

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

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Overview of Invited Talks and Sessions

(lecture rooms ZEU 222, ZEU 160 and ZEU 114; Poster P3 (ZEU 250))

Invited talks of the focus session 'Amphiphilic Systems'

CPP 1.1	Mon	10:45–11:15	ZEU 222	How to make mesoscopic single-crystals — ●STEPHAN FÖRSTER, STEFFEN FISCHER, KATHRIN ZIELSKE, PETER LINDNER, ANDREAS TIMMANN, STEPHAN ROTH
CPP 2.1	Mon	14:00–14:30	ZEU 222	Structure transformations in surfactant bilayer systems — ●OLSSON ULF
CPP 2.2	Mon	14:30–15:00	ZEU 222	Structural Transitions in Self-aggregating Systems Studied by Means of the Stopped-flow Technique — ●MICHAEL GRADZIELSKI
CPP 2.5	Mon	15:45–16:15	ZEU 222	Molecular Reorganization during Membrane Adhesion and Fusion — ●REINHARD LIPOWSKY
CPP 3.1	Mon	18:00–18:30	ZEU 222	Formation and exchange kinetics of block copolymer micelles — ●REIDAR LUND

Invited talks of the focus session 'Magnetic Soft Matter'

CPP 19.1	Tue	9:30–10:00	ZEU 222	Ferrofluids and their Rheology — ●STEFAN ODENBACH
CPP 19.2	Tue	10:00–10:30	ZEU 222	Field-dependent structure and rheology of magnetic fluids as seen from theory and simulations — ●PATRICK ILG
CPP 19.4	Tue	11:00–11:30	ZEU 222	Mechanical Properties of Uniaxial Magnetic Gels — ●PHILIPPE MARTINOTY
CPP 20.1	Wed	9:30–10:00	ZEU 222	Truncated patterning in the normal field instability — ●ANDREAS BOUDOUVIS
CPP 20.6	Wed	11:15–11:45	ZEU 222	Using triaxial magnetic fields to form optimized particle composites — ●JAMES MARTIN

Topical talks of the focus session 'Conjugated Polymers'

CPP 22.1	Wed	9:30–10:00	ZEU 160	Charge transport in doped poly(p-phenylene vinylene) — Y. ZHANG, B. DE BOER, ●P. W. M. BLOM
CPP 22.2	Wed	10:00–10:30	ZEU 160	A realistic description of the charge carrier wavefunction in microcrystalline polymer semiconductors — ●ALESSANDRO TROISI, DAVID L. CHEUNG, DAVID P. MCMAHON
CPP 22.3	Wed	10:30–11:00	ZEU 160	Influence of microstructure on transport and recombination in conjugated polymer:fullerene blend films — ●JENNY NELSON, AMY BALLANTYNE, MARIANO CAMPOY-QUILES, TOBY FERENCZI, JARVIST FROST, PANOS KEIVANIDES, JI-SEON KIM, JAMES KIRKPATRICK, CHRISTIAN MUELLER, DONALD BRADLEY, JAMES DURRANT, PAUL SMITH, NATALIE STINGELIN
CPP 22.4	Wed	11:00–11:30	ZEU 160	Charge transport along isolated conjugated molecular wires — ●FERDINAND C. GROZEMA, LAURENS D.A. SIEBBELES
CPP 22.5	Wed	11:30–12:00	ZEU 160	Charge transport: a multiscale model in polymers — ●JAMES KIRKPATRICK

CPP 22.6 Wed 12:00–12:30 ZEU 160 **From amorphous polymers to discotic liquid crystals - Measuring charge carrier mobility with the time-of-flight technique** — •FREDERIC LAQUAI, DIRK HERTEL, MARCEL KASTLER, KLAUS MUELLEN, GERHARD WEGNER

Topical talks of the focus session 'Microfluidics'

CPP 35.1 Thu 14:00–14:30 ZEU 160 **Simulations of lubrication force experiments** — •JENS HARTING, CHRISTIAN KUNERT, OLGA I. VINOGRADOVA
 CPP 36.1 Thu 15:45–16:15 ZEU 160 **Modifying Single Particle Diffusion by Chemical Surface Patterning** — MARTIN PUMPA, •FRANK CICHOS

Invited talks of the joint symposium 'Self-Organizing Surfaces and Interfaces'

See SYSO for the full program of the Symposium.

SYSO 1.1 Wed 14:00–14:30 BAR SCHÖ **Pattern formation in epitaxial growth and ion beam erosion** — •THOMAS MICHELY
 SYSO 1.2 Wed 14:30–15:00 BAR SCHÖ **Patterns and Pathways in Far-from-equilibrium Nanoparticle Assemblies** — •PHILIP MORIARTY, ANDREW STANNARD, EMMANUELLE PAULIAC-VAUJOUR, MATTHEW BLUNT, CHRIS MARTIN, IOAN VANCEA, UWE THIELE
 SYSO 1.3 Wed 15:00–15:30 BAR SCHÖ **Block-Copolymer Derived Inorganic Functional Materials** — •ULLRICH STEINER
 SYSO 2.1 Wed 15:45–16:15 BAR SCHÖ **Crystallisation of polymers at surfaces and in thin films** — •GÜNTER REITER
 SYSO 2.2 Wed 16:15–16:45 BAR SCHÖ **Active Organisation of Cell Surface Molecules by Cortical Actin** — KRIPA GOWRISHANKAR, DEBANJAN GOSWAMI, SUBHASRI GHOSH, ABHISHEK CHAUDHURI, BHASWATI BHATTACHARYA, SATYAJIT MAYOR, •MADAN RAO
 SYSO 2.3 Wed 16:45–17:15 BAR SCHÖ **Phase Behaviour and Dynamics in Lipid Mixtures** — •PETER OLMSTED

Invited talks of the joint symposium 'Organic Photovoltaics'

See SYOP for the full program of the Symposium.

SYOP 2.1 Thu 9:30–10:00 BAR SCHÖ **Material Design for Organic and Hybrid Solar Cells – structural to functional control on all length scales** — •MUKUNDAN THELAKKAT, MICHAEL SOMMER, RUTH LOHWASSER, SEBASTIEN MARIA
 SYOP 2.2 Thu 10:00–10:30 BAR SCHÖ **Triplet exciton formation in organic photovoltaics** — XUDONG YANG, SEBASTIAN WESTENHOFF, IAN HOWARD, THOMAS FORD, RICHARD FRIEND, JUSTIN HODGKISS, •NEIL GREENHAM
 SYOP 2.3 Thu 10:30–11:00 BAR SCHÖ **Charge Carrier Dissociation and Recombination in Polymer Solar Cells** — •VLADIMIR DYAKONOV, CARSTEN DEIBEL
 SYOP 2.4 Thu 11:00–11:30 BAR SCHÖ **Modeling exciton diffusion and dissociation at organic-organic interfaces** — •DAVID BELJONNE
 SYOP 2.5 Thu 11:30–12:00 BAR SCHÖ **Correlation of Interfacial Composition and Bulk Morphology to Device Performance in Organic Bulk Heterojunction Solar Cells** — DAVID GERMACK, •JOSEPH KLINE, DANIEL FISCHER, LEE RICHTER, CALVIN CHAN, DAVID GUNDLACH, MICHAEL TONEY, DEAN DELONGCHAMP
 SYOP 2.6 Thu 12:00–12:30 BAR SCHÖ **Developments on the acceptor side in plastic PV** — •JAN C. HUMMELEN

Sessions

CPP 1.1–1.6	Mon	10:45–12:30	ZEU 222	Focus: Amphiphilic Systems I
CPP 2.1–2.8	Mon	14:00–17:00	ZEU 222	Focus: Amphiphilic Systems II
CPP 3.1–3.4	Mon	18:00–19:15	ZEU 222	Focus: Amphiphilic systems III
CPP 4	Mon	11:00–13:15	ZEU 260	Biopolymers (joint session BP/CPP)
CPP 5.1–5.9	Mon	10:30–12:45	ZEU 160	Interfaces
CPP 6.1–6.11	Mon	14:00–17:00	ZEU 160	Thin Films
CPP 7.1–7.6	Mon	18:00–19:30	ZEU 160	Liquids
CPP 8.1–8.8	Mon	10:30–12:30	ZEU 114	Nanoparticles I
CPP 9.1–9.11	Mon	14:00–17:00	ZEU 114	Nanoparticles II
CPP 10.1–10.6	Mon	18:00–19:30	ZEU 114	Polymer Physics I
CPP 11.1–11.9	Tue	14:00–16:30	P3	POSTERS Amphiphilic Systems
CPP 12.1–12.13	Tue	14:00–16:30	P3	POSTERS Magnetic Soft Matter
CPP 13.1–13.34	Tue	14:00–16:30	P3	POSTERS Polymer Physics
CPP 14.1–14.14	Tue	14:00–16:30	P3	POSTERS Nanoparticles
CPP 15.1–15.15	Tue	14:00–16:30	P3	POSTERS Dynamics and Diffusion
CPP 16.1–16.22	Tue	14:00–16:30	P3	POSTERS Polyelectrolytes and Biological Systems
CPP 17.1–17.10	Tue	9:30–12:15	ZEU 160	Confined Fluids
CPP 18.1–18.11	Tue	9:30–12:30	ZEU 114	Polyelectrolytes
CPP 19.1–19.8	Tue	9:30–12:30	ZEU 222	Focus: Magnetic Soft Matter I
CPP 20.1–20.9	Wed	9:30–12:30	ZEU 222	Focus: Magnetic Soft Matter II
CPP 21.1–21.11	Wed	9:30–12:30	ZEU 114	Polymer Physics II
CPP 22.1–22.6	Wed	9:30–12:30	ZEU 160	Fokus: Conjugated Polymers
CPP 23.1–23.11	Wed	14:00–17:00	ZEU 114	Electronic and Optical Properties
CPP 24.1–24.5	Wed	14:00–15:15	ZEU 160	Colloids
CPP 25.1–25.7	Wed	15:30–17:15	ZEU 160	Diffusion and Dynamics
CPP 26.1–26.12	Wed	14:00–17:00	ZEU 222	Organic Photovoltaics I
CPP 27	Wed	14:00–17:15	BAR SCHÖ	Symposium Self-Organizing Surfaces and Interfaces
CPP 28.1–28.27	Wed	17:00–19:00	P3	POSTERS Interfaces and Thin Films
CPP 29	Thu	9:30–12:30	BAR SCHÖ	Symposium Organic Photovoltaics
CPP 30	Thu	9:30–12:30	GÖR 226	Symposium Self-Organizing Surfaces and Interfaces
CPP 31	Thu	14:00–17:00	GÖR 226	Symposium Self-Organizing Surfaces and Interfaces
CPP 32.1–32.9	Thu	9:30–12:00	ZEU 222	Polymer Physics III
CPP 33.1–33.8	Thu	14:00–16:00	ZEU 222	Organic Photovoltaics II
CPP 34.1–34.11	Thu	9:30–12:30	ZEU 160	Microfluidics I: Applications and Devices
CPP 35.1–35.5	Thu	14:00–15:30	ZEU 160	Microfluidics II: Boundary conditions
CPP 36.1–36.4	Thu	15:45–17:00	ZEU 160	Microfluidics III: Soft Objects in Flow
CPP 37.1–37.11	Thu	14:30–17:30	ZEU 114	Biopolymers (joint session CPP/BP)
CPP 38.1–38.15	Thu	17:00–19:30	P3	POSTERS Micro- and Nanofluidics
CPP 39.1–39.34	Thu	17:00–19:30	P3	POSTERS Colloids and Liquids
CPP 40.1–40.19	Thu	17:00–19:30	P3	POSTERS Electronic and Optical Properties
CPP 41.1–41.11	Fri	10:30–13:15	ZEU 222	Organic Photovoltaics III
CPP 42.1–42.10	Fri	10:30–13:00	ZEU 160	Polymer Physics IV
CPP 43.1–43.7	Fri	10:30–12:15	ZEU 114	New Materials

Annual General Meeting Chemical and Polymer Physics Division

Mittwoch 19:00–20:00 Raum ZEU 160

- Begrüßung und Bericht
- Wahl
- Verschiedenes

CPP 1: Focus: Amphiphilic Systems I

Time: Monday 10:45–12:30

Location: ZEU 222

Invited Talk

CPP 1.1 Mon 10:45 ZEU 222

How to make mesoscopic single-crystals — ●STEPHAN FÖRSTER¹, STEFFEN FISCHER¹, KATHRIN ZIELSKE¹, PETER LINDNER², ANDREAS TIMMANN³, and STEPHAN ROTH³ — ¹Institut für Physikalische Chemie, Universität Hamburg, Grindelallee 117, D-20146 Hamburg, Germany — ²Institut-Lau-Langevin, 6 rue Jules Horowitz, F- 38042 Grenoble Cedex 9, France — ³DESY (HASYLAB), Notkestrasse 85, 22603 Hamburg, Germany

Amphiphilic molecules can spontaneously assemble into micelles that can further assemble into cubic superlattices. The local order of these lattices is remarkably high on length scales of up to several hundred nanometers. However, on macroscopic scales the resulting materials contain many defects and have a multi-domain structure with random orientations so that samples are macroscopically isotropic.

For many applications it would be highly desirable to have well-defined macroscopic single crystals. This can be achieved by the application of external fields such as shear. Using in-situ SAXS- and SANS-experiments we have investigated how random multi-domain structures can be arranged into single crystals. Single crystals are prepared with unit cells in the range of 10 to 100 nm showing more than 100 Bragg-peaks. We observe that the orientation pathways show many similarities to the plastic flow behaviour of metals. These pathways can also be used to prepare magnetic and semiconductor nanoparticle superlattices with very high quality and tunable unit cell dimensions.

