developed extension of the MMM2D and ELC algorithms for electrostatics. The influence of the dielectric jump and of the charge distribution on the confining plates (uniform vs. discrete) is investigated and compared with theoretical predictions.

CPP 21.10 Wed 16:00 Poster B

Is lithium hydride LiH or LiH_{0.5}? This is just a question of time! — ●TYNO ABDUL-REDAH — Inst. f. Chemie, TU Berlin, Str. d. 17. Juni 135, 10623 Berlin, Germany.

The interactions of the particles in a macroscopic system lead to quantum correlated states in which the particles become invisible. The survival time of these states in condensed matter is generally expected to

be very short because of the fast and effective decoherence due to interaction with the remaining environment. However, it is indeed possible to measure their effects if the experimental technique is fast enough, e.g., using neutron Compton scattering (NCS) with scattering times of attoseconds. NCS experiments on various solid compounds like metal hydrogen systems have been done [1]. The effect manifests itself by a strong anomalous decrease of the scattering cross section density. E.g., the ionic hydride lithium hydride appears then as $\text{LiH}_{0.5}$ rather than LiH in the subfemtosecond time scale of the experiment [2]. The anomaly varies among others with scattering time and with temperature depending on the chemical bond and the electronic environment of the hydrogen in the particular chemical compound. The effect suggests that the protons do not scatter individually. New experimental results on solid LiH , LaH_x , NbH_x will be presented. The importance of this effect for chemistry and physics will be outlined.

[1] T. Abdul-Redah, C. A. Chatzidimitriou-Dreismann, E. B. Karlsson, *Neutron News* 15 (2004) 14.

[2] T. Abdul-Redah and C. A. Chatzidimitriou-Dreismann, *Physica B* 350 (2004) 1035.

CPP 21.11 Wed 16:00 Poster B

The dielectric properties of ionic liquids — ●JOSHUA SANGORO¹, ANATOLI SERGHEI¹, FRANK BORDUSA², and FRIEDRICH KREMER¹ — ¹Institut für Experimentelle Physik I, Universität Leipzig, Linnestraße 5, 04103, Leipzig, Germany — ²Max-Planck-Forschungsstelle für Enzymologie der Proteinfaltung, Weinbergweg 22, D-06120 Halle (Saale), Germany

Broadband Dielectric Spectroscopy (in the frequency range from 0.01 Hz to 10 MHz) at temperatures varying between 190 K to 330 K is employed to study molecular relaxations and ionic charge transport in ionic liquids. The former are observed at low temperatures (~ 200 K) with the latter giving rise to pronounced increases in the real part of conductivity and respectively the imaginary part of the complex dielectric function, both quantities have pronounced temperature dependence indicating the thermal activities of the underlying ionic charge transport. A remarkably low threshold of the applied electric field E is found to be at 0.3 V/cm, above which non-linear responses take place. Electrode polarization - usually neglected as an unwanted effect - contributes as well depending on various factors as geometry, concentration and the material of the electrode. The results are discussed with respect to recent and old (Debye-Falkenhagen) theories of ionic conduction.

CPP 22: POSTER: INTERNAL SYMPOSIUM Optical Spectroscopy

Time: Wednesday 16:00–18:30

Location: Poster B

CPP 22.1 Wed 16:00 Poster B

FTIR and EPR Studies of the Adsorption Complexes of Benzene and Oxygen on Cu/HZSM5 Zeolites — ●AUGUSTA ENE, TANJA ARCHIPOV, and EMIL RODUNER — Institute of Physical Chemistry, University of Stuttgart

Today phenol is produced mostly by the Cumene process, a three-step process which yields phenol and acetone in an 1:1 ratio. An alternative to this synthesis is the oxidation of benzene to phenol with molecular oxygen on Cu-exchanged zeolite catalysts. In order to understand the catalytic process on a molecular level one needs to understand the structures and geometry of the reactants on the surface. Vibrational spectroscopy offers information on both the strength of the acid sites and the nature of the adsorbate. Thus we study the adsorption complexes of benzene and oxygen on Cu-containing and Cu-free HZSM-5 zeolites by means of FTIR spectroscopy in order to determine the orientation of the adsorbed molecules on the zeolite surface. As the Cu^{2+} ions (3/2 spin) are EPR active, the oxidation state of Cu can be observed as well. Information on the surroundings of the active Cu species can be gained from the g and hyperfine anisotropy, offering us the chance to determine which Cu containing sites are more active during the catalytic process.

CPP 22.2 Wed 16:00 Poster B

Revealing the Electron-Phonon Coupling in a Conjugated Polymer by Single-Molecule Spectroscopy — ●RICHARD HILDNER¹, ULRICH LEMMER², ULLRICH SCHERF³, MARIN VAN HEEL⁴, and JÜRGEN KÖHLER¹ — ¹Experimentalphysik IV, Universität Bayreuth, 95440 Bayreuth, Germany — ²Lichttechnisches Institut, Universität Karlsruhe (TH), 76131 Karlsruhe, Germany — ³Fachbereich C, Universität Wuppertal, 42097 Wuppertal, Germany — ⁴Department of Biological Sciences, Imperial College London, London SW7 2AY, United Kingdom

The efficiency of charge- and energy-transfer processes in π -conjugated polymers is strongly determined by their electron-phonon coupling strength. However, the inherent pronounced structural disorder as well as the strong spectral diffusion in this class of functional materials prevented a direct determination of this parameter as yet. Here we employ single-molecule spectroscopy in combination with pattern recognition techniques which allows us to retrieve the profile of the electronic spectrum and concomitantly the electron-phonon coupling strength in a methyl-substituted ladder-type poly(*para*-phenylene) (MeLPPP). From these data we find a weak electron-phonon coupling for this polymer at low temperatures consistent with the fast excitation energy transfer processes that have been observed for this polymer. Moreover, we find strong evidence that the low-frequency vibrational modes, which are coupled to the electronic transitions, stem from vibrations of the surrounding host matrix indicating an even weaker intra-chain

electron-phonon coupling in MeLPPP.

CPP 22.3 Wed 16:00 Poster B

Fluorescence Lifetime Imaging Microscopy (FLIM) in the Frequency Domain — WILHELM HÜTTNER and ●LOTHAR KADOR — Universität Bayreuth, Physikalisches Institut und Bayreuther Institut für Makromolekülforschung (BIMF), 95440 Bayreuth

We report the design and construction of a confocal fluorescence lifetime imaging microscope (FLIM) based on a cw laser which is amplitude-modulated in the MHz range. Fluorescence lifetimes are calculated from the phase shift between the fluorescence signal and the excitation. The concept is inspired by a recent publication by Booth and Wilson [1] and allows one to choose different modulation frequencies between about 28 and 50 MHz. First experimental data are presented for blotting paper stained with a laser dye.

[1] M. J. Booth and T. Wilson, *J. Microsc.* **214**, 36 (2004).

CPP 22.4 Wed 16:00 Poster B

Mapping the Diffusional Landscape of a Porous Nanostructure — ●JOHANNA KIRSTEIN, ANDREAS ZÜRNER, STEFFEN SCHMIDT, MARKUS DÖBLINGER, THOMAS BEIN, and CHRISTOPH BRÄUCHLE — Dept. Chemie und CeNS, LMU München, Germany

Single Molecule Spectroscopy (SMS) is used in combination with Transmission Electron Microscopy (TEM) to trace out the internal structure of mesoporous thin films and to gain insight into the diffusion dynamics with respect to the underlying structure of the host. Individual dye molecules acting as molecular beacons are incorporated into the pores and their diffusion pathway through the pore system is observed by optical widefield microscopy. However, structural features on the nanometer scale can not be observed by optical methods. To resolve the pore structure in detail TEM measurements are needed. Usually, the sample preparation for TEM is either time-consuming, when it involves the preparation of cross-sections, or it lifts the film off its substrate by scratching. With such methods it is thus not possible to directly correlate the nanopore structure of the film and the trajectories of the dye molecules obtained by SMS.

Here, we present the synthesis of thin mesoporous films loaded with fluorescent dye molecules that can be successively investigated by optical widefield microscopy and TEM. We developed a method to overlay the images obtained by the two methods. This is the first time that dynamical information from single particle diffusion can be directly correlated with the structural details of the porous host obtained by TEM.

CPP 22.5 Wed 16:00 Poster B

Tunneling Events in Methyl-Substituted Terrylene in a Hexadecane Matrix — ●ALFRED SIGL¹, ANDRE GOURDON², MICHEL ORRIT³, and JOSEF FRIEDRICH¹ — ¹TUM, München, Germany —

²CEMES, Toulouse, France — ³MoNOS, Leiden, Netherlands

We investigated methyl-substituted terrylenes in a crystalline hexadecane matrix via hole-burning and single-molecule spectroscopy with the goal to detect single rotational tunneling events of the methyl group. A methyl group is a perfect tunneling system since there is no energy asymmetry. The rotational tunneling states correlate strictly with the nuclear spin states of the hydrogens. The hole burning experiments show a very unusual pattern: symmetric to the central hole appear two extremely sharp (200 MHz broad) antiholes, two broader antiholes and two sideholes. We associate the sharp antiholes, shifted by 1.3 GHz from the central hole, with the rotational tunneling states of the terrylene methyl group and the remaining features (5.1 and 6.4 GHz from the central hole) with a structural Two Level System involving the hexadecane lattice. The jumps in the frequency trajectories of single β -terrylene molecules reflect the 5.1 and 6.4 GHz features found in the hole-burning experiments. However, light-induced frequency jumps of single molecules corresponding with the 1.3 GHz features could not be detected. A possible reason could be that the high intensities in the single-molecule experiment pump the tunneling system to one of its substates.