CPP 1.2 Mon 11:15 ZEU 222

Interfaces in bicontinuous surfactant phases — ●MAXIM BELUSHKIN and GERHARD GOMPPER — Theoretical Soft-Matter and Biophysics, IFF, Forschungszentrum Juelich, Juelich, Germany

Surfactant molecules added to an oil-water system self-assemble into a large variety of structures on the mesoscopic scale. In particular, bicontinuous and lamellar structures are observed. In bicontinuous phases, the surfactant monolayer separates continuous channels of oil and water. In regions of the phase diagram close to the lamellar phase, bicontinuous phases with long-range order emerge. In these cubic phases the surfactant monolayer forms triply periodic minimal surfaces. In amphiphilic systems many kinds of interfaces occur: between two ordered phases, between ordered and disordered phases, and between two grains of the same ordered phase.

Using a Ginzburg-Landau theory of ternary amphiphilic systems we study two classes of interfaces in bicontinuous surfactant phases - twist grain boundaries in cubic phases and microemulsions in contact with hydrophilic/hydrophobic surfaces. Twist grain boundaries are found to be minimal surfaces. The interfacial tension is very small and exhibits a non-monotonous dependence on the twist angle. For microemulsions near a hydrophilic wall, the nucleation of a lamellar phase at the surface is observed for regions in the phase diagram close to the microemulsion-lamellar phase transition.

CPP 1.3 Mon 11:30 ZEU 222

Microemulsions near planar surfaces — ●MICHAEL KERSCHER¹, HENRICH FRIELINGHAUS², and DIETER RICHTER¹ — ¹Institute for Solid State Research, Forschungszentrum Jülich GmbH D-52425 Jülich — ²Jülich Centre of Neutron Science, Forschungszentrum Jülich GmbH, Lichtenbergstr. 1, D-85747 Garching

Microemulsions have a great variety of uses in industrial application. Most of these applications like oil productions and cleaning imply the presence of huge surfaces. The influence of such surfaces on the domain structure of microemulsions is studied using the example of a planar, hydrophilic wall. In our studies, it shows that the ordering near the wall is locally elevated, while the bulk state is reached far from the surface. Using neutron reflectometry and grazing incidence small angle neutron scattering (GISANS) the alternating domain sequence and the lateral order in the sample is recorded. The sample is studied in GISANS, where we varied the overall scattering length density in order to vary the penetration depth of the evanescent wave, while the bulk contrast remains dominating. In this way the lateral order is resolved as a function of the depth, and the local ordering near the surface can be resolved. These measurements are the first of their kind. The reflectometer measurements aim mainly at the structure in the normal direction. Thus, the thickness of an ordered phase near the surface can be measured. The collected information will be used to improve

the microemulsion behavior near surfaces in the static state and under flow. By using amphiphilic polymers as additives the response of the system to the surface and the flow will be tailored.

CPP 1.4 Mon 11:45 ZEU 222

Adsorption and Near-Interface Structure of Tri-block Copolymer Micelles — ●NICOLE VOSS¹, MARCO WALZ¹, STEFAN GERTH¹, PHILIPP GUTFREUND², MAX WOLFF², HARTMUT ZABEL², and ANDREAS MAGERL¹ — ¹Chair for Crystallography and Structural Physics, University of Erlangen-Nürnberg, Staudtstr. 3, 91058 Erlangen, Germany — ²Chair for Solid State Physics/EP IV, Ruhr-University Bochum, Universitätsstr. 150, 44780 Bochum, Germany

Micellar solutions of block copolymers have rich phase diagrams and they are an excellent model system for the study of crystallization in soft matter. Further, the surface active properties of these systems lead to a distinct sensitivity of micellar structures on the wettability of a solid boundary.

In our studies we investigated the tri-block copolymer EO(20)-PO(70)-EO(20) solved in water using in-situ rheometry, Grazing Incidence Small Angle Neutron Scattering (GISANS) and neutron reflectometry to extract the structural arrangements close to a solid interface in concentrated and dilute solutions. We report on the dependence of structural properties and interfacial adsorption of micelles on surface energy and temperature. After the cessation of applied shear we find a relaxation of the crystalline structure which is determined by the type of micellar structure as well as by the chemical potential of the adjacent surface.

CPP 1.5 Mon 12:00 ZEU 222

Switching of Electrical Conductivity in Microemulsions — ●THOMAS WOLFF and MARKUS BUFE — Technische Universität Dresden, Physikalische Chemie, 01062 Dresden

Microemulsions exhibit three types of macroscopically monophasic solutions structures: water droplets in oil (w/o), oil droplets in water (o/w), and bicontinuous (sponge-like). In the latter two structures water forms a continuous phase. As a consequence these two structures show electrical conductivity in contrast to w/o. Transitions between the solutions states can be achieved by varying composition or temperature. The onset of electrical conductivity in conductivity versus temperature curves can be taken as the percolation temperature indicating the transition o/w - bicontinuous.

We have reported systems in which percolation temperatures are influenced by the presence of certain solubilizers. Photochemically reactive solubilizers allow isothermal switching of conductivity (without turning a mechanical contact), provided photoelect and photoproduct induce different percolation temperatures. The solubilizers thus act as large response triggers for varying the solution structure. However, the systems described so far [1 and references therein] allow switching in one way only, i.e. from conductive to non-conductive or vice versa.

Here we present AOT systems, in which thermally reversible photo-reactions of solubilizers are used, so that the conductivity can be switched on under light (e.g. at daytime) and disappears in the dark (e.g. at night).

[1] M. Bufe, T. Wolff, Phys. Chem. Chem. Phys. 8 (2006) 4222-4227

CPP 1.6 Mon 12:15 ZEU 222

Thermodiffusion of non-ionic sugar surfactants — ●BASTIAN ARLT¹, SASCHA DATTA², THOMAS SOTTMANN², and SIMONE WIEGAND¹ — ¹IFF - Weiche Materie, Forschungszentrum Jülich, Germany — ²Institut für Physikalische Chemie, Universität zu Köln, Germany

Thermodiffusion describes the formation of a concentration gradient due to a temperature gradient in a solution. The strength of this effect is described by the Soret coefficient (S_T): a positive Soret coefficient of a component implies that this component moves to the cold side.

In this work we investigate the thermal diffusion behavior of non-ionic sugar surfactants in water using the IR-TDFRS [1] and the classical TDFRS [2]. First studies on C_8G_1 (n-Octyl β -D-glucopyranoside) indicate a pronounced change in S_T at the critical micelle concentration (cmc) which coincides with an observation by Santos *et al.* [3], who observed a significant change in the strength of the thermal lens signal at the cmc. Furthermore, we observed a temperature dependent

sign change in S_T for higher concentrated solutions. With the classical TDFRS setup which uses a dye, we observe that S_T is independent of the presence of dye, if the concentration is below the cmc, while S_T differs for higher concentrations. We can conclude that the dye

molecules are incorporated as a cosurfactant into the micelles.

[1] H. Ning *et al.*, *J. Phys. Chem. B*, **112**, 10927 (2008) [2] H. Ning *et al.*, *J. Phys. Chem. B*, **110**, 10746 (2006) [3] M. P. Santos *et al.*, *Phys. Rev. E* **77**, 011403 (2008)

CPP 2: Focus: Amphiphilic Systems II

Time: Monday 14:00–17:00

Location: ZEU 222

Invited Talk CPP 2.1 Mon 14:00 ZEU 222
Structure transformations in surfactant bilayer systems — ●OLSSON ULF — Div. of Physical Chemistry Lund University Box 124 SE-221 00 Lund, Sweden

Surfactants and lipid bilayers in solution may form closed shells as in vesicles, planar films as in lamellar phases or multiply connected or branched films as in the sponge phases. Structural transformations between these different topologies involves the fusion or fission of bilayer films. Bilayer fusion and fission are also important biological events, like in endocytosis and exocytosis, and it is of some interest to study these processes in more simple surfactant model systems. Using non-ionic surfactants, where structural transformations are conveniently triggered by small temperature changes, we have studied kinetics in a sponge phase and the kinetics of a lamellar-sponge phase transition. In another study we have focused on vesicle stability. Since Ostwald ripening like processes in these systems are very slow and may be anti-coarsening, vesicle dispersions may have a very long shelf-life if vesicle fusion is a rare event. Vesicle stability depends on the surfactant monolayer spontaneous curvature.

Topical Talk CPP 2.2 Mon 14:30 ZEU 222
Structural Transitions in Self-aggregating Systems Studied by Means of the Stopped-flow Technique — ●MICHAEL GRADZIELSKI — Stranski-Laboratorium, Institut für Chemie, Technische Universität Berlin, Germany

Typically self-aggregating structures are highly dynamic species where characteristic times for structural reorganisations may range from μ s to weeks. Such structural changes can be triggered by mixing with other surfactants, polymers, or solubilisates. In our experiments rapid mixing was done by the stopped-flow technique and followed with turbidity, conductivity, and fluorescence detection or by coupling it to high-flux SANS/SAXS instruments which allows to obtain detailed structural information with a time-resolution of 5-50 ms. Using this method a variety of different structural transitions has been investigated, e. g. the formation of unilamellar vesicles by admixing oppositely charged surfactant or a cosurfactant, solubilisation processes in microemulsions, or the formation of interpolyelectrolyte complexes (IPECs) by admixing oppositely charged polyelectrolytes with charged block copolymer micelles. These processes were followed in structural detail and especially with respect to intermediate, non-equilibrium structures involved. These dynamic processes can be described by invoking simple elementary steps and analysing growth processes for instance in terms of Ostwald ripening or coalescence processes. In particular, in our experiments we are interested in how such intermediate structures differ from the final states and allow for a control of the structures formed.

CPP 2.3 Mon 15:00 ZEU 222
Dissolution of amphiphiles: a time- and space-resolved study — ●HELEN E HERMES and STEFAN U EGELHAAF — Physik der weichen Materie, Heinrich-Heine-Universität Düsseldorf, D-40225 Düsseldorf

Amphiphiles in solution can self-assemble into a variety of structures. Due to their molecular architecture, lipids and non-ionic surfactants tend to form lamellae over a wide range of sample conditions. Upon contact with water these stacks of bilayers swell due to the influx of the water. During this non-equilibrium dissolution process fascinating interface instabilities, so-called myelins, may be observed. To date, information about how such interfacial instabilities form and grow has been obtained using optical techniques. Recently, it has become possible to quantitatively determine the evolution of the microscopic concentration profiles using neutron imaging. Due to latest technical improvements in this method, time- and space-resolved water profiles can now be determined in-situ. In this presentation, an overview of current understanding of the dissolution of amphiphiles and the formation of non-equilibrium structures will be given. Particular emphasis will be

placed on the new quantitative data obtained using neutron imaging and the knowledge gained by a comparison with computer simulations of the processes occurring during amphiphile dissolution.

CPP 2.4 Mon 15:15 ZEU 222
Dynamics of Morphological Transitions in Self-Aggregating Systems Studied by Stopped-Flow Experiments — ●ANINA BARTH¹, MICHAEL GRADZIELSKI¹, ISABELLE GRILLO², and THEYENCHERI NARAYANAN³ — ¹Stranski-Laboratorium für Physikalische und Theoretische Chemie, Institut für Chemie, Technische Universität Berlin, D-10587 Berlin, Germany — ²Institut Max von Laue-Paul Langevin (ILL), F-38042 Grenoble Cedex 9, France — ³European Synchrotron Radiation Facility (ESRF), BP 220 F-38043 Grenoble Cedex

The question of the dynamic behaviour of amphiphilic systems has been investigated. One way to study rapid kinetics is the stopped-flow method in which two volumes of solutions are rapidly mixed and the properties of the mixed solution followed as a function of time, for instance by fluorescence spectroscopy, turbidity, conductivity measurements and small-angle x-ray or neutron scattering. A topic of broad interest is the interaction of surfactants in aqueous solution with hydrophobic material. Although there has been a deep interest in the dynamics of micellar solutions some years ago, less is known about the more complex process of solubilisation. For that purpose quaternary systems of surfactant, cosurfactant, oil, and water were employed and by a systematic variation of their molecular architecture a comprehensive understanding of the solubilisation dynamics is to be achieved. Stopped-Flow fluorescence measurements were done in order to study the formation process of and exchange dynamic between microemulsion droplets.

15 min. break

Invited Talk CPP 2.5 Mon 15:45 ZEU 222
Molecular Reorganization during Membrane Adhesion and Fusion — ●REINHARD LIPOWSKY — Max Planck Institute of Colloids and Interfaces, Potsdam/Golm, Germany

The molecules within biomimetic and biological membranes are rather mobile and can reorganize themselves in various ways. During membrane adhesion, this reorganization leads to the formation of domain patterns induced by the topography of the underlying substrate [1] or by the clustering of adhesion molecules [2,3]. During membrane fusion, the molecules of the adjacent membranes are reorganized to form a fusion pore (or neck). One particularly simple way to induce fusion is provided via membrane tension. [4,5,6] One fusion pathway consists of interbilayer flips and nucleation of a hemifused membrane segment with two tension-dependent energy barriers. [5] Another pathway involves hemifusion via the rupture of one membrane. [6]

[1] B. Rozycki, T. Weikl, and R. Lipowsky, *Phys. Rev. Lett.* **100**, 098103 (2008) [2] T. Weikl and R. Lipowsky, *Biophys. J.* **87**, 3665 (2004) [3] M. Asfaw, B. Rozycki, R. Lipowsky, and T. Weikl, *Europhys. Lett.* **76**, 703 (2006) [4] J. Shillcock and R. Lipowsky, *Nature Materials* **4**, 225 (2005) [5] A. Grafmueller, J. Shillcock, and R. Lipowsky, *Phys. Rev. Lett.* **98**, 218101 (2007) [6] L. Gao, R. Lipowsky, and J. Shillcock, *Soft Matter* **4**, 1208 (2008)

CPP 2.6 Mon 16:15 ZEU 222
Pressure Jump Relaxation Investigations of Lipid Bilayers Using FTIR Spectroscopy — ●MARTIN SCHIEWEK and ALFRED BLUME — Martin-Luther-Universität Halle-Wittenberg, Institut für Chemie, Mühlpforte 1, 06108 Halle(Saale)

The relaxation kinetics of aqueous lipid dispersions after a pressure jump (p-jump) were investigated using time-resolved FTIR spectroscopy with a time resolution of ca. 10 ms. The methylene stretching vibrational bands and the carbonyl band were analyzed to detect changes in conformational order of the hydrocarbon chains and to fol-

low the degree of hydration of the head group, respectively. The kinetics of the transition was found to consist of multiple processes with relaxation constants from seconds down to milliseconds. Faster processes are also present, but could not be resolved by our instrument.

This is the first investigation showing directly the time resolved change in chain order in lipid bilayers induced by a pressure jump using IR spectroscopy. The results obtained with this IR detection method support previous results obtained with light scattering and fluorescence techniques that the change in chain order after a perturbation is a multi-step process with the initial molecular events occurring with time constants shorter than milliseconds.

CPP 2.7 Mon 16:30 ZEU 222

Pressure-jump time-resolved NMR experiments on Phospholipides up to 250 bar and 3 ms jump time — ●GÜNTER HEMPEL¹, MARINA KRUMOVA², UWE HEUERT³, MARTIN SCHIEWEK⁴, and ALFRED BLUME⁴ — ¹Martin-Luther-Universität Halle, Institut für Physik, D-06099 Halle, Germany — ²Universität Konstanz, Fachbereich Chemie, D-78457 Konstanz, Germany — ³Fachhochschule Merseburg, D-06217 Merseburg, Germany — ⁴Martin-Luther-Universität Halle, Institut für Chemie, D-06099 Halle, Germany

Pressure is an important thermodynamic and kinetic variable in the investigation of soft condensed matter and biomolecular systems. It is recognized that conformational properties, aggregation and crystallization processes etc. are widely affected by the pressure.

Design and performance of a pressure-jump instrument for time-resolved NMR experiments are described. A special feature is the

need of using non-ferromagnetic materials for all parts placed in or near the magnet. Fast pressure release at a time resolution of 3 ms is achieved opening a fast acting valve driven by piezo stack. The pressure-jump cell is placed in an especially constructed NMR probe, which can be used in standard spectrometers.

We investigated a pressure-driven order/disorder phase transition of a chain-deuterated dimyristoyl-phosphatidyl*choline (DMPC)-water dispersion. First changes from ordered towards disorder-phase spectra could be detected after some 100 ms; the transformation process finished after about 30 s.

CPP 2.8 Mon 16:45 ZEU 222

Structural changes in aqueous lecithin and bile salt mixtures: dependence on ionic strength — ●DILEK MADENCI and STEFAN U. EGELHAAF — Physik der weichen Materie, Heinrich-Heine Universität, Düsseldorf, Germany

Mixtures of lecithin and bile salt form mixed micelles and vesicles in aqueous solution. Their properties have been well-studied under physiological conditions (150 mM electrolyte, pH 7-8), while other conditions are still hardly explored. Upon increasing ionic strength the formed structures and the transitional pathways (micelles, coexistence of micelles and vesicles, and vesicles), change the generated structures completely from those observed under physiological conditions. We quantitatively determined these structures formed in a broad range of electrolyte concentrations with various scattering techniques, x-ray, light and neutron scattering and calorimetry.

CPP 3: Focus: Amphiphilic systems III

Time: Monday 18:00–19:15

Location: ZEU 222

Invited Talk

CPP 3.1 Mon 18:00 ZEU 222

Formation and exchange kinetics of block copolymer micelles — ●REIDAR LUND — Donostia International Physics Center/ University of the Basque Country, Paseo Manuel de Lardizabal 4, 20018 San Sebastián

In this presentation, we will review results of both the kinetics associated with unimer exchange in the equilibrium state and the non-equilibrium formation kinetics of block copolymer micelles. For the former, we have shown in a series of experiment using TR-SANS and a novel deuteration scheme, that the unimer exchange of block copolymer micelles is characterized by a very slow logarithmic decay [1]. This opposes the theoretically predicted exponential kinetics proposed by Halperin and Alexander a long time ago. For the latter micellization kinetics, we will show some very recent results [2] using time resolved synchrotron x-ray scattering in combination with stopped-flow where the birth of block copolymer micelles can be directly seen on the millisecond time range. We will further demonstrate that the self-assembly process can be quantitatively described as a special nucleation & growth process where the dominating elemental growth mechanism is stepwise unimeric (single chain) addition without invoking any more complicated higher order mechanism such as fusion/fission.

References [1]R. Lund; L. Willner; J. Stellbrink and D. Richter Phys. Rev. Lett. 96 068302 (2006) [2]R. Lund; L. Willner; M. Monkenbusch; P. Panine; T. Narayanan; J. Colmenero and D. Richter submitted

CPP 3.2 Mon 18:30 ZEU 222

Responsive Polymer Cushions for Lipid Bilayer Manipulation — ●MARTIN KAUFMANN¹, DIRK KUCKLING², CARSTEN WERNER¹, and TILO POMPE¹ — ¹Leibniz Institute for Polymer Research, Dresden, Germany — ²University of Paderborn, Department of Chemistry, Germany

Supported lipid bilayer membranes (sLBM) are used to study the function of membranes of living cells. We introduce a pH- and thermoresponsive polymer cushion platform which allows for a switching of the interaction of the sLBM and incorporated transmembrane biomolecules with the solid support. Copolymers composed of N-isopropylacrylamide (NiPAAm) and varying amounts of acrylamide derivatives bearing carboxylic groups at different spacer length were immobilized as thin films and characterized by quartz crystal microbalance. Cushion thickness could be switched between 15–150 nm in response to changes in pH and temperature with lower critical solution temperatures in biological relevant ranges of 15–45 °C. sLBM

were successfully formed from a lipid mixture composed of 90 % DOPC and 10 % DOTAP. First sLBM mobility measurements using fluorescence recovery after photobleaching revealed diffusion coefficients on swollen copolymer films ($8.0 m^2 s^{-1}$) distinctly higher than on SiO₂ sLBM ($6.0 m^2 s^{-1}$). This finding proposes a reduced friction between lipids and the copolymer cushion in comparison to SiO₂. The copolymer cushion responsiveness will be used to further adjust lipid-support interaction and to vary the characteristics of incorporated transmembrane proteins.

CPP 3.3 Mon 18:45 ZEU 222

Temperature dependent swelling and switching kinetics of gold coated end-capped PNIPAM thin films — ●WEINAN WANG¹, JAN PERLICH¹, GUNAR KAUNE¹, ACHILLE M. BIVIGOU KOUMBA², ANDRE LASCHEWSKY², CHRISTINE M. PAPADAKIS¹, ROBERT CUBITT³, and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik - Department E13, James-Franck-Str. 1, D-85747 Garching, Germany — ²Uni. Potsdam, Inst. Chemie, Karl-Liebknecht-Str. 24-25, D-14476 Potsdam-Golm, Germany — ³ILL, b.p. 156, 38042 Grenoble, France

Poly(N-isopropylacrylamide) (PNIPAM) is one of the prominent stimuli-sensitive hydrogels for the construction of nanoscale sensors which are sensitive to water and to water vapour (humidity). We choose PNIPAM end-capped with n-butyltrithiocarbonate (nbc-PNIPAM), a very short hydrophobic end group, to introduce an internal ordering and increase the mechanical stability in the films without sacrificing the swelling ability seriously. Two different gold layers with 0.4 nm and 5 nm thickness are coated on the nbc-PNIPAM surface by sputtering. The surface and internal structure of the dry films are characterized with AFM and GISAXS. The lower critical solution temperature (LCST) of the films in the water vapour is determined with white light interferometry. The temperature dependent swelling and switching kinetics in water vapour of such sensor films is probed by in-situ neutron reflectometry. The real time water diffusion and thickness changes for the two different gold layer thicknesses are compared and discussed in the framework of sensor applications. [1] W. Wang et al., Macromolecules 41, 3209-3218 (2008)

CPP 3.4 Mon 19:00 ZEU 222

Self-Assembly of Symmetric Single-Chain Bolaamphiphiles: The Formation of Temperature, Ionic Strength and pH-Responsive Hydrogels — ●ANNETTE MEISTER¹, SIMON DRESCHER², MARTIN BASTROP¹, GÖRAN KARLSSON³, VASIL GARAMUS⁴, BODO DOBNER², and ALFRED BLUME¹ — ¹Martin-Luther-University Halle-

Wittenberg, Institute of Chemistry, Halle, Germany — ²Martin-Luther-University Halle-Wittenberg, Institute of Pharmacy, Halle, Germany — ³Uppsala University, Department of Physical Chemistry, Uppsala, Sweden — ⁴GKSS Research Centre, Geesthacht, Germany

The bolaamphiphile dotriacontane-1,w-diyl-bis[2-(dimethylammonio)-ethylphosphate] was found to be an excellent hydrogelator by forming a dense network of nanofibers [1]. The temperature, ionic strength and pH dependent aggregation behaviour of this bolaamphiphile in water was investigated using DSC, rheological measurements, SANS and cryo-TEM. SANS and cryo-TEM indicate the formation of a dense

network of nanofibers below the first and second DSC transition temperature and the presence of micelles above the second and third transition temperature. However, rheological measurements point out that the formation of stable hydrogels is only possible at low pH, where the headgroups are in a zwitterionic state. At higher pH values, where the headgroup is deprotonated and negatively charged, a fluid with Newtonian behaviour is obtained.

[1] Meister, A.; Bastrop, M.; Koschoreck, S.; Garamus, V. M.; Sine-mus, T.; Hempel, G.; Drescher, S.; Dobner, B.; Richtering, W.; Huber, K.; Blume, A. *Langmuir*, 2007, 23, 7715.

CPP 4: Biopolymers (joint session BP/CPP)

Time: Monday 11:00–13:15

Location: ZEU 260

see BP 2 for the program of the session

CPP 5: Interfaces

Time: Monday 10:30–12:45

Location: ZEU 160

CPP 5.1 Mon 10:30 ZEU 160

Tracing physio-chemical changes at the solid liquid interface with single molecule microscopy. — ●TÄUBER DANIELA, SCHUSTER JÖRG, and VON BORCZYKOWSKI CHRISTIAN — TU-Chemnitz, Institut für Physik, 09107 Chemnitz, and FOR 877

Hydrodynamics at the solid-liquid interfaces are subject of recent studies in experiment and simulations. Scaling down to nanoscience X-ray and other investigations revealed structural ordering of liquids close to interfaces. However on the molecular level there are still open questions which interactions with the solid interface are accountable for dynamic and structural effects. In previous single molecule tracking experiments [1] we were able to show that diffusion within ultrathin liquid films is vertically heterogeneous and drastically slowed down in comparison to the bulk behavior. Furthermore it is characterized by adsorption events interrupting the diffusional motion.

In series of recent experiments we focussed on details of molecular interactions. By the use of charged and neutral dyes we could reveal spontaneously occurring physio-chemical changes at the solid liquid interface within days leading to a decrease in adsorption probability and thus enhancement of dye diffusion. A simple surface chemistry model is presented to explain those observations.

[1] J. Schuster, F. Cichos, Ch. von Borczykowski: *Euro. Phys. J. E.* 12 (2003), 75-80

CPP 5.2 Mon 10:45 ZEU 160

Wetting and surface tension dynamics of aqueous anionic surfactant/cationic polyelectrolyte mixtures — RADOMIR SLAVCHOV^{1,2}, BORJAN RADOEV¹, GUDRUN PETZOLD², BURKHARD BREITZKE³, and ●VICTORIA DUTSCHK² — ¹Faculty of Chemistry, University of Sofia, Bulgaria — ²Leibniz Institute of Polymer Research — ³Sasol Germany, Marl

Surfactant-polyelectrolyte interactions in aqueous mixtures were studied using dynamic surface tension, polyelectrolyte titration, nephelometric turbidity and dynamic light scattering. A cationic polyelectrolyte (hydroxyethylcellulose, HEC) was used in combination with two anionic surfactants in surfactant classes AS (alkyl or fatty alcohol sulphates) and LES (lauryl ether sulphates) of similar structure but different hydrophobicity.

Systematic studies of the dynamic surface tension and contact angles of aqueous solutions of single components as well as of their mixtures led to an indirect estimation of the interactions both at the liquid-vapour and solid-liquid (highly hydrophobic) interfaces. Here, differences in the wetting kinetics depend on adsorption mechanisms.

Evidently, hydrophobic surfaces show the same or similar adsorption kinetics at the solid-liquid interface as to be expected in the case of the liquid-vapour interface. Besides, the current state of the air interface (dynamic surface tension) at the instance of the drop-surface contact determines the contact angles on hydrophobic surfaces.

CPP 5.3 Mon 11:00 ZEU 160

Large molecules near metal surfaces: A density functional based scale-bridging approach — ●LUIGI DELLE SITE — Max-

Planck-Institute for Polymer Research, PO Box 3148,D-55021 Mainz

We present a hierarchical quantum-classical scale-bridging approach for modeling and simulating large molecules, in bulk and in solution, on inorganic (metal) surfaces. Some examples of its application are illustrated, in particular the study of the adsorption of oligopeptides on a Pt(111) in solution.