CPP 22.6 Wed 16:00 Poster B

Incorporation of in vitro Synthesized GPCRs into Peptide Tethered Artificial Membran Sensor Platforms — ●RUDDOLF ROBELEK¹, MARCEL LEUTENEGGER², THEO LASSER², WOLFGANG KNOLL¹, and EVA-KATHRIN SINNER¹ — ¹Max-Planck-Institute for Polymer Research; Ackermannweg 10; 55128 Mainz; Germany — ²Laboratoire d'optique biomédicale; EPFL; Lausanne; Switzerland

In the last decade the optical spectroscopy techniques and biosensors have made a tremendous progress. Against this background it strikes that the study of complex membrane proteins, including the pharmacologically very important class of G protein coupled receptors, is rarely covered by this development. The main reason therefor is the difficult accessibility and availability of these proteins in biosensoric systems that are adapted for optical spectroscopic techniques. To overcome the named problems we here present a new concept using an in vitro expression strategy to directly insert complex membrane proteins into peptide tethered lipid bilayers. The result of this approach, which is demonstrated for the odorant receptor OR5, is a vectorial insertion of the protein under full conservation of its biological function. The protein / biosensor system can then be characterized in detail by different kinds of optical spectroscopic techniques. In our case we applied SPFS, SEIRAS and TIRF-Imaging to characterize the odorant receptor OR5 in a peptide tBLM. The successful transfer of this concept to further protein examples indicates, that the presented strategy could be a versatile platform to make the broad field of complex membrane proteins available to a multitude of optical spectroscopic techniques.

CPP 22.7 Wed 16:00 Poster B

Optical properties of rubrene crystals and films as a function of temperature — OLGA KRYLOVA¹, DOMINK BERG¹, ●MATTHIAS MÜLLER¹, JENS PFLAUM², and MORITZ SOKOLOWSKI¹ — ¹Institut für Physikalische und Theoretische Chemie, Universität Bonn, — ²3. Physikalisches Institut, Universität Stuttgart

We have investigated the optical absorption and photoluminescence (PL) of high quality rubrene (Rub) single crystals and thin vacuum deposited Rub films as a function of temperature. Interestingly, very strong changes are found in the PL spectra of Rub crystals upon cooling. Whereas room temperature (RT) spectra show the strongest emission at about 2000 cm⁻¹ below the electronic origin, spectra at low temperatures (LT), i.e., 5 K, have a very strong emission on the electronic origin and are very similar to spectra of thin Rub films. Going to low T increases the PL yield by a factor of more than 100. These results are tentatively interpreted with an emission from H-aggregates at RT and from J-aggregates at LT. A detailed comparison with the spectra of Rub films and Rub in solution will be given. Funding by the DFG research unit 557 is acknowledged.

CPP 22.8 Wed 16:00 Poster B

Diffusion of biomolecules in mesoporous silica materials — ●TIMO LEBOLD, CHRISTOPHE JUNG, JOHANNA KIRSTEIN, LEA MÜHLSTEIN, THOMAS BEIN, and CHRISTOPH BRÄUCHLE — Center for Nanoscience, Ludwig-Maximilians-Universität München, Department Chemie und Biochemie, Butenandtstraße 5-13, Haus E, 81377 München, Germany

Nanoporous channel systems, for example M41S-materials, form a class

of very promising host systems. Various guests can be embedded into their pores. A highly interesting application could be drug-delivery systems based upon such mesoporous silica materials. However, an essential prerequisite for the development of such systems is the detailed knowledge of the molecular dynamics and the host-guest interactions within the porous network. The diffusional behaviour of fluorescent molecules is elucidated in our group by highly-sensitive single-molecule microscopy techniques: wide-field and confocal fluorescence microscopy. They provide a unique insight into the molecular trajectories and the underlying mechanisms. This study focuses on fluorescently labelled biomolecules which are incorporated as guests into calcined mesoporous structures as well as structures with an internal functionalization of the pores. Their dynamics and their interaction with the pore inner surface are investigated in detail. This allows us to characterize the diffusion processes that are essential for the release of biomolecules from mesoporous silica materials in their role as drug-delivery systems.

CPP 22.9 Wed 16:00 Poster B

Femtosecond Resolved Transient Absorption Spectroscopy of Silicon Quantum Dots — ●VOLKER KUNTERMANN^{1,2}, CARLA CIMPEAN¹, DIETRICH HAARER², and CAROLA KRYSCH¹ — ¹Department for Physical Chemistry I, Friedrich-Alexander-Universität — ²Experimentalphysik/BIMF, Universität Bayreuth

We report about femtosecond resolved transient absorption spectroscopy of quantum dot semiconductor nanoparticles. The silicon nanoparticles with a diameter of 5 nm were synthesized by a gas phase process. The diameter is in the order of the exciton radius. The time resolved experiments are always in the limit of strong confinement. Performing stationary fluorescence spectroscopy we find two characteristic bands, which arise on the one hand from bulk excitons of the nanoparticles and on the other hand from surface states in the outer shell. The basis for all possible applications, e.g. photovoltaics, is a well defined and stable surface. With time resolved spectroscopic investigations we get insight in the surface quality and in the passivation of the quantum dots since the observed surface luminescence is highly sensitive to physisorbed compounds (e.g. different functionalisations).

CPP 22.10 Wed 16:00 Poster B

Photothermal Microscopy of Single Gold Nanoparticles in Polymers — ●ROMY RADÜNZ and FRANK CICHOS — Molecular Nanophotonics, Universität Leipzig, Linnéstraße 5, 04103 Leipzig

Photothermal microscopy is an optical imaging technique, which is based on the release of heat of an absorbing nanoobject to its local surrounding. The temperature rise in the surrounding induces a local refractive index change, which can be detected optically. Thus non-fluorescent nanoobjects such as gold particles of only a few nanometer in size become visible. It is generally expected that the photothermal signal scales with the volume of the nanoobject due to the dependence of the absorption cross-section on the volume. We show that this relation does not hold due to the influence of the nanoparticle surface on the heat transfer from the gold particle to the environment. Numerical calculations and experimental results demonstrate that the dependence of the photothermal signal on the particle size is weaker than expected due to the surface conductivity of the nanoparticle. As a consequence, this type of experiments provides new routes to explore local thermal properties as well as the physics of heat conduction on the nanoscale.

CPP 22.11 Wed 16:00 Poster B

Vibrational Sum Frequency Scattering on Biomedical Poly (lactic acid) Microspheres — ●ALBERT SUGIHARTO¹, CLAES MAGNUS JOHNSON¹, MARC SMITS², JOHANNES NIJSEN³, and SYLVIE ROKE¹ — ¹MPI for Metals Research, Stuttgart, Germany — ²FOM-Institute AMOLF, Amsterdam, The Netherlands — ³Departement of Nuclear Medicine, University Hospital, Utrecht, The Netherlands

Biodegradable poly(lactic acid)(PLA) microspheres have recently been applied as a medicine against liver cancer [1]. In this proposed treatment, one injects polymer particles loaded with radioactivated heavy metal (Ho) complex into hepatic artery. The particles are transported to the tumor site, and from there irradiate and destroy the tumor cells. To understand the interaction of these particles with the body, it is important to investigate the bulk and surface structure of these particles on a detailed molecular level.

We have probed the particle structure using vibrational sum frequency scattering [2], a novel technique that combines all the advantages of vibrational sum frequency generation (SFG) with light scat-

tering. This means one can obtain information about both the bulk and the surface structure on the molecular level as well as particle shape and size. We find that the PLA microspheres consist of crystallite domains, in which two adjacent helical PLA chains are arranged anti-parallel to each other. Furthermore we observed crucial structural changes between microspheres with and without medicinal complex.

[1] J.F.W. Nijssen et al., *Eur. J. Nucl. Med.* **26**, 699 (1999)

[2] S. Roke et al., *Phys. Rev. Lett.* **91**, 258302 (2003)

CPP 22.12 Wed 16:00 Poster B

Characterization of novel acceptor materials for photovoltaic application by optical spectroscopy methods

— •MORITZ LIEDTKE^{1,2}, ANDREAS WÖRLE¹, JOHANNES SIEGER¹, CARSTEN DEIBEL¹, VLADIMIR DYAKONOV^{1,2}, INGO RIEDEL², and NAZARIO MARTIN³ — ¹Experimental Physics VI, Physical Institute, Julius-Maximilians University of Würzburg, Am Hubland, D-97074 Würzburg, Germany — ²Div. Functional Materials for Energy Technology, ZAE Bayern e.V., Am Hubland, D-97074 Würzburg, Germany — ³Departamento de Química Organica, Facultad de Química, Universidad Complutense, E-28040 Madrid, Spain

Polymer-Fullerene composites are used in photovoltaic applications due to their efficient charge carrier generation. One approach to improve power efficiencies of bulk heterojunction solar cells are new material combinations in which the low absorbing C60 derivative (PCBM) is replaced by an optically active C70 based methanofullerene. We compared blends of poly(3-hexylthiophene) (P3HT) and [6,6] phenyl-C61-butyric acid methyl ester to blends of two C70 based fullerene molecules mixed with P3HT. We studied the formation of excited states, their lifetimes and charge transfer reactions with respect to blend ratio and temperature by optical spectroscopy techniques such as photoinduced absorption (PIA) and frequency dependent PIA measurements.

CPP 22.13 Wed 16:00 Poster B

Photophysics of functionalized perylenebisimides as building blocks for dye - quantum dot nanoassemblies

— •DANIELA TÄUBER, DANNY KOWERKO, JÖRG SCHUSTER, and CHRISTIAN VON BORCZYKOWSKI — Center of nanostructured materials and analytics, TU-Chemnitz, 09107 Chemnitz

Organic - inorganic building blocks promise numerous applications in nanoelectronics, biology and physics. Organic dye molecules in combination with semiconductor quantum dots are good candidates to study chemistry and physics of organic-inorganic interfaces at molecular level. However, characterization of such complexes first requires careful analysis of the elementary building blocks. Thus we report here on polarization resolved single molecule spectroscopy as a powerful tool for characterizing the different rotational and conformational dynamics of functionalized perylenebisimides. Such functionalized dyes with different anchor groups are used by us in prototype dye quantum dot nanoassemblies. Perylenebisimide dyes are known to show rich dynamics, including intramolecular flips which will result in intensity fluctuations. Polarization resolved detection allows for a discrimination of those intramolecular flips against rotations of the complete molecule.

CPP 22.14 Wed 16:00 Poster B

Single-laser-pulse-induced switching of molecular spin states

— •SÉBASTIEN BONHOMMEAU¹, NIKO PONTIUS¹, HERMANN DÜRR¹,

WOLFGANG EBERHARDT¹, SAIOA COBO², GABOR MOLNÁR², and AZZEDINE BOUSSEKSOU² — ¹Berliner Elektronenspeicherring-Gesellschaft für Synchrotronstrahlung m.b.H (BESSY), Albert-Einstein-Straße 15, 12489 Berlin, Germany — ²Laboratoire de Chimie de Coordination, CNRS UPR-8241, Route de Narbonne 205, 31077 Toulouse, France

Light-induced phenomena in spin crossover complexes have aroused a lot of interest since the discovery of the LIESST (Light-Induced Excited Spin State Trapping) effect in solid state. Here, we demonstrate by means of Raman spectroscopy that a bi-directional spin transition can be obtained at room temperature when applying a nanosecond laser pulse in the hysteresis loop of the spin crossover complex Fe(pyrazine)[Pt(CN)₄]. This phenomenon is interpreted as a photo-induced phase transition exhibiting a threshold energy density. In order to provide a deeper insight on the electronic properties of such polymeric materials, X-ray photoemission and absorption experiments have also been performed on a multilayer assembly of thin films of Fe(azopyridine)[Pt(CN)₄] that display spin crossover. This information is of paramount importance to shed new light on the photo-induced dynamics, in the subpicosecond time scale, which will be investigated using the femtoslicing facility now available at BESSY GmbH.

CPP 22.15 Wed 16:00 Poster B

Spectra of molecular aggregates and energy transfer dynamics: a novel approach

— •LARS ERIK WÜRFLINGER, WOLFGANG WOLFF, and WALTER STRUNZ — Physikalisches Institut, Universität Freiburg, Hermann-Herder-Straße 3, D-79104 Freiburg

Although dye polymer aggregates have been studied since the mid-thirties (J-band), in the last few years there has been a feverish reawakening of interest in this area [1, 2]. Based on a recently developed stochastic Schrödinger equation [3], we study exciton transfer dynamics fully including the influence of intramolecular vibrations of arbitrary spectral density. The efficiency of our approach allows us to calculate absorption spectra of aggregates composed of an arbitrary number of monomers. Furthermore we are able to describe the full range from coherent to incoherent transfer in a unified way.

[1] V. May, O. Kühn, *Charge and Energy Transfer Dynamics in Molecular Systems* (Wiley-VCH)

[2] A. Eisfeld, J. S. Briggs, *Chem. Phys.* **281**, 61, *Chem. Phys.* **324**, 376

[3] T. Yu, L. Diósi, N. Gisin, W.T. Strunz, *Phys. Rev. A* **60**, 91

CPP 22.16 Wed 16:00 Poster B

Monitoring of Single-Chromophore Lifetime Fluctuations by Single-Photon Autocorrelation

— RUBEN SCHMIDT¹, •THOMAS BLAUDECK¹, ACHIM GRUBER^{1,2}, and FRANK CICHOS^{1,2} — ¹Photonics and Optical Materials, TU Chemnitz, 09107 Chemnitz, Germany — ²Molecular Nanophotonics, 04103 Leipzig, Germany

We report on a technique of time-resolved single-photon counting to monitor the fluctuations in the fluorescence lifetime of single chromophores. When analyzing the single-photon data in terms of a lifetime-intensity correlation, fluctuations can be assigned to either the radiative or the non-radiative decay rate of the excited state. In particular, the case of highly non-exponential fluorescence decays observed for semiconductor nanocrystals is discussed. Here, single-photon autocorrelation allows to assign a change of the fluorescence lifetime on the timescale of several microseconds. This reveals the emissive state to be rather a distribution of states than a single one.

CPP 23: POSTER: JOINT SYMPOSIUM Polyelectrolytes

Time: Wednesday 16:00–18:30

Location: Poster B

See session SYPE 1 for details about the presented posters.

CPP 24: Micro and Nano Fluidics II: Soft Objects in Flow + Slippage

Time: Thursday 9:30–12:30

Location: H37

Invited Talk

CPP 24.1 Thu 9:30 H37

Fluctuating 2d vesicles in hydrodynamic Stokes flow — ●REIMAR FINKEN and UDO SEIFERT — II. Institut für Theoretische Physik, Pfaffenwaldring 57, 70550 Stuttgart, Germany

The behaviour of soft objects in hydrodynamic flow has received increasing attention in recent years, both theoretically and experimentally. An important and intriguing aspect is the interaction of the flow with thermal fluctuations in this non-equilibrium situation. As a paradigmatic model system we study the stochastic motion of a vesicle with a one dimensional membrane in a planar shear flow. At large shear rate the hydrodynamic forces stretch out the membrane fluctuations. The simplified geometry allows easier analytic treatment and makes the system amenable to computer simulations. We develop a theory which takes advantage of small deviations from a circular shape and obtain Langevin type equations of motion for the deformation amplitudes. Analytic expressions are obtained for the stationary state and for the correlation functions of the deformation. Our analytic results are compared with simulation data. This work was funded by the DFG Priority Program SPP 1164 “Nano- and Microfluidics”.

CPP 24.2 Thu 10:00 H37

Spontaneous stretching of DNA in a two-dimensional nanoslit — ●MADHAVI KRISHNAN and PETRA SCHWILLE — Institut für Biophysik, Biotechnologisches Zentrum der TU Dresden, 01307 Dresden, Germany

We report a novel regime of polyelectrolyte behaviour manifested in the stretching of DNA molecules confined in solution to two dimensions that arises from the combined effects of confinement and electrostatics in nanoslits. We observe that a proportion of DNA molecules in slit-shaped silicon dioxide-glass channels, a few microns wide and 50 to 100 nm deep, spontaneously assumes axially extended configurations at the lateral sidewalls of the slit, exhibiting thermal fluctuations in contour length predominantly along the major axis of the slit. The situation resembles that of extension of a physically confined polymer chain in a nanochannel, with the important exception that the nanochannel confines the DNA molecule in two of three spatial dimensions, while the nanoslit involves actual physical confinement in only one spatial dimension; confinement in the second spatial dimension is gratuitous, and appears to be electrostatically mediated. The spontaneous ordering and extension of DNA molecules in fluidic slits with depths comparable to persistence length of DNA, is not only of fundamental relevance in understanding electrostatic interactions between confined charged entities but also offers a novel, greatly simplified method to stretch DNA in solution for DNA-protein interaction studies.

CPP 24.3 Thu 10:15 H37

Brownian dynamics of microswimmers — ●VLADIMIR LOBASKIN — Physics Department T37, Technical University of Munich, 85747 Garching, Germany

We perform computer simulation of few simple model microswimmers consisting of three spheres and propelling themselves in a fluid by non-reciprocal body reshaping cycle at low Reynolds numbers. We find that the stationary velocity of the swimmers can be described by an universal scaling law and grows as a square of the beating amplitude and linear in the beating frequency. We show that the performance of coupled swimmers scales linearly with their number. In presence of fluctuations, the microswimmers display random walk trajectories. The characteristics of the trajectory and the velocity distribution change qualitatively upon variation of the stationary swimming velocity at fixed temperature. We observe a Gaussian random walk and Maxwellian velocity distribution in the weak-beating regime and crater-like velocity distribution, typical for driven systems, in the strong-beating regime. The transition to the driven regime as well as the corresponding force-velocity relation for the microswimmers can be described by a Langevin theory of active Brownian motion.

CPP 24.4 Thu 10:30 H37

Determination of density, viscosity and activation energy of small liquid volumes using an atomic force microscope — ●NEAL MCLOUGHLIN, STEPHEN LEE, and GEORG HÄHNER — *EaStCHEM* School of Chemistry and *SUPA* School of Physics; University of St Andrews; St Andrews KY16 9ST UK

We demonstrate that the viscosity and density of small liquid volumes can be determined with good precision from the resonance spectra of both magnetically driven and thermally excited AFM cantilevers. Recording spectra depending on the temperature allows for the determination of activation energy values. Data recorded in water were employed to extract parameters characteristic of the resonance behaviour of the system. These parameters were then used to determine the properties of further liquid samples. The method we present is fast and reliable and does not require a calibration of the force constant of the cantilever or knowledge of its geometry. It can be performed with commercial instruments and has the potential to be incorporated in microfluidic systems [1].