CPP 5.4 Mon 11:15 ZEU 160

A thermodynamically consistent view of ion adsorption at interfaces — ●DOMINIK HORINEK, NADINE SCHWIERZ, and ROLAND R. NETZ — Physik Department, Technische Universität München, 85748 Garching, Germany

The implications of ion adsorption at water/solid interfaces are relevant in many biological, chemical, and physical processes. The adsorption shows a very ion-specific behavior, which leads to the so-called Hofmeister series. In recent years this subject has moved into the focus of atomistic computer simulations. In such simulations, one key problem is the proper choice of the ionic force field: the bulk solvation properties and the affinity to interfaces are very sensitive on the ion parameterization. We demonstrate that a thermodynamically consistent description of bulk solvation is compatible with ion adsorption of large anions at hydrophobic interfaces even if the force field is free of atomic polarizabilities. At polar interfaces, the Hofmeister series is reversed, and small ions have a higher affinity to the interface than large ions.

CPP 5.5 Mon 11:30 ZEU 160

Polymer Adsorption Transitions at Attractive Substrates: Analysis from Canonical and Microcanonical Perspectives — ●MONIKA MÖDDEL, MICHAEL BACHMANN, and WOLFHARD JANKE — Institut für Theoretische Physik, Universität Leipzig

Multicanonical simulations allow not only for a precise determination of canonical expectation values over a wide range of temperatures, they also provide a very precise estimation of the density of states. We used thermal fluctuations of energetic and structural quantities to identify the variety of pseudophases of a semiflexible off-lattice homopolymer near an attractive substrate [1]. Introducing a solvent parameter related to the strength of the surface attraction, the solubility-temperature phase diagram is constructed and discussed. Apart from the adsorption transition, several other structural transitions such as the freezing transition between energy-dominated crystalline low-temperature structures and globular entropy-dominated structures as well as the layering transition between single- and double-layered conformations are identified. With the density of states, we then performed a microcanonical analyses focused on the adsorption transition, where a convex intruder of the microcanonical entropy can be observed for short chains, which is a typical signal for a phase separation process. However, for longer chains, the latent heat decreases and seems to vanish in the thermodynamic limit. Thus, we interpret the adsorption process as a second-order phase transition.

[1] M. Möddel, M. Bachmann, and W. Janke, submitted to *J. Phys. Chem. B* (2008).

CPP 5.6 Mon 11:45 ZEU 160

Lateral structures of buried interfaces in ABA-type tri-block copolymer films — ●PETER MÜLLER-BUSCHBAUM¹, LEANDER SCHULZ², EZZELDIN METWALLI¹, JEAN-FRANCOIS MOULIN^{1,3}, and ROBERT CUBITT⁴ — ¹TU München, Physikdepartment E13, James-Franck-Str.1, 85747 Garching (Germany) — ²Uni. de Fribourg, Phys. Dept., Chemin du Musée 3, 1700 Fribourg (Switzerland) — ³Inst. für Werkstofforschung, GKSS, 21502 Geesthacht (Germany) — ⁴ILL, 6 rue Jules Horowitz, 38042 Grenoble (France)

The lateral structure of an A-B-A type tri-block copolymer polyparamethylstyrene-block-polystyrene-block-polyparamethylstyrene at the buried silicon substrate interface is studied as a function of different substrate surface energies. With grazing incidence small angle neutron scattering (GISANS) high interface sensitivity is reached. With GISANS the orientation and the degree of order of the morphology are probed. The powder-like oriented lamellar structure in the bulk becomes oriented along the surface normal in the vicinity of the substrate. A modification of the short-ranged interface potential of the substrate introduces a stretching of the lateral spacing of this lamellar structure up to 8 % as compared to the bulk. The decay of the stretching towards the volume structure is probed with depth profiling. It extends at least up to a distance of 51 nm from the solid surface. [1]

[1] P.Müller-Buschbaum, et al.; Langmuir Letter, 24, 7639-7644 (2008) and P.Müller-Buschbaum, et al.; Langmuir ASAP (DOI 10.1021/la802471p)

CPP 5.7 Mon 12:00 ZEU 160

Free volume distribution at a polymer-solid interface investigated by a slow positron beam — ●STEPHAN HARMS¹, KLAUS RÄTZKE¹, VLADIMIR ZAPOROJTCHEKNO¹, FRANZ FAUPEL¹, WERNER EGGER², and PETER SPERR² — ¹Technische Fakultät der CAU, Lehrstuhl für Materialverbunde, Kaiserstr. 2, 24143 Kiel, Germany — ²Universität der Bundeswehr München, Neubiberg, Germany and FRM II München

Polymer-solid contacts are important for many applications such as adhesion, coating and nanocomposites. Mechanical and permeability properties of polymers are strongly connected to the free volume cavity size and fractions, which might be different at the boundary layer. Positron annihilation lifetime spectroscopy is a widely accepted experimental technique to study the free volume in polymers. The ortho-positronium lifetime is directly connected to the mean free volume size. A tunable low-energy positron beam allows us to measure the free volume as a function of the depth on a nm scale. For the first time we investigated several Teflon AF2400/silicon interfaces at different positron beam energies which corresponds to various depths from surface to interface. By this we obtain information about free volume, the thickness of the interphase region and changes in the free volume in this area. First evaluation shows a decrease in free volume fraction at the interface while the size of the cavities stays constant. We acknowledge the financial support by the DFG within the priority program (SPP) 1369 (Ra 796/5-1).

CPP 5.8 Mon 12:15 ZEU 160

Tuning of surface properties by self assembled mixed monolayers — ●DAVID POLSTER, HARALD GRAAF, and CHRISTIAN VON BORCZYKOWSKI — Center of Nanostructured Materials and Analytics, University of Technology Chemnitz, 09107 Chemnitz, Germany

Self assembled monolayers covalently bond on silicon surfaces were prepared from different mixture ratios of 1-decene (DEC) and methyl-10-undecenoate (UND). A two step radical reaction induced by heat treatment was used to prepare the monolayers. The prepared films have been studied with contact angle measurements, using water as polar liquid and diiodomethane as dispersive liquid as well as atomic force microscopy (AFM). For the mixed monolayers a decrease in the water contact angle, 110° to 75°, was found with increasing ratio of UND in the monolayer. Smaller contact angles could be explained by increasing polarity of the surface induced by the increasing amount of ester groups containing beside dispersive also polar character. Furthermore work of adhesion increases by higher polarity of the mixed monolayers and thereby the process of wetting happens easier and liquids spreads wider. In addition angle hysteresis and mole free energy of dewetting were constant. Beside contact angle investigations scanning probe measurements showed that all surfaces were extremely smooth. By AFM force spectroscopy it could be shown that with increasing polarity of the surface also a slight increase of adhesive force between AFM tip and surface was found.

CPP 5.9 Mon 12:30 ZEU 160

Direct measurement of normal and shear forces between grafted-from polyelectrolyte layers — ●IAIN DUNLOP^{1,4}, WUGE BRISCOE¹, SIMON TITMUS¹, ROBERT JACOBS¹, VICKY OSBORNE², STEVE EDMONDSON², WILHELM HUCK², and JACOB KLEIN^{1,3} — ¹Dept. Chemistry, University of Oxford, South Parks Road, Oxford, OX1 3QZ, U.K. — ²Melville Laboratory for Polymer Synthesis, University Chemistry Laboratory, Lensfield Road, Cambridge, CB2 1EW, U.K. — ³Dept. Materials and Interfaces, Weizmann Institute of Science, PO Box 26, Rehovot 76100, Israel — ⁴Present address: Dept. New Materials and Biosystems, Max-Planck-Institute for Metals Research, Heisenbergstraße 3, 70569 Stuttgart, Germany, and University of Heidelberg, Biophysical Chemistry, INF 253, D-69120 Heidelberg.

We present direct measurements, using the surface force balance (SFB), of the normal and shear forces in aqueous solutions between grafted-from polyelectrolyte layers that were grown by surface-initiated atom transfer radical polymerization on mica substrates. The successful formation of the grafted-from polyelectrolyte layers was confirmed using X-ray reflectometry. Normal force measurements in water showed a long-range force due to an electrical double layer that extended beyond the swollen polyelectrolyte layers, as well as a stronger repulsion when the layers were in contact. Upon addition of 1:1 electrolyte, the long-range force became undetectably small, due to screening effects. Shear force measurements in pure water showed a measurable friction that may arise from the bridging of polymer chains between the surfaces.

CPP 6: Thin Films

Time: Monday 14:00–17:00

Location: ZEU 160

CPP 6.1 Mon 14:00 ZEU 160

Mimicry of natural structural colours — ●MATHIAS KOLLE¹, MAIK SCHERER¹, HEATHER WHITNEY², and ULLRICH STEINER¹ — ¹Cavendish Laboratories, University of Cambridge, UK — ²School of Biological Sciences, University of Bristol, UK

For many organisms in nature intense and distinctive colours play an important role in inter- and intra-species communication. The most impressive natural colours arise from micrometre- to nanometre-sized structures, which often consist of intrinsically transparent materials. Most of the underlying physical principles that create colour from mere transparent materials are well understood and the challenge lies in applying them to create artificial replicas of natural photonic structures

Outstanding structural colours result in general from a balanced combination of various optical effects. We aim to create coatings based on nature-similar structures that optimally exploit different optical effects such as multilayer interference, diffraction from lateral structures as well as fluorescence. Efficient, simple procedures such as nanoim-

printing and nanosphere-lithography and a variety of polymers and inorganic materials are used and will be subject of this presentation. Structural colour coatings promise a wide range of applications only to mention unique labels in security applications to protect for instance credit cards, passports or banknotes from forgery.

CPP 6.2 Mon 14:15 ZEU 160

Surface enrichment layers in pressure sensitive adhesive films — ●ALEXANDER DIETHERT¹, STEPHAN V. ROTH², and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik Department LS E13, James-Franck-Str.1, 85748 Garching (Germany) — ²HASYLAB at DESY, Notkestr. 85, D-22603 Hamburg (Germany)

Pressure sensitive adhesives (PSAs) are used for many different applications, such as for example adhesive foils or binding materials. A prominent class of PSA films is based on statistical copolymers. Typically, two or three different monomers are combined to balance the different requests of the PSA. The adhesive properties of the PSA

films are mainly determined by surface-near regions. However, detailed structural information about this region is still missing.

In the presented work we focus on PSA model systems of statistical copolymers consisting of two different types of monomers: a tacky monomer (e.g. ethyl hexylacrylate) and a glassy monomer (e.g. methyl methacrylate). The PSA films were prepared with solution casting.

From a naive point of view, one would have expected homogenous films which are characterized by the average monomer composition. To investigate the surface structure, we probed the density profile perpendicular to the PSA surface using x-ray reflectivity (XRR). We detected an oscillating composition profile depending on the chosen monomers, the molecular weight of the polymer and the sample age.

Lateral structures within the surface near region are probed with grazing incidence small angle x-ray scattering (GISAXS).

CPP 6.3 Mon 14:30 ZEU 160

Electron irradiation on thin polymer films and its use for biosurface engineering — ●SINA BURKERT, UHLMANN PETRA, and MANFRED STAMM — Leibniz-Institut für Polymerforschung Dresden e.V. Hohe Str. 6, 01069 Dresden

Surface-active materials have been attracting considerable attention in recent years. Especially the tuning of thin polymer films at surfaces has achieved high interest for applications in micro- and nanotechnology, as well as in biotechnology. In this work we will present the effect of electron irradiation on polymer brushes, which represent thin functional films. Those films have shown to be a versatile tool to create, in dependence on the grafting density and chemical composition, e.g. as mixed brushes, stable responsive functional coatings. It is possible to switch the surface properties of a mixed film between the properties of two incompatible polymers by external stimuli, such as temperature. During electron irradiation specific modifications of the respective polymers occur, which have been investigated by various characterization techniques and will be discussed in detail. The knowledge about the interaction of specific polymer brushes with electrons was then used to control the physico-chemical brush properties and to generate a lateral wettability gradient within the film. Those modified surfaces influence protein adsorption in a special manner, which will be also discussed in this contribution. In terms of application in biotechnology first results of cell growth experiments will be presented.

CPP 6.4 Mon 14:45 ZEU 160

Brillouin spectroscopy on thin polymer films — ●JOHANNES WIEDERSICH, ALEXANDER DIETHERT, PETER MÜLLER-BUSCHBAUM, and WINFRIED PETRY — Physikdepartment E13, TU München, Garching

Conventional Brillouin light scattering spectroscopy is a versatile tool for the contact free investigation of mechanical properties of polymers. This makes Brillouin scattering an interesting method for the investigation of thin films, where contact methods have difficulties discerning contributions from the thin film and the substrate. Substantial progress of the Brillouin light scattering technique allows acquisition from scattering volumes in the femto litre range, and thus from films merely tens of nm thick.

We present our first results on Brillouin spectroscopy on thin, transparent polymer films on a glass substrate. Depending on the sample thickness (in the range from less than 100 nm up to bulk dimensions) we observe several film-guided phonons, propagating parallel to the surface.