[1] N. McLoughlin, S. L. Lee, G. Hähner *Appl. Phys. Lett.* **89**, 184106 (2006)

15 min. break

CPP 24.5 Thu 11:00 H37

Rupture and collapse dynamics of thin liquid films — ●FRANK MÜLLER and RALF STANNARIUS — Institut für Experimentelle Physik, Otto-von-Guericke Universität, 39106 Magdeburg, Germany

Equilibrium shapes of thin free-standing liquid membranes are well understood. On the other hand, when such films undergo fast configurational transitions like the rupture of spherical bubbles or the collapse of catenoids [1], different dynamical mechanisms are involved, and such processes are in general poorly understood. We study such phenomena experimentally, using smectic liquid crystal membranes and a fast camera (up to 100 kfps). From the time resolved image analysis, we determine the influences of different processes involved, like collection of the excess material in a rim, global flow in the film towards the meniscus and global thickening of the film. The role of these mechanisms is controlled by the viscosity, the thickness of the film and influences of the surrounding air.

[1] Müller F and Stannarius R: Collapse dynamics of catenoid-shaped smectic films, *Europhys. Lett.* 2006, in press

CPP 24.6 Thu 11:15 H37

Ratchet driven microfluidic transport: the case of two liquid layers — ●UWE THIELE¹ and KARIN JOHN² — ¹Max-Planck-Institut fuer Physik komplexer Systeme, Noethnitzer Str. 38, 01187 Dresden, Germany — ²Laboratoire de Spectrométrie Physique, Université Joseph Fourier Grenoble I, BP 87 - 38402 St.-Martin-d'Hères Cedex, France

We extend our previously derived model for ratchet-driven microfluidic transport [1] to the case of two layers of immiscible liquids confined in a capacitor.

The transport relies on field-induced morphological changes of the free liquid-liquid interface based on a switchable, spatially asymmetric, periodic interaction of the liquid-liquid interface and the substrates. The concept is exemplified using an evolution equation for the profile of the interface between two dielectric liquid layers under an spatially inhomogeneous, time-periodic voltage. We analyse the influence of the various phases of the ratchet cycle on the transport properties.

We discuss conditions for maximal transport for the case of periodic switching between two potentials differing by translation in space by half a period. This constellation allows for the transport of droplets of liquid 1 in liquid 2.

[1] K. John and U. Thiele, <http://arxiv.org/abs/physics/0611144> (2006).

CPP 24.7 Thu 11:30 H37

Microrheology on (DNA-grafted) colloids using Optical tweezers — ●CHRISTOF GUTSCHE¹, ULRICH KEYSER¹, KATI KEGLER¹, MATHIAS SALOMO², and FRIEDRICH KREMER¹ — ¹Univ Leipzig, Inst Expt Phys 1, Leipzig, Germany — ²Univ Leipzig, Inst Biochem, Leipzig, Germany

Optical Tweezers are employed to measure the forces of interaction within single pairs of (DNA-grafted) colloids in media of monovalent and divalent ionic aqueous solutions of varying concentrations. For monovalent ions the data for the blank colloids are well described by

the DLVO theory but as well by a novel Poisson-Boltzmann approach. Additional parameters to be varied for grafted colloids are the length of the DNA and the grafting density. From the measured force-separation dependence an interaction length at a given force is deduced. It shows in the "mushroom" regime a scaling with the grafting density which levels off for brushes [1]. The flow resistance of single blank or DNA-grafted colloids is determined and compared. The degree of swelling of the grafted DNA is adjusted by exchanging the ion concentration of the surrounding medium. For all examined flow velocities one observes an interesting deviation from Stokes law which can be traced back to a shear-dependent conformational change of the brush layer [2].

[1] K. Kegler, M. Salomo, and F. Kremer, in *Press Phys. Rev. Lett.* (2006) [2] C. Gutsche, M. Salomo, Y.W. Kim, R.R. Netz and F. Kremer, *MICROFLUIDICS AND NANOFUIDICS* 2 (5): 381-386 SEP (2006)

CPP 24.8 Thu 11:45 H37

Motion of polymer droplets on soft substrates: A Molecular Dynamics Study — ●MARCUS MULLER¹, CEM SERVANTIE¹, and CLAUDIO PASTORINO² — ¹Institut fuer Theoretische Physik, Georg-August Universitaet, Goettingen — ²Comission National de Energia Atomica, Physics, Buenos Aires, Argentina

Brushes are soft, elastically deformable substrates giving rise to a rich wetting behavior and additional molecular dissipation mechanisms for the motion of droplets. We study thin polymer films and droplets on flat brush-covered substrates by non-equilibrium molecular dynamics simulation of a coarse-grained bead-spring model. The brush consists of identical polymers as the droplets.

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 in equilibrium and under shear. The velocity profile across a thin polymer film is investigated. The slip length adopts large positive values (perfect slip) for low grafting densities, but decreases and becomes negative for densely grafted, autophobic brushes.

At high grafting density the polymer melt dewets from the brush and forms droplets. Nanoscopic polymer droplets driven by volume forces are investigated in their steady state.

CPP 24.9 Thu 12:00 H37

Impact of the solid/liquid interface on the flow dynamics of thin polymer films — ●OLIVER BÄUMCHEN, RENATE FETZER, and KARIN JACOBS — Saarland University, Experimental Physics, D-66041 Saarbrücken, Germany

We investigate the boundary conditions at the solid/liquid interface

of thin film flow of highly viscous Newtonian liquids. To induce flow, we use the dewetting process which starts by the nucleation of holes. In our system, low molecular weight polystyrene melts dewet from hydrophobic substrates after annealing above their glass transition temperature. By investigating the radii of growing circular holes, we find that the dewetting velocity at a constant temperature strongly depends on the type of substrate. We could show that in the case of silicon wafers covered by different silane brushes (octadecyltrichlorosilane and dodecyltrichlorosilane) hole growth can be described by a superposition of viscous flow and slippage. A novel data analysis method is used to identify the two velocity contributions, viscous flow and slippage, and to extract the slip length. The numbers for the slip length are consistent with results obtained from SPM analysis of rim profiles [1]. This latter method could be connected to a lubrication model derived from the Navier-Stokes equations with a Navier-slip condition and enables us to determine the slip length as well as the viscosity of the polymer melt. The variation of further system parameters such as substrate properties allows us to obtain more detailed information about the mechanism of slippage at the interface on a molecular level.

[1] R. Fetzer et al., *Europhys. Lett.* 75 (2006) 638

CPP 24.10 Thu 12:15 H37

Boundary flow on superhydrophobic surfaces — ●AUDREY STEINBERGER¹, CECILE COTTIN-BIZONNE², and ELISABETH CHARLAIX² — ¹MPI for Dynamics and Self-Organization, Göttingen, Germany — ²Laboratoire de Physique de la Matière Condensée et Nanostructures – Université Claude Bernard Lyon 1 and CNRS, Lyon, France

With the development of microfluidic systems it becomes important to control flows at small scales for systems characterized by a large surface to volume ratio. A slip hydrodynamic boundary condition can both increase the flow rate at a given pressure gradient, and reduce the hydrodynamic dispersion. Trapping gas in superhydrophobic surfaces has been suggested as a good way to obtain high and controlled slippage.

We have investigated the boundary flow of water-glycerol mixtures on superhydrophobic surfaces, using a dynamic Surface Force Apparatus. Firstly, we show that the entrapped bubbles confer elastic properties to superhydrophobic surfaces. Measuring those elastic properties allowed us to probe the meniscus shape of the bubbles. Secondly, we have shown that, contrary to conventional notions, microbubbles at the solid-liquid interface do not systematically lubricate the interface. Protruding microbubbles can strongly reduce the slippage instead. The control of the meniscus shape is thus a key point to control the slippage and has to be integrated into the conception of the design of microsystems.

CPP 25: Micro and Nano Fluidics III: Lab-on-Chip Geometries

Time: Thursday 17:15–19:00

Location: H37

Invited Talk

CPP 25.1 Thu 17:15 H37

Coupled electro-hydrodynamic force fields for the manipulation of objects in solutions — ●MAGNUS JAEGER¹, MAIKA FELTEN², GUENTER FUHR¹, MICHAEL STUKE³, and CLAUS DUSCHL² — ¹Saarland University, Faculty Clinical Medicine, Department Medical Technology, Ensheimer Strasse 48, 66386 St. Ingbert, Germany — ²Fraunhofer Institute for Biomedical Engineering, Am Muehlenberg 13, 14476 Potsdam, Germany — ³Max Planck Institute for Biophysical Chemistry, Am Fassberg 11, 37077 Goettingen, Germany

Presently, pumping of fluids in lab-on-chip systems still suffers from serious limitations. Theoretical and experimental investigations have shown that high-frequency travelling electric waves are well-suited to pump liquids through microchannels. The absence of any moving parts predestines this method for the design of microscaled fluid pumps. Depending on the frequency of the electric field used, different mechanisms lead to an effective fluid transport. We used impedance measurements to quantify the processes in the different frequency regimes. To analyse the flow profile above the electrodes, Fluorescence Correlation Spectroscopy was carried out. Furthermore, we scaled the whole system down to the nanometer range. Since the electrodes that generate the force on the fluid are installed at the channel walls, this method shows great promise for overcoming the enormous frictional forces in nanostructures. This work is part of the Priority Programme 1164 "Nano- & Microfluidics: Bridging the Gap between Molecular Motion

and Continuum Flow" and funded by the Deutsche Forschungsgemeinschaft under the reference number JA 17 17 / 1 - 2.

CPP 25.2 Thu 17:45 H37

Field mediated self assembly and actuation of highly parallel microfluidic devices — ●STEFAN BLEIL¹, TOBIAS SAWETZKI¹, DAVID MARR², and CLEMENS BECHINGER¹ — ¹2. Physikalisches Institut, Universität Stuttgart, Germany — ²Colorado School of Mines, USA

The use of microfluidic devices requires active components (pumps, valves and mixers) which can direct and control liquids in such structures. We present a novel approach where pumps and valves are created by a self assembly process which allows the realization of thousands of pumps at the same time. This is achieved by subjecting superparamagnetic colloidal particles to a rotating magnetic field, which results in a rotation of particles and thus leads to a fluid flow. The rotating field induces attractive interactions between particles and thus leads to the self assembly process. To control single pumps and valves individually we use optical tweezers, which can stop or slow down the motion of particle clusters. In addition to the advantage of forming large arrays of individually addressable devices, our approach allows also to scale the devices down to the nanometer range by using smaller particles.

S. Bleil, D.W.M. Marr and C. Bechinger; *Appl. Phys. Lett.*, 88,

263515 (2006)

CPP 25.3 Thu 18:00 H37

Mesoscopic modeling of microfluidic colloidal devices — ●ARTHUR STRAUBE¹ and ARD LOUIS² — ¹Department of Physics, University of Potsdam, Am Neuen Palais 10, PF 601553, D-14415 Potsdam, Germany — ²Rudolph Peierls Centre for Theoretical Physics, Oxford University, 1, Keble Road, Oxford, OX1 3NP, UK

We address the problem of microfluidic colloidal devices and focus on a peristaltic micropump and a colloidal valve, which have recently been implemented experimentally [1]. To model these microfluidic systems, we apply the method of stochastic rotation dynamics, where the motion of colloids is assumed to be imposed through the use of optical traps. We investigate the efficiency of the devices and are particularly interested in the effects of Brownian motion of the colloids. Here, we aim at answering a fundamental question of how small such a device can be made before it stops functioning.

The research is funded by DFG Priority Program SPP 1164 "Nano- and microfluidics," (project STR1021/1-1) and partially supported by HPC-EUROPA Visitor program (RII3-CT-2003-506079).

[1]. A. Terray, J. Oakey, D.W.M. Marr, Microfluidic control using colloidal devices, *Science* **296**, 1841 (2002).

CPP 25.4 Thu 18:15 H37

separation of liquid mixtures on chemically patterned surfaces — ●PAGRA TRUMAN, LEONID IONOV, SMRATI GUPTA, PETRA UHLMANN, and MANFRED STAMM — Leibniz Institute of Polymer Research Dresden, Hohe Str. 6, Germany

The use of chemically patterned surfaces is an interesting tool to drive liquid flow along surfaces, micro- or nano-channels. In this work we investigate novel applications of chemically patterned surfaces namely the separation of liquid mixtures. The liquid dynamics on chemically patterned surfaces is highly complex since interfacial phenomena and flow inside the liquid influence the dynamics. As a simple model liquid mixture to study fundamental aspects of this process we apply Toluene/Water mixtures to two types of surfaces: Firstly flow on surfaces with a wetting gradient is studied. Secondly flow on surfaces with an abrupt change of wettability (hydrophilic/ hydrophobic) is investigated. Wetting gradients are prepared by binary polymer brushes made of two incompatible polymers by introducing a gradient of hydrophilicity/ hydrophobicity or surface charge via variations in the grafting density. A surface with an abrupt change of wettability is fabricated by casting an epoxy resin into the cavity of a teflon block and subsequent milling. Besides presenting experimental results the perspectives to carry out such processes in confinement for applica-

tions in microfluidics systems will be discussed.

CPP 25.5 Thu 18:30 H37

Juggling with droplets: manipulation of monodisperse gel emulsions in microchannels — ●ENKHTUUL SURENJAV, CRAIG PRIEST, STEPHAN HERMINGHAUS, and RALF SEEMANN — Max-Planck Institute for Dynamics and Self-Organization, Bunsenstr. 10, D-37073, Göttingen, Germany

Emulsions with a continuous phase volume fraction of a few percent only are called gel emulsions. These emulsions are topologically analogous to foam and the monodisperse compartments (droplets) assemble into well-defined arrangements. Hence, the position of a single droplet within an ensemble of droplets is fully determined while being transported through microfluidic channels. We studied the online generation, organization, and manipulation of monodisperse gel emulsions using a variety of microchannel geometries. In particular, the topological change between a zigzag structure and a bamboo structure is considered. "Passive" reorganization, based on fixed channel geometries, can be supplemented by "active" manipulation of an incorporated ferrofluid phase. A ferromagnetic continuous phase facilitates reorganization of liquid compartments on demand using an electromagnetic trigger. Moreover, coalescence between adjacent compartments of a well-defined gel emulsion can be induced via spinodal instability of their lamellae when applying an electrical potential of a few volts across a lamella. We anticipate that microfluidic processing of compartmented liquid will be well-suited for applications in combinatorial chemistry, DNA sequencing, drug screening and protein crystallizations.

CPP 25.6 Thu 18:45 H37

Atomistic simulation of nanoscale wicking — ●BJÖRN HENRICH¹, MARK SANTER^{1,2}, and MICHAEL MOSELER^{1,3} — ¹Fraunhofer Institut für Werkstoffmechanik IWM, Wöhlerstraße 11, D-79108 Freiburg — ²IMTEK-Institut für Mikrosystemtechnik, Lehrstuhl für Anwendungsentwicklung, Georges-Köhler-Allee 106, D-79110 Freiburg — ³Freiburger Materialforschungszentrum (FMF), Stefan-Meier-Straße 21, D-79104 Freiburg

We present extensive molecular dynamics simulations of fluid propane in gold nanopores. In particular, the impregnation dynamics into a slit is investigated and compared to a continuum model, namely an extended Washburn equation which takes into account inertia, slip induced by an atomistic precursor film and the evolution of the dynamic contact angle. The latter is also extracted from stationary plug flow simulations and is found to agree with those found in the wicking simulation after a short period dominated by inertial effects.

CPP 26: INTERNAL SYMPOSIUM Optical Spectroscopy I

Time: Thursday 10:00–12:30

Location: H40

Invited Talk

CPP 26.1 Thu 10:00 H40

Efficient coupling of single molecules with light — ●VAHID SANDOGHDAR — Laboratory of Physical Chemistry, ETH Zurich, CH-8093 Zurich, Switzerland, www.nano-optics.ethz.ch

We examine the coherent interaction of strongly confined light with a single molecule at cryo-genic temperatures [1, 2, 3] and show that a single molecule can leave a fingerprint larger than 10% on a laser beam. Furthermore, we discuss experiments and theoretical calculations for enhancing the coupling between a single molecule and light. We show how a single spherical gold nanoparticle can act as a nano-antenna to modify the excitation, radiation and dissipation processes of a single molecule by more than an order of magnitude [4] and provide guidelines for designing more complex antenna structures that result in even larger effects [5]. [1] I. Gerhardt, G. Wrigge, P. Bushev, G. Zumofen, M. Agio, R. Pfab, V. Sandoghdar, to appear in *Phys. Rev. Lett.* [2] I. Gerhardt, G. Wrigge, M. Agio, P. Bushev, G. Zumofen, V. Sandoghdar, submitted. [3] G. Wrigge, I. Gerhardt, J. Hwang, V. Sandoghdar, in preparation. [4] S. Kühn, U. Hakanson, L. Rogobete, V. Sandoghdar, *Phys. Rev. Lett.* **97**, 017402 (2006). [5] L. Rogobete, F. Kaminski, M. Agio, V. Sandoghdar, in preparation.

Invited Talk

CPP 26.2 Thu 10:30 H40

Charge and Energy Transfer in Photosynthetic Systems - Some Principles of Photosynthetic Light Harvesting — ●VILLY

SUNDSTRÖM — Department of Chemical Physics, Lund University, Box 124, S-221 00 Lund, Sweden

Photosynthesis is Nature's way of converting solar energy into energy rich molecules. The molecular machinery to achieve this consists of two coupled pigment-protein systems - a light-harvesting antenna to collect the light and a photochemical reaction center to convert short-lived excited state energy of antenna pigments into more stable charge separated states. With the need to find artificial systems for solar energy conversion it is interesting to find out what are the structures and processes by which photosynthesis fulfils its task. Light harvesting and charge transfer has been studied in many different antennas and reaction centers. In this lecture a few examples will be given with the aim to highlight key concepts and some principles of operation.

CPP 26.3 Thu 11:00 H40

The Interplay between Symmetry and Electronic Structure of Pigment-Protein Complexes from Purple Bacteria — ●SILKE OELLERICH¹, MARTIN RICHTER¹, JÜRGEN BAIER¹, THOMAS PREM¹, FRANCESCO FRANCA², GIOVANNI VENTUROLI², DIETER OESTERHELT³, JUNE SOUTHALL⁴, RICHARD COGDELL⁴, and JÜRGEN KÖHLER¹ — ¹Experimentalphysik IV, Universität Bayreuth — ²University of Bologna — ³MPI für Biochemie, Martinsried — ⁴University of Glasgow

A recent rather low resolution X-ray crystal structure of the RC-LH1 core complex from the photosynthetic purple bacterium *Rps. palustris* showed the presence of a physical gap in the LH1 ring. The presence of such a gap, though functionally critical for the cyclic electron transport in the photosynthetic process, has become very controversial. We have now applied single-molecule spectroscopy to the RC-LH1 complexes of the purple bacteria *Rps. palustris* and *Rb. sphaeroides* (pufX- strain) to demonstrate that there is such a gap in the LH1 ring structure.

More than 80% of the complexes from *Rb. sphaeroides* only show broad absorption bands, whereas all of the measurable complexes from *Rps. palustris* also have a narrow line at the low-energy end of their spectrum. We describe how the presence of this narrow feature indicates the presence of a gap in the electronic structure of the LH1 from *Rps. palustris*, which provides strong support for the physical gap that was previously modelled in its X-ray crystal structure.