CPP 6.5 Mon 15:00 ZEU 160

"Micro-structure - Macro-response" Relationship in Swollen Block Copolymer Films — JULIA GENSEL and ●LARISA TSARKOVA — Physikalische Chemie II, Universität Bayreuth, Bayreuth 95440, Deutschland

We present experimental evidence on the correlation between micro-structure and macro-response of diblock copolymer films towards swelling in a selective solvent. The starting morphology of poly(styrene)-*b*-poly(2-vinylpyridin) (SV) films has been adjusted by the fast quench from selective or non selective solvents. The structure at films surface was characterized by scanning force microscopy (SFM), while grazing-incidence small-angle X-ray scattering (GISAXS) measurements have been used to access the microstructure in the interior of the films. The swelling under controlled atmosphere of selective solvent was monitored by *in-situ* spectroscopic ellipsometry. The long-term annealing under atmosphere of a selective solvent (toluene) revealed up to 10% stronger swelling of the films with the initial bulk lamella morphology as compared to the films with the non-bulk micellar phase.

Moreover, we observed clear dependence of the degree of swelling on the film thickness in a thickness range of 0.5-10 layers irrespective to the initial microstructure. These findings bring novel insights into the solvent processing of block copolymer films and indicate roots for designing nano-structured responsive materials.

CPP 6.6 Mon 15:15 ZEU 160

Highly Ordered Block Copolymer Templates for the Generation of Nanostructured Materials — ●ERATHIMMANNA BHOJE GOWD¹, BHANU NANDAN¹, MANFRED STAMM¹, NADJA C BIGALL², and ALEXANDER EYCHMÜLLER² — ¹Leibniz Institute of Polymer Research Dresden, Hohe Strasse 6, 01069 Dresden, Germany — ²Physical Chemistry, TU Dresden Bergstrasse 66b, 01062 Dresden, Germany

Among many different types of self-assembled materials, block copolymers have attracted immense interest for applications in nanotechnology. Block copolymer thin film can be used as a template for patterning of hard inorganic materials such as metal nanoparticles. In the present work, we demonstrate a new approach to fabricate highly ordered arrays of nanoscopic inorganic dots and wires using switchable block copolymer thin films. Various inorganic nanoparticles from a simple aqueous solution were directly deposited on the surface reconstructed block copolymer templates. The preferential interaction of the nanoparticles with one of the blocks is mainly responsible for the lateral distribution of the nanoparticles in addition to the capillary forces. Subsequent stabilization by UV- irradiation followed by pyrolysis in air at 450 oC removes the polymer to produce highly ordered metallic nanostructures. This method is highly versatile as the procedure used here is simple, eco-friendly and provides a facile approach to fabricate a broad range of nanoscaled architectures with tunable lateral spacing.

CPP 6.7 Mon 15:30 ZEU 160

Single molecule tracing to analyze the surface morphology of block-copolymer thin films — ●MUSTAFA YORULMAZ¹, ALPER KIRAZ¹, and ADEM LEVENT DEMIREL² — ¹Department of Physics, Koç University, Rumelifeneri Yolu, 34450 Sariyer, Istanbul, Turkey — ²Department of Chemistry, Koç University, Rumelifeneri Yolu, 34450 Sariyer, Istanbul, Turkey

Single molecules are sensitive reporters that can provide detailed information on their host matrices. In our studies, Terrylene molecules are embedded in Polybutadiene-Polyethylene Oxide (PB-PEO) block-copolymer thin films which reveal cylindrical channels of PB (diameters of ~40-80 nm) that are oriented parallel to the substrate inside the PEO matrix[1]. Samples are prepared by spin coating a Terrylene/Toluene (~20 nM) and PB-PEO/Toluene (~40 mg/mL) mixture on cover glass. Thin films are then annealed for better channel formation. Terrylene molecules are monitored by using the total internal reflection fluorescence (TIRF) microscopy technique. TIRF microscopy images are then recorded with an Electron Multiplied Charge Coupled Device camera (Hamamatsu-ImagEM). Our experiments revealed single molecule traces matching the thin film morphology observed in AFM images. In some of the traces, single molecules are also observed to switch between parallel cylindrical channels. Mean square displacement curves also revealed parabolic dependences to the lag time, suggesting directed diffusion within the channels. This is attributed to the variations in the channel diameters in those cases. [1] M. Y. Yuce, A. L. Demirel, and F. Menzel, Langmuir 21, 5073-5078 (2005).

15 min. break

CPP 6.8 Mon 16:00 ZEU 160

Thermoresponsive PNIPAM Microgel Films — ●ANNA BURMISTROVA, MATTHIAS KARG, MARTIN MEDEBACH, and REGINE VON KLITZING — Stranski-Laboratorium, Institut für Chemie, TU Berlin, Strasse des 17. Juni, 10623 Berlin

During the last decades microgels made of N-isopropylacrylamide (NIPAM) have attracted much interest and were studied by several techniques like microscopy and light scattering [1]. These polymer particles show thermoresponsive behaviour and can therefore be classified as "smart" materials. We synthesize monodisperse PNIPAM microgel with different contents of acrylic acid (AAc) to receive thermosensitive as well as pH-sensitive particles [2,3]. The films were prepared by spin coating and dip coating methods. Characterisation has been done using Atomic Force Microscopy (AFM) and ellipsometry. While AFM allows obtaining information about the particle size and arrangement [4], ellipsometry focuses on the overall film thickness [4]. In order

to study the films under various conditions such as temperature and solvent composition we used liquid cells which allowed studying the surfaces against solution. The results show that the way of preparation and external stimuli like pH, ionic strength and temperature influences strongly the film structure. The internal correlation length was measured by SANS. [1] K. Kratz, T. Hellweg, W. Eimer, *Polymer* (2001) 42, 6531. [2] S. Höfl, I. Zitzler, T. Hellweg, S. Herminghaus, F. Mugele, *Polymer* (2007) 48, 245. [3] S. Nayak, L.A. Lyon, *Angew. Chem.* (2005) 117, 7862. [4] S. Schmidt, H. Motschmann, T. Hellweg, R. v. Klitzing, *Polymer* (2008) 49, 749.

CPP 6.9 Mon 16:15 ZEU 160

Stability of smectic films in water — ●YASUTAKA IWASHITA¹, CHRISTIAN BAHR¹, RALF SEEMANN^{1,2}, and STEPHAN HERMINGHAUS¹ — ¹MPI for Dynamics and Self-Organization, D-37073 Goettingen — ²Experimental Physics, Saarland University, D-66041, Saarbrücken

Free-standing smectic films in air, consisting of plane layers parallel to the film surfaces (homeotropic alignment), have been widely studied for decades [1]. In liquids like water, on the other hand, such stable films have not been observed due to the planar alignment of thermotropic liquid crystals (LCs) at the interface. However, it has been shown that LCs can align homeotropically at the interface to water with the aid of surfactants [2]. An advantage of this system is the tunable anchoring potential via the concentration of the surfactant [3].

Here we focus on smectic-A (S_A) films of the cyanobiphenyl series (nCB, n = 10 and 12) in water stabilized by a surfactant, monoolein. These systems show surface smectic ordering at the LC-water interface in a range of about 2 K above the isotropic - S_A transition temperature, T_A [3]. First we studied smectic films separating water droplets in microfluidic channels: the foam-like structure made up by the water droplets shows a coarsening time which diverges as $T \rightarrow T_A^+$. The voltage for electrocoalescence of the water droplets also increases towards T_A . In addition, we demonstrate the generation of large-area ($5 \times 5 \text{ mm}^2$) S_A films showing layer-by-layer thinning on heating around T_A .

[1] P. Pieranski *et al.*, *Physica A* **194**, 364 (1993).

[2] J.M. Brake *et al.*, *Langmuir* **19**, 6436 (2003).

[3] C. Bahr, *Phys. Rev. Lett.* **99**, 057801 (2007).

CPP 6.10 Mon 16:30 ZEU 160

Ion specific effects in thin aqueous films — ●NATASCHA SCHELERO and REGINE V. KLITZING — Stranski-Laboratorium, Institut für Chemie, TU Berlin, Germany

The specific effects of electrolytes are omnipresent in all systems and processes based on liquid water. For instance the question arises, why salty water is foaming in a more pronounced way than salt free water. Therefore, the effect of addition of different types of salt on the

(de)stability and functionality of single thin aqueous films (foam films) is of interest.[1] Within this work the stability and the interactions between film surfaces is determined in a so-called thin film pressure balance (TFPB). This apparatus is normally used to investigate free-standing symmetrical foam films. In recent studies our group showed that a TFPB also can be used for the investigation of wetting films (air/ water/ solid)[2]. A great advantage of measurements of asymmetrical films is that one can modify the charge of both interfaces independently e.g. by charged polyelectrolytes. The stability of aqueous wetting films on a solid substrate depends on the charge of the substrate and on the ionic strength of the liquid. These results indicate that the force within a water film is controlled by electrostatic interactions[3] and give evidence for negative charges at the air/ water interface[1,4]. Further on, we will present a new insight into ion specific effects in foam films and wetting films. [1] K. Ciunel, *et al.* *Langmuir* 2005, 21, 4790 [2] R. v. Klitzing, *Adv. Coll. Int. Sci.* 2005, 114/115, 253 [3] K. Hänni-Ciunel, *et al.* *Soft Materials*, 2007, 5, 61 [4] K. Hänni-Ciunel, N. Schelero, R. v. Klitzing, *Faraday Discussion*, 2008, in press

CPP 6.11 Mon 16:45 ZEU 160

Tuning of interactions in foam films from oppositely charged polyelectrolyte/surfactant mixtures — ●NORA KRISTEN¹, VASILE SIMULESCU¹, REINHARD MILLER², and REGINE V. KLITZING¹ — ¹Stranski-Laboratorium, TU Berlin, Berlin, Germany — ²Max Planck Institute of Colloids and Interfaces, Potsdam-Golm, Germany

Polyelectrolyte/surfactant mixtures in foams play an important role in many technical applications, e.g. in decalcification processes and cosmetics. In order to control the properties of the foam it is important to investigate single free-standing foam films. A quantitative measure of the interactions between the two opposing film interfaces is the disjoining pressure, which is the sum of repulsive electrostatic, attractive van der Waals and steric forces. The disjoining pressure as a function of film thickness is measured with a Thin Film Pressure Balance.

In this work we study the interactions between polyelectrolytes and surfactants in foam films at low surface charge. To tune the surface charge the concentration of negatively charged polyelectrolyte is varied. Starting with a cationic surfactant films with positively charged surfaces are formed. With the addition of more polyelectrolyte the surface charge is reduced and then reversed. Low and high polyelectrolyte concentrations induce the formation of thick Common Black Films but what happens at very low surface charges? Is a thin Newton Black Film formed or does the film break? Results on the stability of films with different polyelectrolytes are presented and compared with surface tension and elasticity measurements. The effect of polyelectrolytes is compared to the influence of their monomers.

CPP 7: Liquids

Time: Monday 18:00–19:30

Location: ZEU 160

CPP 7.1 Mon 18:00 ZEU 160

Doppler-broadening (DB) measurement of ionic liquids using a monoenergetic positron beam. — ●PHILIP PIKART¹, CHRISTOPH HUGENSCHMIDT², and KLAUS SCHRECKENBACH² — ¹Physik-Department E21, Technische Universität München, James-Frank-Strasse, 85748 Garching, Germany — ²ZWE FRM II, Technische Universität München, Lichtenbergstrasse 1, 85747 Garching, Germany

In this project, room-temperature ionic liquids are studied by positron annihilation spectroscopy which is a standard method for defect characterization of solid state samples. These "organic salts" contain essentially only weakly coordinated ions, resulting in a remarkably low melting point. One of their key properties is the low vapour pressure of less than 10^{-6} mbar at liquid state, which enables measurements of the bare substances in high-vacuum and therewith the application of positron beam studies. 1-Butyl-3-methyl-imidazolium-hexafluorophosphat is chosen for this study, that has well known thermal properties like glass-transition- and triple-point temperature.

The (C)DB-spectrometer and the high intense monoenergetic positron beam of the NEPOMUC beam facility located at the FRM II in Garching are used. The measurements demonstrate the diffusion effects of positrons in a liquid as well as phase transitions, induced by variation of sample temperature between 80K and 300K during the

measurement.

CPP 7.2 Mon 18:15 ZEU 160

Cation Dynamics in Ionic Liquids as seen by QuasiElastic Neutron Scattering — ●JAN PETER EMBS^{1,2} and ROLF HEMPELMANN² — ¹Laboratory for Neutron Scattering, ETH Zurich & Paul Scherrer Institut, CH - 5232 Villigen-PSI — ²Physical Chemistry, Saarland University, D-66041 Saarbrücken

Quasi-elastic Neutron Scattering (QENS) is a powerful tool to investigate the dynamics of species containing protons on a picosecond (ps) time and Angstrom length scale. With this method one can investigate crystalline as well as liquid samples. We use QENS to probe the cation dynamics in pyridinium and imidazolium based ionic liquids containing anions that are not visible due to their negligible scattering cross sections. In this contribution we will present data obtained using different time-of-flight (FOCUS@SINQ, TOFTOF@FRM-II) as well as backscattering spectrometers (MARS@SINQ, IN10@ILL). Different spectrometers are needed in order to obtain experimental results on different time and spatial scales and thus deepen the insight into the dynamical processes occurring in ionic liquids. Our results show that even in the liquid phase the corresponding cations perform localized motions (translational and rotational jump processes inside confining regions (cages) built up by surrounding ions) together with slower pro-

cesses that can be attributed to rearrangements of the ions forming the confining cages. Furthermore using QENS we also can get insight into inelastic processes and thus completing the inelastic region that can be probed by far-infrared spectroscopy.