CPP 26.4 Thu 11:15 H40

Electronic properties of dendrimers — ●PETER REINEKER, CHRISTOPH SUPRITZ, and VASILIOS GOUNARIS — Institute of Theoretical Physics, University of Ulm, 89069 Ulm, Germany

Dendrimers, regular star like polymers, are of interest from a fundamental point of view, but also because of various possible applications, such as in light harvesting systems, in solar cells, as carriers for drug delivery or for gene manipulation, or in catalysis, etc. In our investigation of the dendrimers we have focused on optical and energy transport properties of dendrimers with C3 and C2 symmetries. We have calculated optical absorption line shapes and the time dependence of the energy transport in dependence on the size for compact and extended dendrimers. Our Frenkel exciton model takes into account the geometry of the dendrimers, local electronic excitation energies, transfer integrals, and the influence of vibrational degrees of freedom via a stochastic description.

CPP 26.5 Thu 11:30 H40

Optimal Control of Femtosecond Time-Resolved Four-Wave Mixing for the Selective Excitation of Molecular Modes — ●ARNULF MATERNY — International University Bremen (Jacobs University Bremen as of spring 2007), Campus Ring 1, 28759 Bremen

A selective excitation of vibrational modes even for complex molecules would be of considerable interest for the control of chemical reactions. Due to the fast intramolecular vibrational energy redistribution (IVR) process, the selectivity can usually not be achieved. The internal energy transport takes place on a time scale of few picoseconds or even less. Therefore, the use of ultrashort laser pulses in the femtosecond range seems to open up a possibility to overcome the IVR problem. However, now at least all modes within the broad frequency spectrum of the pulses are excited. A solution to this problem is the phase and/or amplitude modulation of the pulse spectrum. It will be demonstrated that by an optimization of the pulse shape in a self-learning loop arrangement guided by an evolutionary algorithm the control of mode excitations can be achieved. Using a coherent anti-Stokes Raman scattering interaction the enhancement as well as suppression of molecular vibrations are demonstrated for both electronically resonant

and non-resonant stimulating laser pulses.

CPP 26.6 Thu 12:00 H40

Large-scale heterogeneity in supercooled glycerol probed by single-molecule fluorescence and by rheology — ●FLORIAN KULZER¹, ROB ZONDERVAN¹, TED XIA¹, HARMEN VAN DER MEER¹, CORNELIS STORM², WIM VAN SAARLOOS², and MICHEL ORRIT¹ — ¹Leiden Institute of Physics, Leiden University, P.O. Box 9504, NL-2300 RA Leiden — ²Instituut-Lorentz for Theoretical Physics, Leiden University, P.O. Box 9506, NL-2300 RA Leiden

We employ variable-temperature single-molecule microscopy to study heterogeneity in supercooled glycerol in the temperatures range of 5 to 25 K above the glass transition ($T_g = 190$ K). By following the rotational diffusion of perylene guest molecules we get direct access to the distribution of local viscosities, which vary by a factor of five or more for different individual fluorophores at a given temperature. By following the same single molecules at various temperatures, we find that the distribution of local viscosities itself broadens upon approaching the glass transition temperature. This spatial heterogeneity relaxes extremely slowly and can persist over hours or even days. These results convey a picture of heterogeneous liquid pockets separated by solid-like walls, which exist already well above the viscosimetric glass transition. To corroborate this surprising result, we have conducted rheological measurements to find evidence for the solid-like network in the macroscopic mechanical response of supercooled glycerol. In agreement with the conclusions from our single-molecule experiments, we can detect typical features of soft glassy rheology in the properties of glycerol in the same temperature range.

CPP 26.7 Thu 12:15 H40

Single-molecule traffic in mesoporous materials — ●CHRISTOPHE JUNG, JOHANNA KIRSTEIN, TIMO LEBOLD, JENS MICHAELIS, and CHRISTOPH BRÄUCHLE — LMU, München

In the last decade single molecule methods play a major role in material science because they can reveal structural and dynamic features which are otherwise obscured by ensemble averaging in conventional spectroscopic methods. Here we show how single dye molecules can be used as nanoscale probes to map out the structure of mesoporous thin films, and to provide valuable insight into the dynamics/interactions of guests molecules within the host porous matrix. In a first study, the translational and orientational movement of single TDI molecules was observed simultaneously in CTAB templated films with hexagonal pores (M41S). The molecules show linear movement, with their transition dipole moment aligned along their trajectories, reflecting the structural features of the underlying material, i.e. unidimensional, straight, cylindrical pores. A second system containing a mixture of hexagonal and lamellar phase was obtained using the non-ionic Block-copolymer Brij-56 as template. The structure of the trajectories, the diffusivities and the orientation of single molecules are distinctive for molecules travelling in the hexagonal and the lamellar mesophases. Moreover, transitions between the different types of surroundings can be observed for the same individual dye molecule.

CPP 27: INTERNAL SYMPOSIUM Optical Spectroscopy II

Time: Thursday 14:30–17:00

Location: H40

Invited Talk

CPP 27.1 Thu 14:30 H40

Controlling intermolecular interactions in organic semiconductors — ●LAURA HERZ — University of Oxford, Clarendon Laboratory, Parks Road, Oxford OX1 3PU

Conjugated polymers and molecules have emerged over the last decade as cheap and flexible alternatives to existing inorganic semiconductor technology. Light-emitting displays based on these materials are now at commercial standards with several products on the market, with transistors and photovoltaics being at the research and development stage. This talk will summarize our recent research into the mechanisms governing the femtosecond dynamics of electronic processes at the interface formed between two organic semiconductor components. We have examined the Coulombic interactions at the interface in a blend of two copolymers with intramolecular charge-transfer character and optimized band offsets for photoinduced charge generation. Through a combination of both time-resolved measurements of photo-

luminescence, and quantum-chemical modeling of the heterojunction, we demonstrate that the relative molecular orientation at the heterojunction can lead to either a repulsive barrier or an attractive interaction. For the latter case, charge transfer across the heterojunction may occur, but is followed by rapid relaxation into a coulombically bound state (exciplex) across the interface. I will follow on to show that electronic delocalization across more than one conjugated polymer chain may be tailored effectively through supramolecular self-assembly strategies, as for example shielding of chains with insulating macrocycles, or complexation with inert macromolecules.

CPP 27.2 Thu 15:00 H40

A real time, real space approach for calculating 2D spectra in heterogeneous systems — ●BEN BRÜGGEMANN^{1,2}, PÄR KJELLBERG¹, and TONU PULLERITS¹ — ¹Department of Chemical Physics, Lund University, Sweden — ²Institut für Physik, Humboldt-

Universität zu Berlin

A non-perturbative approach is used to calculate nonlinear spectra using a multi-exciton density matrix theory. All interaction orders are reproduced simultaneously, but analog to the experiment they can be distinguished by the different phase matching directions. This is possible due to the summation of the polarizations for a number of randomly placed molecules, but since orientational averaging and energetic disorder can be included at the same time the additional computational effort is moderate. The method is applied to the FMO complex to calculate 2D frequency resolved spectra, which show good agreements with experimental data [1]. The advantage of the presented method is that the intensity dependence of the 2D spectrum can be investigated, as well as the signal from higher order phase matched directions. [1] T. Brixner et al. Nature 434, 625 (2005).

CPP 27.3 Thu 15:15 H40

Proteins under pressure: spectroscopic determination of compressibilities — ●JOHANNES WIEDERSICH¹, VLADIMIR PONKRATOV¹, MARK SOMOZA¹, JANE VANDERKOOI², and JOSEF FRIEDRICH¹ — ¹Lehrstuhl für Physik Weihenstephan, Physikdepartment, TU München — ²Department of Biochemistry and Biophysics, University of Pennsylvania, Philadelphia, Pennsylvania

By means of optical spectroscopy we determine the local compressibility of proteins. At low temperatures the pressure shift of optical spectra can be precisely determined employing hole burning techniques. The values for the compressibility of ubiquitin and Zn horseradish peroxidase obtained at low temperatures are compared with those from high pressure experiments at ambient temperature. The results of both experiments show the same compressibility, indicating that the compressibility of proteins is the same whether the protein is surrounded by liquid at ambient conditions or whether it is frozen at low temperatures. In both cases the observed values are typical for solids.

Invited Talk

CPP 27.4 Thu 15:30 H40

Coherent control of single spins in diamond — ●FEDOR JELEZKO and JÖRG WRACHTRUP — 3. Physikalisches Institut, Universität Stuttgart

Defects in diamond may have a large impact on solid state quantum physics in general and quantum information processing and communication in particular. This contribution will highlight recent results on the nitrogen-vacancy center (NV). Experiments on optical detection and manipulation of single electron spins will be reviewed. The experimental background of optical detection of single quantum systems in solids will be introduced. Well established single electron and nuclear spin measurement of NV defect is a key step in solid-state quantum information processing. Another important application of single spin manipulation is of more fundamental character. Experiments with single spins are suitable for experimental test of quantum mechanics. Projective measurements of single spins can be used as a test of the quantum Zeno effect and Bell's inequalities.

CPP 27.5 Thu 16:00 H40

Optical Spectroscopy On Nanoparticles in a Linear Paul Trap — ●ALEXANDER KUHLLICKE, STEFAN SCHIETINGER, and OLIVER BENSON — AG Nano-Optik, Institut für Physik, Humboldt-Universität zu Berlin Hausvogteiplatz 5-7, 10117 Berlin

Linear radio frequency ion traps, so-called Paul traps, are widely-used tools for high-resolution spectroscopy on atom ions and have also been utilized for the trapping of micrometer-sized particles. We have narrowed the gap between these size regimes by trapping single nanoparticles with sizes down to 20 nm within a linear Paul trap. This opens a way to investigate nanoparticles without the interaction with supporting surfaces. We observed ion chains and Coulomb-crystals within the trap and performed spectroscopy on trapped dye-doped particles and N-V centers in diamonds. Future experiments aim at the spectroscopy on mesoscopic quantum emitters.

CPP 27.6 Thu 16:15 H40

Resonant Energy Transfer Monitoring Self-Assembly of Functionalized Dye Molecules on Semiconductor Nanocrystals — ●THOMAS BLAUDECK^{1,2}, MOHAMED ABDEL-MOTTALEB², EDUARD ZENKEVICH³, ALEXANDER SHULGA³, and CHRISTIAN VON BORCZYKOWSKI² — ¹POM, TU Chemnitz, 09107 Chemnitz, Germany — ²OSMP, TU Chemnitz, 09107 Chemnitz, Germany — ³Institute of Molecular and Atomic Physics, National Academy of Science, Minsk 220072, Belarus

Targeted generation of multichromophoric aggregates comprising inorganic (NCs) and organic (dye molecules) parts encounters growing interest in biology, medicine, and molecular electronics. We report on the properties of such aggregates designed from pyridyl-substituted free-base porphyrin dye molecules and CdSe NCs, formed via spontaneous self-assembly and monitored by steady-state and time-resolved spectroscopy. The results clearly identify an excitation energy transfer from the NC to the dye molecules and are discussed in the framework of Stern-Volmer quenching and Förster resonant energy transfer (FRET) theory. The results are generalized on the self-assembling formation of antenna arrays comprising NCs and other classes of molecules.

Invited Talk

CPP 27.7 Thu 16:30 H40

Optical spectroscopy on single carbon nanotubes — ●ACHIM HARTSCHUH¹, HUIHONG QIAN¹, TOBIAS GOKUS¹, MATHIAS STEINER², and ALFRED MEIXNER² — ¹Department Chemie und Biochemie and CeNS, LMU Muenchen, Germany — ²Institut fuer Physikalische und Theoretische Chemie, Universitaet Tuebingen, Germany

Semiconducting single-walled carbon nanotubes (SWNTs) are photoluminescent quasi-one-dimensional quantum wires with great promise for applications in photonics, nanoelectronics and optical sensing. Light emission from SWNTs is dominated by excitonic recombination with a low quantum yield of typically 10e-3 for embedded nanotubes. Recent measurements on single nanotubes using confocal Raman and photoluminescence microscopy revealed variations of both emission energies and excited-state lifetimes from nanotube to nanotube [1, 2]. Lifetime variations appear to result from defect mediated non-radiative transitions to non-luminescent states while energetic variations can be attributed to fluctuations in the dielectric environment of the nanotube. Since nanotubes consist of surface atoms only, dielectric screening and thus the emission energy of excitonic states are highly susceptible to the local environment making them ideally suited as nanoscale optical sensors (see e.g. [3]).

[1] A. Hartschuh et al., Science 301, 1293 (2003). [2] A. Hagen et al., Phys. Rev. Lett. 95, 197401 (2005). [3] D. A. Heller et al., Science 311, 508 (2006).

CPP 28: Polymer Physics V

Time: Thursday 17:15–18:15

Location: H40

CPP 28.1 Thu 17:15 H40

Lifetimes of photoexcited states in P3HT:PCBM heterojunctions — ●JOHANNES SIEGER¹, ANDREAS WÖRLE¹, ANDREAS SPERLICH¹, MORITZ LIEDTKE^{1,2}, CARSTEN DEIBEL¹, and VLADIMIR DYAKONOV^{1,2} — ¹Experimental Physics VI, Physical Institute, Julius-Maximilians University of Würzburg, Am Hubland. D-97074 Würzburg — ²Div. Functional Materials for Energy Technology, ZAE Bayern e.V., Am Hubland, D-97074 Würzburg

The photoinduced charge transfer and the resulting charge carrier generation in polymer-fullerene bulk heterojunctions are essential for organic photovoltaics. We present our investigations on the efficiency of singlet exciton dissociation and polaron generation in poly(3-

hexylthiophene) (P3HT) : [6,6] phenyl-C61-butyric acid methyl ester (PCBM) blends by performing photoluminescence measurements, photoinduced absorption spectroscopy (PIA) and light-induced electron spin resonance (LESr). Particularly, we focus on the temperature dependence of the lifetime of the photoinduced states. The PIA measurements were possible at room temperature due to a high sensitivity of the setup and are relevant for applications of organic semiconductors such as solar cells.

CPP 28.2 Thu 17:30 H40

Low temperature mobility of Frenkel excitons on amphi-PIPE J-Aggregates — ●CHRISTIAN SPITZ, ANTONIO SAGHATI, and

RALF MENZEL — Universität Potsdam

The mobility of optically excited excitons on J-aggregates can be demonstrated by the phenomena of exciton exciton annihilation. In this intensity dependent process the collision of two excitons results in their annihilation and hence in a shortening of the mean excitation lifetime. By measuring the intensity dependent fluorescent lifetime in contrast to the predicted immobilization of the excitons at low temperature we could prove the excellent mobility of the excitons on the ampi-PIPE J-aggregates of the octyl derivate of 5,5,6,6-tetrachloro-1,1-diethyl-3-3 bis(4-sulpho-n-butyl) benzimidacarbocyanine (TDBC) at a temperature (4 K), which is far below their expected freezing point. The high mobility is further approved by fluorescence depolarisation at low temperatures.

CPP 28.3 Thu 17:45 H40

Integrated spin-on barrier layers a reasonable idea? — ●MINE MEMESA¹, YA-JUN CHENG¹, JAN PERLICH², PETER MÜLLER-BUSCHBAUM², and JOCHEN GUTMANN^{1,3} — ¹Max-Planck Institute for Polymer Research, Ackermannweg 10, D-55128, Mainz, Germany — ²TU München, Physik-Department LS E13 James-Franck-Str. 1, 85747 Garching, Germany — ³Institute of Physical Chemistry, University Mainz, D-55099, Mainz, Germany

Titanium dioxide (TiO₂) nanoparticles were prepared by using polystyrene block poly (ethyleneoxide) (PS-b-PEO) copolymer as a template. As a preliminary study whether poly (dimethylsiloxane) (PDMS) is a suitable polymeric replacement for barrier layers PDMS was spin coated over the TiO₂ nanoparticles and subsequently etched away by oxygen plasma cleaning. The surface characteristics of the particles were investigated using Scanning Electron Microscopy (SEM) and photoluminescence (PL). The PL measurements indicated the for-

mation of exciton traps close to the particle surface after plasma treatment. The stability of the TiO₂ nanoparticles upon sealing with PDMS followed by etching of the polymer overcoating was confirmed with microbeam grazing incidence small angle x-ray scattering (μ GISAXS) measurements.

CPP 28.4 Thu 18:00 H40

Accurate forces in Quantum Monte Carlo calculations with non-local pseudopotentials — ●ALEXANDER BADINSKI and R. J. NEEDS — Cavendish Laboratory, Cambridge, United Kingdom

Calculating accurate inter-atomic forces within variational and diffusion Monte Carlo (VMC and DMC) methods is a challenging and long-standing problem [1-2]. VMC and DMC methods have become quite successful for calculating ground state total energies of many-electron systems. However the lack of an accurate and efficient method for calculating forces usually requires one to perform VMC and DMC calculations with geometries obtained from either density functional theory or conventional quantum chemistry methods. We present a novel approach to calculate Hellmann-Feynman forces within these two methods using non-local pseudopotentials. The use of pseudopotentials allows one to overcome the severe problem of infinite variance in the sampling distribution of the force estimator which is vital when using statistical methods. Equilibrium geometries and harmonic vibrational frequencies are derived from the forces and compared with those obtained from the energies at the Hartree-Fock, VMC and DMC levels. Results for five small molecules show that the equilibrium bond lengths obtained from the force and energy calculations are in excellent agreement.

[1] R. Assaraf, M. Caffarel, J. Chem. Phys. 119, 10536 (2003) [2] S. Chiesa, D. M. Ceperley, and S. Zhang, Phys. Rev. Lett. 94, 036404 (2005)

CPP 29: JOINT SYMPOSIUM Polyelectrolytes I

Time: Thursday 14:00–17:00

Location: H37

See session SYPE 2 for details about the presented talks.

CPP 30: JOINT SYMPOSIUM Polyelectrolytes II

Time: Friday 10:30–12:30

Location: H1

See session SYPE 3 for details about the presented talks.

CPP 31: New Materials

Time: Friday 10:30–12:30

Location: H40

CPP 31.1 Fri 10:30 H40

Piezoelectric properties of polyester ferroelectrets made from polyethylene terephthalate — ●OLENA VORONINA, MICHAEL WEGENER, WERNER WIRGES, and REIMUND GERHARD — University of Potsdam, Institute of Physics, 14469 Potsdam, Germany

Ferroelectrets are cellular polymer foams with macroscopic electric dipoles that are formed by charges trapped on the internal void surfaces. The piezoelectricity of ferroelectrets arises from changes of the void heights (and thus of the dipole sizes) when mechanical or electrical stress is applied. Ferroelectrets are usually relatively soft in the thickness direction which leads to high piezoelectric activities with coefficients up to hundreds of pC/N [1].

Here, we describe the preparation and the resulting properties of new polyethylene-terephthalate (PETP) ferroelectrets [2]. An optimized sequence of steps for preparation is described. It includes foaming of commercial PETP films in supercritical CO₂ accompanied by a heat treatment as well as biaxial stretching and electric charging. The optimized PETP ferroelectrets exhibit piezoelectric thickness coefficients up to 500 pC/N for which the low elastic stiffness of only around 0.3 MPa is essential. The PETP ferroelectrets show unclamped thickness-extension resonance frequencies between approximately 120 and 250 kHz, and are thus particularly suitable for ultrasonic-transducer applications.