CPP 7.3 Mon 18:30 ZEU 160

Charge transport and glassy dynamics in ionic liquids — ●JOSHUA SANGORO, CIPRIAN IACOB, ANATOLI SERGHEI, SERGEJ NAUMOV, JORG KÄRGER, and FRIEDERICH KREMER — Institute of Experimental Physics I, University of Leipzig, Linnéstr. 5, 04103, Leipzig, Germany

Charge transport and glassy dynamics of a variety of glass-forming ionic liquids (ILs) are investigated in a wide frequency and temperature range by means of Broadband Dielectric Spectroscopy (BDS), Pulsed Field Gradient Nuclear Magnetic Resonance (PFG NMR), AC Calorimetry, Differential Scanning Calorimetry and Rheology. While the absolute values of dc conductivity and viscosity vary over more than 11 decades with temperature and upon systematic structural variation of the ILs, quantitative agreement is found between the characteristic frequency of charge transport and the structural α -relaxation. This is traced back to dynamic glass transition assisted hopping as the underlying mechanism of charge transport. A novel approach is applied to extract diffusion coefficients from BDS spectra in quantitative agreement with PFG NMR values but in a much broader range. References: [1] J. R. Sangoro, A. Serghei, S. Naumov, P. Galvosas, J. Kärgner, C. Wespe, F. Bordusa, and F. Kremer, *Phys. Rev. E* 77, 051202 (2008); J. R. Sangoro et al, *J. Chem. Phys.* 128, 214509 (2008); J.R. Sangoro, C. Iacob, A. Serghei, C. Friedrich, F. Kremer, *Phys. Chem. Chem. Phys.*, In press.

CPP 7.4 Mon 18:45 ZEU 160

Tetrahydrofuran clathrate hydrate formation studied by non-resonant inelastic x-ray scattering — ●FELIX LEHMKÜHLER¹, CHRISTIAN STERNEMANN¹, HEIKO CONRAD¹, ARTO SAKKO², MIKKO HAKALA², KIM NYGÅRD³, DIETMAR PASCHEK⁴, OMID FEROUGH¹, THOMAS BUSLAPS⁵, LAURA SIMONELLI⁵, METIN TOLAN¹, and KEIJO HÄMÄLÄINEN² — ¹TU Dortmund, Fakultät Physik/DELTA, Dortmund, Germany — ²Division of Materials Physics, Department of Physics, FIN-00014 University of Helsinki, Finland — ³Paul Scherrer Institut, Villigen PSI, Switzerland — ⁴Rensselaer Polytechnic Institute, Troy, 12180 NY, USA — ⁵ESRF, 38043 Grenoble, France

Clathrate hydrates are ice-like inclusion compounds where guest molecules are embedded in water nano-cages. A possible future application of hydrates is the storage of gases, especially H₂ in THF hydrate for fuel cells. In general, the hydrate formation on a microscopic level is still not understood. Competing formation models are reported in literature, which predict hydrate precursors in a supercooled state before the hydrate formation starts or a stochastic formation without any hydrate pre-structures.

The bulk formation in the system water-THF was investigated by measuring x-ray Compton profiles and non-resonant x-ray Raman spectra of the hydrate, a mixture at temperatures above the region of hydrate stability, and the supercooled liquid mixture in order to

detect hydrate precursors. The measurements were compared with DFT calculations employing local structures obtained from molecular dynamics simulation snapshots.

CPP 7.5 Mon 19:00 ZEU 160

Chelation in a water/triamine mixture: investigation of structure formation in space and time — ●ULRICH MÜLLER¹, MARTINE PHILIPP¹, JÖRG BALLER¹, ROLAND SANCTUARY¹, PIERRE SECK¹, MICHAEL VEITH², and JAN KRISTIAN KRÜGER¹ — ¹Université du Luxembourg, FSTC, Campus Limpertsberg, 162a avenue de la Faiencerie, L-1511 Luxembourg — ²Universität des Saarlandes, Anorganische Chemie, Fachbereich 8.11, Gebäude C 4.1, Postfach 151150, D-66041 Saarbrücken

Chelation is the binding or complexation of a bi- or multidentate ligand. Usually this term refers to complexes of metal ions and the chelating agent but can also refer to the complexation of water by polyamines. We will present first results of the chelation of water by diethylene triamine (DETA). DETA is tridentate ligand and exhibits a good miscibility with water. Our study comprises the investigation of the DETA concentration dependence of the mass density, of the refractive index and the longitudinal elastic modulus as well as time and space dependence of the chelation process at a water/DETA interface as measured by time resolving Brillouin microscopy. The results show that the longitudinal elastic modulus and the mass density possess a maximum over concentration whereas the refractive index does not. This strong deviation from the Lorenz-Lorentz behaviour indicates a significant influence of chelation and the accompanying change in structure on the electronic polarizability. Furthermore we are able to show a complex structure formation process at the water-DETA interface leading to an astonishingly asymmetric interphase.

CPP 7.6 Mon 19:15 ZEU 160

Molecular motions in liquid medium-chain *n*-alkanes — ●TOBIAS UNRUH¹, CHRISTOPH SMUDA¹, SEBASTIAN BUSCH¹, and GERD GEMMECKER² — ¹Technische Universität München, Forschungsneutronenquelle Heinz Maier-Leibnitz (FRM II), D-85747 Garching — ²Technische Universität München, Bayerisches NMR-Zentrum, Chemie Department

Different diffusive motions in liquid medium-chain *n*-alkanes could be disentangled by resolution resolved quasielastic time-of-flight neutron spectroscopy (TOF-QENS). It was found that the dominating motion causes a Q^2 -dependence of the QENS signal for any observation time in the picosecond time range. For the longest times the Q^2 -dependence describes the long range center-of-mass diffusion of the alkane molecules as confirmed by PFG-NMR measurements. By comparison with molecular dynamics simulations, the identified motions for short times are attributed to displacements of hydrogen atoms reflecting local molecular trajectories. Despite the rod-like shape of the molecules the center-of-mass diffusion was found to be essentially isotropic. A coherent picture of the diffusional process ranging from the fast tumbling of CH₂ groups to the slow long range molecular diffusion will be presented.

CPP 8: Nanoparticles I

Time: Monday 10:30–12:30

Location: ZEU 114

CPP 8.1 Mon 10:30 ZEU 114

Nanoscale pH-sensing with Polymer coated Gold Nanorods — ●IRENE AMENT, JAN BECKER, ANDREAS HENKEL, SEBASTIAN PIERRAT, LUIGI CARBONE, and CARSTEN SÖNNICHSEN — Institute for Physical Chemistry, University of Mainz, Germany

We report a reversible nanoscale pH-sensor consisting of a gold nanorod covered with the pH sensitive polymer Poly(acrylic acid). This polymer is covalently bound to the gold particle by cystein side groups and deprotonates under basic conditions. At high pH, the backbone is therefore stretched by the repelling forces of the negative charges and the packing becomes less dense, lowering the refractive index around the particle. This change in the refractive index induces a shift in the plasmon resonance, which we detect with single particle dark field spectroscopy. With such a reversible system we detect pH variations at the nanometer scale and could potentially map pH landscapes with high precision.

CPP 8.2 Mon 10:45 ZEU 114

Investigation of nucleation and growth processes of gold nanoparticles via coupled in situ SAXS/XANES — ●JÖRG POLTE¹, FRIEDMAR DELISSEN¹, TORSTEN T. AHNER², SERGEY SOKOLOV², RALPH KRAEHNERT², MARTIN RADTKE¹, UWE REINHOLZ¹, HEINRICH RIESEMEIER¹, FRANZISKA EMMERLING¹, and ANDREAS F. THÜNEMANN¹ — ¹BAM Federal Institute for Materials Research and Testing Richard-Willstätter-Str. 11, 12489 Berlin — ²LIKAT - Leibniz Institute for Catalysis, Richard-Willstätter-Str. 12, 12489 Berlin

Gold nanoparticles (AuNP) are among the most studied nanoscale material due to prospective applications in areas such as medicine, biotechnology and catalysis [1, 2]. To control the size and shape of metal nanoparticles, a detailed understanding of the mechanism and kinetics of precursor reduction and particle growth is essential. We report on a new method to determine in parallel the oxidation state of the reactants as well as the size, number and polydispersity of formed par-

ticles in-situ. The method relies on time-resolved XANES and SAXS measurements carried out on sample droplets exposed to synchrotron radiation. Supplemented by in-situ UV-Vis and SEM, the evolution of AuNP during reduction and particle formation was explored using different reducing agent. From the data, a mechanistic scheme is developed explaining the different phases of particle formation and growth, thus providing a basis for improved control over the synthesis process. [1] J. Park, J. Joo, S. G. Kwon, Y. Jang, T. Hyeon, *Angewandte Chemie-International Edition* 2007, 46, 4630. [2] M. C. Daniel, D. Astruc, *Chemical Reviews* 2004, 104, 293.

CPP 8.3 Mon 11:00 ZEU 114

Kinetic study of binding of multivalent ligands on size selected gold nanoparticles — ●SUGUNA PERUMAL, ANDREAS HOFMANN, CHRISTINA GRAF, and ECKART RÜHL — Physikalische und Theoretische Chemie, Institut für Chemie und Biochemie, Freie Universität Berlin, Takustr. 3, 14195 Berlin

A kinetics study of binding of multivalent ligands on different kinds of nanoparticles is presented. The enhanced binding of multiple ligands in one entity to multiple receptors is known as the multivalency effect. Flexible thiol functionalized multivalent ligands are synthesized by using reported procedures. Pyrene bound nanoparticles are prepared by wet colloidal chemistry and characterized by transmission electron microscopy. The multivalency effects are investigated by exchanging pyrene bound to gold nanoparticles with multivalent ligands and studying this process via fluorescence spectroscopy. The fluorescence of the pyrene moiety is completely quenched when it is directly bound to gold nanoparticles. It recovers completely after desorption from nanoparticles after an exchange with mono- or multivalent ligands. The change of the fluorescence intensity of the pyrene moiety is measured as a function of time. Multivalency effects are observed by comparing the rate constants of monovalent and di- or trivalent thiol ligands. However, no enhancement effects are observed between trivalent and divalent thiol ligands on gold nanoparticles. Hence, we assume that only two thiol groups are binding in case of the trivalent ligands. Further, the influence of the particle size on the exchange kinetics is discussed.

CPP 8.4 Mon 11:15 ZEU 114

Nanoscale Characterization of Single Metal Nanoparticles by their Scattering Patterns — ●TINA ZÜCHNER¹, FRANK WACKENHUT¹, ANTONIO VIRGILIO FAILLA^{1,2}, and ALFRED J. MEIXNER¹ — ¹Eberhard-Karls-Universität Tübingen, Institute of Physical and Theoretical Chemistry, Tübingen, Germany — ²University of Cambridge, The Cancer Research UK, Cambridge, UK

We present a novel route to detect the environment of metal nanoparticles by means of confocal interference scattering microscopy in combination with higher order laser modes. Each scattering pattern results as the sum of the light reflected at the interface between two dielectric media and the light scattered by the particles. The images not only show directly the orientation of individual Au nanorods [1-3], but are also extremely sensitive on variations of the local environment [4]. In fact, changing the refractive index of the surrounding medium strongly influences e.g. the signal to noise ratio, the amplitude and the contrast sign which in addition reveals the nature of the interface between two dielectric media. A quantitative understanding of the refractive index's influence on the scattering pattern was achieved by comparing the experimental results and our theoretical calculations.

[1] A.V. Failla, H. Qian, H. Qian, A. Hartschuh and A.J. Meixner, *Nano Lett.* 6, 1374 (2006). [2] A.V. Failla, S. Jäger, T. Züchner, M. Steiner and A.J. Meixner, *Opt. Expr.* 15, 8532 (2007). [3] T. Züchner, A.V. Failla, A. Hartschuh and A.J. Meixner, *J. Microsc.* 229, 337 (2008). [4] T. Züchner, A.V. Failla, M. Steiner and A.J. Meixner, *Opt. Expr.* 16, 14635 (2008).

CPP 8.5 Mon 11:30 ZEU 114

Strukturelle und elektronische Eigenschaften von Biomolekülen auf isolierten Goldnanopartikeln — ●RENE LEWINSKI, CHRISTINA GRAF, BURKHARD LANGER, BERNHARD GRUNDKÖTTER, BERNHARD WASSERMANN and ECKART RÜHL — Institut für Chemie und Biochemie, Freie Universität Berlin, Takustr. 3, 14195 Berlin

Die Oberflächenmodifikation von Nanopartikeln (NP) mit einfachen Biomolekülen wie z.B. Aminosäuren ermöglicht neue Anwendungen als Sensoren und Diagnostika. Zur Optimierung dieser Systeme ist ein detailliertes Verständnis der Wechselwirkungen zwischen den Biomolekülen und den NP erforderlich. NEXAFS (Near Edge X-ray Absorption Fine Structure)-Spektroskopie ist eine empfindliche Methode zur

Untersuchung der lokalen elektronischen Struktur sowohl organischer Moleküle als auch der NP. Ihr Einsatz führt aber durch die intensive Röntgenstrahlung oft zu Strahlenschäden. Wir haben deshalb NP in einem freien Partikelstrahl mittels NEXAFS untersucht. Die Lösungen wurden versprüht, getrocknet und mit einer aerodynamischen Linse in den Bereich der Synchrotronstrahlung überführt. Hierdurch werden sowohl der Kontakt zu einem Substrat als auch Strahlenschäden vermieden. Mit schwefelhaltigen Biomolekülen funktionalisierte Gold-NP wurden mit den Spektren der entsprechenden reinen Liganden verglichen, wobei signifikante spektrale Verschiebungen beobachtet wurden. Insbesondere konnte trotz der relativ stabilen S-Au Bindung, eine partielle Oxidation der Liganden nachgewiesen werden. Auch zwischen mono- und bivalent gebundenen Liganden kann ein signifikanter Unterschied in der lokalen elektronischen Struktur festgestellt werden.