[1] M. Wegener and S. Bauer, ChemPhysChem 6, 1014-1025 (2005).

[2] W. Wirges, M. Wegener, O. Voronina, L. Zirkel and R. Gerhard-Multhaupt, Advanced Functional Materials, in press

CPP 31.2 Fri 10:45 H40

Investigation of structures in diblock copolymer film containing magnetic nanoparticles — ●M. M. ABUL KASHEM¹, J. PERLICH¹, L. SCHULZ¹, S. V. ROTH², and P. MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik-Department LS E13, James-Franck-Str. 1, 85747 Garching, Germany — ²HASYLAB at DESY, Notkestr. 85, 22603 Hamburg, Germany

Nanocomposite materials based on polymeric matrix and inorganic fillers having desired mechanical, electrical and thermal properties have been being reported since long. Rendering magnetic properties to the polymer by using magnetic nanoparticles is a rather new idea. We have investigated the nanostructures supported by superstructures formed in ultra thin films of such a new type of nanocomposite materials. The system is a diblock copolymer p(styrene-block-isoprene) matrix with embedded magnetic nanoparticles (metal oxide) covered with polymeric (PS) hairs. The superstructure is formed due to dewetting of the polymer film and the nanostructure due to self-assembly of diblock copolymer. We were able to produce dewetted structures containing magnetic nanoparticles. The nanoparticles retard the dewetting process and control the orientation from a perpendicular to a parallel lamella. Moreover, roughness correlation between the substrate and the film surface has been observed at different film thicknesses resulting from gradient sample. The investigation has been carried out by atomic force microscopy (AFM) in non-contact mode and by using micro-beam grazing incident small angle X-ray scattering (μ GISAXS).

Funding by the CompInt network is acknowledged.

CPP 31.3 Fri 11:00 H40

Formation and properties of monomolecular nanomembranes

— ●ANDRE BEYER¹, CHRISTOPH T. NOTTBOHM¹, BERTHOLD VÖLKE¹, WOLFGANG ECK², and ARMIN GÖLZHÄUSER¹ — ¹Physik Supramolekularer Systeme, Universität Bielefeld, Universitätsstr. 25, D-33615 Bielefeld (Germany) — ²Institute for Molecular Biophysics, The Jackson Laboratory, 600 Main Street, Bar Harbor, ME 04609 (USA)

Recently, a new way was found to reduce the thickness of polymerized nanomembranes to about 1 nm [1]. These membranes can be clamped over several micrometer wide openings and withstand pressures as high as 10 kPa. They are made from self-assembled monolayers which form stable nanosheets by crosslinking with electrons. Free-standing nanomembranes can be fabricated by preparing nanosheets on silicon nitride membranes which are supported by a silicon frame. After dissolving the silicon nitride, the nanosheets of monomolecular thickness remain clamped over the silicon frame.

In this contribution, we will discuss the fabrication of such nanomembranes as well as first measurements of their mechanical properties. We designed a pressure cell that allows bulge tests with an atomic force microscope. The latter is necessary to determine the membrane deflection. Bulge tests, i.e. measurements of the deflection as a function of an applied pressure difference, allow us to determine the biaxial modulus, changes of the mechanical properties in time and the critical tension at which the nanomembranes start to rupture.

[1] W. Eck, A. Küller, M. Grunze, B. Völkel, and A. Gölzhäuser, *Advanced Materials* 17, 2583 (2005).

CPP 31.4 Fri 11:15 H40

Near-edge x-ray absorption spectroscopy of metalloporphyrins and metalloporphyrin-fullerene dyads

— ●NORMAN SCHMIDT¹, JÖRG DANNHÄUSER², THOMAS STRUNSKUS³, ANDREAS HIRSCH², and RAINER FINK¹ — ¹Universität Erlangen. Physikalische Chemie II, Erlangen, Germany — ²Universität Erlangen, Organische Chemie II, Erlangen, Germany — ³Ruhr-Universität Bochum, Physikalische Chemie I, Bochum, Germany

Metalloporphyrins are well-known as electron donors in photoinduced electron transfer processes. [60]fullerene is an excellent electron acceptor, thus stabilizing radical ion-pair states in dyads of metalloporphyrins and fullerene. In these model systems for photosynthesis, the two chromophores are forced into a rigid stacking arrangement by covalent bonding and crystal packing, which leads to an interaction of the electron density of the central metal and the fullerene π -system on both sides of the porphyrin plane. Also a weak back-bonding is found.

In the current study, the electronic structure of thick films of (Mn, Fe, Co, Zn, Sn)-porphyrins and (Mn, Fe, Co)-dyads on Au-plated Si was investigated with NEXAFS spectroscopy. The presented N1s spectra reflect the electronic interaction of the central metal ion with the surrounding N atoms. Differences in the metal 2p-edge spectra between porphyrin and dyad arise mainly from electron density in the d_{z^2} -orbital (single occupation for Fe^{3+} and Co^{2+}). The measured spectra will also be compared to DFT calculations. This work was funded by DFG (SFB 583).

CPP 31.5 Fri 11:30 H40

Charging dynamics of cellular polypropylene ferroelectrets: a combined optical and acoustic study

— ●AXEL MELLINGER, XUNLIN QIU, MICHAEL WEGENER, WERNER WIRGES, and REIMUND GERHARD — Universität Potsdam, Institut für Physik, 14469 Potsdam, Germany

Ferroelectrets (i.e., charged cellular polymers) are rendered piezoelectric through barrier discharges inside their artificial voids [1]. Controlling and understanding the charging dynamics is a key element in the optimization of present and the development of new materials. In this work, time-resolved imaging has revealed discharge processes in individual voids and led to the discovery of a strong back-discharge glow. Simultaneous acoustic measurements of the inverse piezoelectric d_{33} coefficient show a “butterfly” hysteresis curve. In the framework of the presently accepted electromechanical model [2], their shape can be explained by an effective internal charge density σ_{eff} which depends both on the applied electric field and the charging history. Approx. 75% of the internal charge density is destroyed through back discharges.

[1] S. Bauer, R. Gerhard-Multhaupt and G. M. Sessler, *Physics Today* 57, 37-43 (2004).

[2] M. Paaanen, J. Lekkala and H. Välimäki, *IEEE Trans. Dielectr. Electr. Insul.* 8, 629-636 (2001).

CPP 31.6 Fri 11:45 H40

Fabrication of nano-porous electrode arrays by self-assembly

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Colloidal particles are used as a lithographic tool for the fabrication of a nano-porous electrochemical sensor. The system consists of a bottom and a porous top electrode separated by an insulating layer of predefined thickness. Polystyrene particles of different sizes act as a shadow mask for the deposition of the top electrode. After the particle lift-off, the porous metal layer is used as an etching resist to remove the insulating material. By adjustment of the nanoelectrode spacing and its pore diameter defined electrode arrays are generated. We demonstrate the control of particle films with particle sizes up to 1 μm by a simple dipping procedure. This enables a fast and reproducible processing of a lithographic mask. The particle adsorption is influenced by electrostatic particle/particle and particle/surface interactions, resulting in an extended monolayer of ordered particles on the surface. In this context we present solutions how the pore size and spacing can be adjusted in order to improve the nanopore geometry. Enhanced electrochemical sensitivity is achieved by redox-cycling between the top and bottom electrode. So far, amplification factors > 50 have been demonstrated. Currently the system is optimized to obtain maximum signal amplification.

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Magnetorheology of polymer bottle brushes

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By dispersing polymer bottle brushes [1] in a magnetic liquid synthesized in paraffine oil we are creating a new type of inverse ferrofluid [2]. The brushes differ in their cylindrical symmetry, their semi flexible nature and their ramified nano structure from the compact, spherical objects commonly immersed in ferrofluid [3]. The properties of the new magnetorheological fluid are studied by oscillatory measurements of the storage and loss moduli for varying magnetic induction B . For moderate $B < B_c \approx 10$ mT the storage modulus is hardly affected, whereas for larger B we observe a logarithmic increase. The threshold B_c may be interpreted as the percolation transition of a magnetic field induced network of bottle brushes, connecting the bottom with the top plate. Chain formation of the brushes is corroborated by the magnetic field dependent shear thinning observed in rotational measurements of the viscosity. [1] M. Zhang, A. H. E. Müller, *J. Polym. Sci. Part A: Polym. Chem.* 43, 3641 (2005). [2] A. T. Skjeltorp, *Phys. Rev. Lett.* 51, 2306 (1983). [3] R. Saldivar et al., *J. Chem. Phys.* 125, 084907 (2006).

CPP 31.8 Fri 12:15 H40

Magnetic and structural properties of thin polymer films with embedded superparamagnetic γ - Fe_2O_3 nanoparticles

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We investigate lamellae-forming polystyrene-b-polyisoprene diblock copolymer films with embedded γ - Fe_2O_3 nanoparticles. The used block copolymer is asymmetric and forms a microphase separation structure. For the thin film preparation we apply two techniques, spin coating and solution casting. Magnetisation measurements at 2 K and 300 K show that the saturation magnetisation is linear dependent on the nanoparticle concentration. A constant coercitive field and increasing fields of remanence for different nanoparticle concentrations are verified. AC-susceptibility measurements exhibit non-interacting superparamagnetic behaviour of the nanoparticle ensemble. Ageing effects confirm spin-glasses in the surface of the nanoparticles. Structural composition and distribution of the nanoparticles within the thin films are obtained by grazing incidence small angle X-ray scattering (GISAXS) and X-ray reflectivity. An increasing nanoparticle concentration results in forming smaller characteristic structure sizes. GISAXS experiments are performed at beamline BW4 at HA-

SYLAB/DESY in Hamburg.

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