CPP 8.6 Mon 11:45 ZEU 114

Size-controlled functionalized magnetite nanoparticles and their cellular uptake — ●SEBASTIAN WEIBELS¹, ANJA SOMMER¹, STEFANIE KLEIN¹, JESSICA PLOETTNER¹, KLAUS GIEB², KONSTANTIN PETUKHOV², and CAROLA KRYSCHI¹ — ¹Dept. Chemistry and Pharmacy, Physical Chemistry I, FAU, Egerlandstr. 3, 91058 Erlangen — ²Physical Institute III, FAU, Erwin-Rommel-Str. 1, 91058 Erlangen

Magnetite nanoparticles (MNP) were synthesized by coprecipitating Fe(II)/Fe(III)solutions with an ammonia solution, and their sizes were tuned between 4 and 15 nm by varying the concentrations of the reactants. Repulsive interactions between the MNP and their solubility in polar and nonpolar solvents were obtained by functionalizing the MNP with suited organic acids. FTIR spectra of successfully functionalized MNP indicate covalent binding via the carboxylic group. The MNP sizes were determined under a high-resolution transmission electron microscope, while the magnetic properties in dependence on temperature were investigated using a SQUID magnetometer. The uptake of functionalized MNP by Caco-2 cells were imaged by transmission electron microscopy.

CPP 8.7 Mon 12:00 ZEU 114

Nass-chemisch hergestellte, dotierte Lithiumniobat-Nanopartikel* — ●BASTIAN KNABE, DANIEL SCHÜTZE und KARSTEN BUSE — Physikalisches Institut, Universität Bonn, Wegelerstr. 8, 53115 Bonn

Dotierte Lithiumniobat-Nanopartikel versprechen neue optische Eigenschaften, die der entsprechende Volumenkristall nicht aufweist. Wir demonstrieren einen nass-chemischen Ansatz zur Erzeugung dotierter Lithiumniobat-Nanopartikel aus Metallalkoholaten. Die angestrebte Größe liegt dabei unter 50 nm. Grad und Verteilung der Dotierung werden mit Hilfe energiegefilterter Transmissionselektronenmikroskopie und Elektronenenergieverlustspektroskopie nachgewiesen.

*Wir danken der DFG und der Deutschen Telekom AG für finanzielle Unterstützung.

CPP 8.8 Mon 12:15 ZEU 114

Influence of silicon dioxide nanoparticles on the isothermal cure of a silicone rubber. — ●BARTOSZ ZIELINSKI, ULRICH MÜLLER, MARTINE PHILIPP, JÖRG BALLER, ROLAND SANCTUARY, and JAN KRISTIAN KRÜGER — LPM, University of Luxembourg, Luxembourg

Incorporation of nanoparticles is nowadays widely used to improve physical and chemical properties of polymer materials. This is mainly caused by the fact that very often the polymer nanocomposites show physical properties not found in the corresponding microstructured material. The justifications for that behaviour are: size- and surface-induced properties of the nanoparticles themselves, topological constraints within the matrix material for high concentrations of nanoparticles and last but not least specific surface interactions between the nanoparticles and the polymer matrix. These chemical and/or physical interactions change the properties of the polymer nanocomposites and result in the creation of the so-called interphases.

Because there are already strong interactions between the single components of the silicone rubber and the nanoparticles which lead to the formation of new structures it will be shown how these interactions influence the curing process of the silicone rubber. We will discuss the influence of the nanoparticles on the optical and thermal properties for a two-component silicone rubber system filled with silicon nanoparticles. The results will be interpreted in terms of particles induced structure formation.

Refractometry and temperature modulated calorimetry have been used as experimental techniques.

CPP 9: Nanoparticles II

Time: Monday 14:00–17:00

Location: ZEU 114

CPP 9.1 Mon 14:00 ZEU 114

The influence of interfaces on fluorescence intermittency of single CdSe/ZnS nanocrystals — ●CORNELIUS KRASSELT, JÖRG SCHUSTER, and CHRISTIAN VON BORCZYKOWSKI — TU Chemnitz, Institute of Physics, 09107 Chemnitz

Fluorescence intermittency, characterized by inverse power law distributions for both the bright and dark times, appears to be a common feature of many different classes of individual emitters [1].

Meanwhile it is generally accepted, that this behaviour is due to trapping and detrapping of charges. Two basic approaches, a tunneling model by Verberk [2] and the DCET model by Tang [3] try to explain the experimental circumstances associated with the blinking phenomena.

To contribute to the current discussion of the physical nature of blinking we investigated the influence of static trap sites in the local surroundings of ZnS overcoated CdSe nanocrystals spincoated on thermally grown silicon oxide. Therefore we have modified the trap density by annealing the silicon oxide substrate to reduce the amount of trapping silanol groups on the one hand and by passivation of the silicon oxide with an organic (ODS) monolayer on the other hand. Among the modification of the blinking statistics through the ODS-monolayer we found atypical distributions for the "on" time statistics which are different from a power law or exponential behaviour.

[1] F. Cichos et al.: COCIS 12 (2007), 272

[2] R. Verberk et al.: Phys. Rev. B 66 (2002), 233202

[3] J. Tang et al.: J. Chem. Phys. 123 (2005), 054704

CPP 9.2 Mon 14:15 ZEU 114

Investigations to the Influences of Charges on the Fluorescence of Single CdSe/ZnS Quantum Dots Dependent on Crystal Size — ●NICOLE AMECKE-MÖNNIGHOFF and FRANK CICHOS — Molecular Nanophotonics Group, Institute of Experimental Physics I, University Leipzig, Linnéstraße 5, 04103 Leipzig

The fluorescence properties of semiconductor nanocrystals (quantum dots) are intensively studied due to many potential applications, which want to make use of their tunable emission wavelength, high quantum yield and photon statistics. Considering their fluorescence in more detail many peculiarities can be found. Along those are antibunching, power-law blinking, lifetime-fluctuations and spectral diffusion. Most of those can be explained by charges close to or in the dot center leading to Auger processes (non-radiative energy transfer to those charges) and the quantum confined stark effect. Those charges can arise from ejection of electron or hole via tunneling leaving behind the counterpart and additionally changing the matrix charge constellation. We study all those characteristics on Qdot CdSe/ZnS crystals by time-resolved spectroscopy in particular as a function of crystal size. We find strong indications of fluctuating radiative and non-radiative rates for all sizes, however suggesting that the closer vicinity of the interface in smaller crystals is more stringent in switching the crystal either on or off.

CPP 9.3 Mon 14:30 ZEU 114

The shape of CdSe nanoparticles and its role for their electro-optic properties in hybrid semiconductor-polymer structures — ●FARZANA ASLAM¹ and CHRISTIAN VON FERBER² — ¹Department of Mathematics, Statistics and Engineering Sciences, Coventry University, Coventry, United Kingdom — ²Applied Mathematics Research Centre, Coventry University, Coventry, United Kingdom

CdSe nanoparticles due to their electro-optical efficiency play an important role as sensitizers in hybrid semiconductor-polymer structures. Here, we study the electrostatic and structural trends of CdSe nanoparticles using empirical potentials. The electrostatic and structural properties of CdSe nanoparticles are studied as a function of the size, shape, structure and surface of the nanoparticles. We identify trends in the properties of particles that are either approximately spherical, cut along well defined crystal surfaces or short nano-rods. The aspect ratio of these particles has a significant impact on the energy, dipole moment and internal stress. We observe that the choice of the shape in terms of crystal surfaces and aspect ratio strongly affect the number of dangling bonds present on the surface of the nanocrystal, which in turn may determine the photo-generation and sensitization efficiencies. We study systematically both the mean behaviour of randomly

grown nanocrystals as well as the limiting cases of crystals with ideal crystal surfaces.

CPP 9.4 Mon 14:45 ZEU 114

Study of electronic couplings between molecular and core states of 3-ethenylthiophene terminated Si quantum dots — ●VINCENT GROENEWEGEN, VOLKER KUNTERMANN, CARLA CIMPEAN, ANJA SOMMER, and CAROLA KRYSCHI — Dept. Chemistry and Pharmacy, Physical Chemistry I and ICMM, FAU, Egerlandstr. 3, 91058 Erlangen

One of the central challenges in fabrication of silicon quantum dots (Si qdots) tailored for nano-optoelectronics is to functionalize their surfaces with electronically efficiently coupled molecules which mediate photogenerated carrier injection into the bulk and allow to optically control charge separation as well as luminescence properties of the bulk. We have developed a wet-chemistry procedure that allows to produce Si qdots with adjustable sizes and surface properties. Here we present a fs spectroscopy and a time-dependent density function theoretical (TDDFT) study of Si qdots with sizes around 2 nm which are terminated with 3-ethenylthiophene. The photoluminescence spectra as well as the TDDFT computations unambiguously show quasi-resonant electronic interactions between the excited states of covalently bound 3-ethenylthiophene and conduction band states of the Si core. These results were confirmed by ultrafast rise dynamics of absorption transitions of conduction band electrons which were monitored with the fs transient absorption spectroscopy technique

CPP 9.5 Mon 15:00 ZEU 114

FRET and Non-FRET processes in quantum dot - dye nanoassemblies — ●DANNY KOWERKO, JÖRG SCHUSTER, and CHRISTIAN VON BORCZYKOWSKI — Center of nanostructured materials and analytics, TU-Chemnitz, 09107 Chemnitz

Assemblies of semiconductor quantum dots (QDs - donor) and organic (dye - acceptor) molecules are of increasing interest for numerous applications in science and technology. Recent publications on such systems report on charge and fluorescence resonant energy transfer (FRET), prevalently neglecting an exact quantitative spectroscopic analysis of the acceptor. Recently, calculations of Seifert et al. [1] and Blaudeck and coworkers [2] demonstrated the crucial dependence of trap state emission from the surface coverage. In our contribution we emphasize the role of dye induced surface trap states as one mechanism - besides FRET - for QD quenching. Thus detailed quantitative analysis of titration experiments of differently functionalized perylenebismide molecules and CdSe/ZnS quantum dots will be discussed. By means of single particle spectroscopy we may even compare spectroscopic properties of the free and bound species on one and the same sample under identical conditions. Furthermore, analysis of FRET allows for a distinction between different geometries of the dye-QD assemblies.

[1] J. Frenzel, J.-O. Joswig, G. Seifert, J.Phys.Chem.C 2007, 111, 10761 [2] T. Blaudeck, E. I. Zenkevich, F. Cichos, C. von Borczykowski, J.Phys.Chem.C 2008, accepted

CPP 9.6 Mon 15:15 ZEU 114

Optoelectronic properties of surface-modified Ge quantum dots — ●IVAN LITZOV¹, VINCENT GROENEWEGEN¹, CAROLA KRYSCHI¹, HARTMUT WIGGERS², and DIETRICH HAARER³ — ¹Dept. Chemistry and Pharmacy, Physical Chemistry I and ICMM, FAU, Egerlandstr. 3, 91058 Erlangen — ²Institute for Combustion and Gas Dynamics, University of Duisburg-Essen, Lotharstr.1, 47048 Duisburg — ³BIMF, University of Bayreuth, Universitaetsstr. 1, 95440 Bayreuth

This contribution is targeted to the development of functionalized Ge quantum dots tailored for optoelectronic applications such as solar cells and light emitting diodes. Ge qdots with sizes around 7 nm were successfully surface-modified via HF etching followed by thermal germylation with different unsaturated organic compounds. The surface modified Ge qdots exhibit photoluminescence peaking between 750 and 850 nm, while a fs spectroscopy study gave indication to photo-induced electron transfer from surface bound compounds to conduction band states of the Ge core. The eligibility of surface-modified Ge qdots for hybrid solar cells was studied by measuring photocurrent-action spectra and determining the power conversion efficiency for systematically varied compositions and thicknesses of P3HT:Ge qdot films

sandwiched by an ITO glass substrate and a LiF/Alu contact layer.

15 min. break

CPP 9.7 Mon 15:45 ZEU 114

Enwrapping of tubular J-aggregates by Polyelectrolytes — ●OMAR AL-KHATIB^{1,2}, HELMUTH MÖHWALD¹, JÜRGEN P RABE², CHRISTOPH BÖTTCHER³, and STEFAN KIRSTEIN² — ¹Max-Planck-Institut of Colloids and Interfaces, Potsdam, Germany — ²Humboldt University Berlin, Department of Physics, Germany — ³Free University Berlin, Germany

Amphiphilic carbocyanine dyes are able to form tubular J-aggregates in aqueous solutions by a self-assembly process. The wall of the tubular aggregates is assumed to be formed by a dye bilayer that encloses the hydrophobic alkyl chains and exposes negative surface charges to the inside and outside of the aggregates. The charged surface is utilized to adsorb oppositely charged polyelectrolytes in order to enwrap the aggregate. This mechanism allows further stabilization and even functionalization using polyelectrolytes with functional groups. We show the coating of negatively charged tubular J-aggregates by various polycations such as poly(diallyldimethylammonium chloride) (PDAC), poly(allylamine hydrochloride) (PAH), and poly(ethylene imine) (PEI). The enwrapping was verified by cryogenic transmission electron microscopy (cryo-TEM) and its influence on the optical spectra was investigated. The morphology and the optical spectra of the coated structures vary considerably for the different polyelectrolytes and strongly depend on the ionic strength of the solution. The detailed investigation of these parameters allows to find controlled conditions for the formation of complex functionalized structures in aqueous solution by pure self assembling processes.

CPP 9.8 Mon 16:00 ZEU 114

Polarization Resolved Emission of Single Nanotubular J-Aggregates — ●DÖRTHE M. EISELE¹, STEFAN KIRSTEIN¹, JASPER KNOESTER², JÜRGEN P. RABE¹, and DAVID A. VANDEN BOUT³ — ¹Humboldt University Berlin, Department of Physics, Germany — ²University of Groningen, Institute for Theoretical Physics and Zernike Institute for Advanced Materials, Netherlands — ³University of Texas at Austin, Department of Biochemistry and Chemistry, USA

Presently, the most efficient natural Light Harvesting System (LHS) contains multi-layer tubules of aggregated bacteriochlorophyll (BChl). Nanotubular J-aggregates of amphiphilic carbocyanine dyes constitute an artificial model system, which has been intensively studied in ensembles in solution. New insights into how the aggregate morphology affects its optical properties can be gained by directly probing individual single aggregates.

We deposited the aggregates onto solid transparent substrates by maintaining their optical and morphological properties. Single J-aggregates were identified using Atomic Force Microscopy (AFM). Near-field Scanning Optical Microscopy (SNOM) was used to simultaneously collect both topographic and fluorescent images of the single aggregates. The emission was recorded polarization resolved, and a quantitative analysis of the J-band emission polarization relative to the tube orientation was carried out. The emission is strongly but not perfectly polarized parallel to the long tubular axis, and the reduced linear emission dichroism of single tubes was determined to .

CPP 9.9 Mon 16:15 ZEU 114

Spectroscopic study of the complex formation of DNA and a sequence specific minor-groove binding dye: towards molecular metallization — ●MARKUS SCHUSTER¹, GLENN BURLEY², and ULRICH RANT¹ — ¹Technische Universität München, Germany — ²University of Leicester, UK

The complex formation of small molecules and DNA represents a promising concept to prepare self-assembled nanostructures. We investigate the interaction of DNA with 3,3*-Diethylthiadicarbocyanine iodide (DiSC2(5)), which has been reported to selectively bind to the minor groove along ATATA sequences. Using extinction and fluorescence spectroscopy, we characterize the binding affinity of DiSC2(5) to different DNA sequences. Binding stoichiometries are determined using the method of continuous variation. The thermodynamic stability of the DNA/ DiSC2(5) complex is investigated and melting temperatures are analyzed. DiSC is found to associate with DNA as a dimer with increased, albeit not exclusive, affinity for the ATATA binding cassette.

Aiming to create metal nanoparticles on specific sites along DNA templates, we carried out metallization experiments using DiSC2(5)-dimers as site-selective seeds for metal growth. The development of silver nanoparticles is evidenced by the appearance of plasmon peaks in the absorption spectrum. Dynamic light scattering experiments reveal that the particle diameters range between 10 and 20 nm.

CPP 9.10 Mon 16:30 ZEU 114

STM/CITS investigation of a Co(II) Cubane and a Zn(II) Coordination Polymer — ●MICHAEL STOCKER¹, UTPAL MITRA¹, VIACHESLAV DREMOV¹, NINA FISCHER², FRANK W. HEINEMAN², ANDREAS SCHEURER², AYUK M. AKO², NICOLAI BURZLAFF², ROLF W. SAALFRANK², and PAUL MÜLLER¹ — ¹Department für Physik, Universität Erlangen-Nürnberg, Germany — ²Department für Chemie und Pharmazie, Universität Erlangen-Nürnberg, Germany

A combination of scanning tunneling microscopy (STM) and current imaging tunneling spectroscopy (CITS) has been performed on a Zn(II) coordination polymer ($[Zn(L)(Cl)]_n$) and on a Co(II) cubane ($[Co_4(HL)_4(Cl)_4]$). Both were deposited onto highly oriented pyrolytic graphite (HOPG). In the case of the Zn(II) coordination polymer thick strands as well as single polymer lines were observed. For the Co(II) cubane single molecules were observed. In CITS measurements we found a rather large contrast at the expected location of the Zn and Co metal centers, respectively. This demonstrates that the position of the metal centers within the molecule can be mapped. We discuss local tunneling spectroscopy data.

CPP 9.11 Mon 16:45 ZEU 114

Solid State NMR for Polymer Nanocomposites — ●ANASTASIA VYALIKH¹, FRANCIS COSTA^{1,2}, GERT HEINRICH¹, DOMINIQUE MASSIOT³, and ULRICH SCHELER¹ — ¹Leibniz Institute of Polymer Research Dresden, Germany — ²Borealis Polyolefine GmbH, Linz, Austria — ³Université d'Orléans, France

Incorporating layered double hydroxide (LDH), which belongs to a class of synthetic clays with layered geometry, into polymers can significantly improve the materials properties even at low filler concentration. Compatibility with a non-polar polymer matrix and expansion of interlayer space in LDH are achieved by intercalation of surfactant molecules, that, in fact, can strongly affect the crystal structure of aluminium hydroxide layers.[1, 2] In the present work the 27Al MAS and 27Al triple-quantum (3Q)-MAS NMR has been applied in order to monitor stepwise the structural changes as a result of surfactant modification of LDH and to quantitatively characterise the resulting structures.[3] Additional insight is gained from high-resolution solid-state 1H NMR, which gives detailed information on protons in the layered structure, on water and the surfactant. [1] F.R. Costa, A. Leuteritz, U. Wagenknecht, D. Jehnichen, L. Häußler, and G. Heinrich, Appl. Clay Sci. 38 (2008) 153. [2] J. Rocha, M. del Arco, V. Rives, and Ulibarri, M.A., J. Mater. Chem. 9 (1999) 2499. [3] A. Vyalikh, D. Massiot, U. Scheler, Magn. Reson. Chem. (submitted)

CPP 10: Polymer Physics I

Time: Monday 18:00–19:30

Location: ZEU 114

CPP 10.1 Mon 18:00 ZEU 114

Fabrication of Metallic/Bimetallic Microtubes using Self-rolled Polymer Tubes as Templates — ●KAMLESH KUMAR¹, BHANU NANDAN¹, VALERIY LUCHNIKOV², BHOJE GOWD¹, and MANFRED STAMM¹ — ¹Leibniz Institute of Polymer Research Dresden, Hohe Strasse 6, 01069 Dresden, Germany — ²Institute de Chimie des

Surfaces et Interfaces, rue Jean Starcky 15, 68057 Mulhouse, France.

We present a new approach to fabricate single and bimetallic (Au, Ti, and Au/Ti) microtubes with high aspect ratio using self-rolled polymer tubes as templates. This approach is based on the phenomenon of the stress relaxation of thin multi-layer films via curling. We explore self-rolling of a cross-linked polymer film, capped by metallic or bimetallic

layer, in an organic solvent. In a typical fabrication scheme, the multilayer consists of the bottom poly(4-vinylpyridine) (P4VP) film, the intermediate polystyrene (PS) film, and the top metallic or bimetallic film is used. The internal stress and the bending moment are induced in the film due to swelling of the bottom P4VP layer after dipping the sample into aqueous solution of dodecylbenzenesulfonic acid (DBSA). The length of the tubes and the direction of rolling are determined by mechanical patterning of the film, whereas the tube diameter is tailored by varying the thickness of the polymer and metallic layers. After rolling, polymer template is removed by pyrolysis resulting in pure metal microtubes. Metallic microtubes fabricated by self-rolling approach may find applications in such fields as IR-waveguiding, microfluidics, enzyme bi-reaction, chemical and biochemical sensing.

CPP 10.2 Mon 18:15 ZEU 114

Molecular acoustic studies around the boundary between network-forming reactive liquids — ●ROLAND SANCTUARY, MARTINE PHILIPP, JÖRG BALLER, BARTOSZ ZIELINSKI, ULRICH MÜLLER, and JAN KRISTIAN KRÜGER — Université du Luxembourg, Laboratory of Physics of Condensed Matter and Advanced Materials (LPM), 162a, avenue de la Faïencerie, L-1511 Luxembourg

Scanning Brillouin microscopy is used to investigate chemical reactions and molecular transport processes around the interface between the layered reactive constituents of epoxies. The temporal evolution of the spatial hypersonic landscape behaves significantly asymmetric along the resin and hardener rich region and is attributed to a complicated superposition of polymerization, transport, dissolution and molecular disintegration phenomena. The temporal and spatial distributions of the sound velocity in the hardener and resin rich zones of the samples seem to show chaotic behavior. If in addition alumina nanoparticles are initially present in the resin, interfacial polymerization changes its character in comparison to the system involving the pure resin. According to the hypersonic behavior the penetration of the hardener in the filled resin seems to be hindered by the presence of the nanoparticles. In turn, once the alumina nanoparticles have entered the hardener rich region, they seem to develop a catalytic influence on the epoxy polymerization.

CPP 10.3 Mon 18:30 ZEU 114

Particle-Related Microstructural Investigations of Polymer-Nanoparticle Composites using Scanning Electron Microscopy (SEM) and Stereology — ●MARKUS ZIEHMER, ULRICH MÜLLER, JÖRG BALLER, and ROLAND SANCTUARY — University of Luxembourg, Physics of Condensed Matter and Advanced Materials, 162a, Avenue de la Faïencerie, L-1511 Luxembourg

Epoxy polymers containing nanoparticle fillers represent just one of the manifold possibilities of constructing nanocomposite systems which have achieved great scientific and technical interest during the last decade. A lot of work has been done in order to understand the macroscopic physical properties of such functional materials. At a certain step, knowledge about the particle-related microstructure is indispensable. Thus, suitable microscopic techniques are necessary. Usually, solely Transmission Electron Microscopy (TEM) and Atomic Force Microscopy (AFM) are performed, although both methods show some well-known intrinsic shortcomings. Modern SEM has the means to overcome these problems and can fill the information gap between TEM and AFM measurements, even for difficult materials like polymer-nanoparticle mixtures. Low-voltage SEM provides the opportunity to sample rather thin surface layers. The particles can easily be identified. Established stereological methods can be used to calculate more reliable interparticle distances and to look at the spatial particle distributions. We report about first experiments and results performed on DGEBA/DETA systems filled with different contents of alumina and silica nanoparticles.

CPP 10.4 Mon 18:45 ZEU 114

Curing of epoxy-based nanocomposites: Influence of the

nanoparticles and their surface coating — ●JÖRG BALLER, MARKUS ZIEHMER, MATTHIEU THOMASSEY, BARTOSZ ZIELINSKI, MARTINE PHILIPP, ULRICH MÜLLER, JAN KRISTIAN KRÜGER, and ROLAND SANCTUARY — Université du Luxembourg, Laboratory of Physics of Condensed Matter and Advanced Materials (LPM), 162a, avenue de la Faïencerie, L-1511 Luxembourg

Interaction between inorganic filler particles and polymer matrix in epoxy-based nanocomposites mainly takes place at the giant surface of the nanoparticles. Often these surfaces are coated with a hydrophobic layer e.g. to avoid aggregation of nanoparticles. This coating can dominate the interaction between polymer matrix and dispersed nanoparticles. There are quite a lot of possible interactions imaginable. They range from chemical interactions like catalysis of the epoxy curing by the nanoparticles to physical interactions which may e.g. influence the thermodynamic miscibility of different components constituting the epoxy network. Comparing nanocomposites with coated silica and uncoated alumina particles delivers insight into the manifoldness of possible interactions. Thermal, rheological and spectroscopic methods are used to determine the evolution of physical properties before, during and after cure of epoxy nanocomposites.

CPP 10.5 Mon 19:00 ZEU 114

Shelf Life of one-component epoxy resin system studied by Positron Annihilation Lifetime Spectroscopy — ●M. Q. SHAIKH¹, K. RAETZKE¹, F. FAUPEL¹, and P.-L. M. NOESKE² — ¹Institute for Materials Science, Chair for Multi-component Materials, Faculty of Engineering, Christian-Albrecht-University of Kiel, 24118 Kiel, Germany — ²Fraunhofer IFAM, 28349 Bremen, Germany.

One-component epoxy formulations consist of epoxy resin, hardener, filler and the accelerator. They are preferred for industrial applications, but unlike two-component epoxy resin systems they have a limited shelf-life. Positron annihilation lifetime spectroscopy (PALS) was used to study the curing behavior of epoxy resins of DGEBA with a hardener of dicyandiamide (DICY), from the initial viscous state of the formulation to the solid state of cured polymer. Several isothermal measurements were done in the temperature range from 50°C to 80°C. PALS parameters seem to correlate very well with the curing mechanism in the samples. Gelation was observed as an increase in the intensity of ortho-positronium (*o*-Ps) and a sharp decrease in the lifetime. Change of (*o*-Ps) lifetime was used as a measure for the degree of curing. Applying the Johnson-Mehl-Avrami-Kolmogorov approach under reasonable assumptions, these experimentally observed changes could be characterized by determining the growth exponent '*n*' and reaction constant '*k*'. Thus, we were able to extrapolate the shelf life of this particular one component epoxy formulation at room temperature. Acknowledgements. This work was supported by the BMBF (03X0026F 'Nanomodule').

CPP 10.6 Mon 19:15 ZEU 114

Interfacial Polarization and Field Induced Orientation in Self Assembled Nanostructured Soft Ion Conductors — ●PETER KOHN, KLAUS SCHRÖTER, and THOMAS THURN-ALBRECHT — Institut für Physik, Martin-Luther-Universität Halle-Wittenberg

We report about the effects of interfacial polarization in and upon a self assembled nanostructured ion conductor, consisting of an ordered, lamellar block copolymer with a Lithium salt dissolved selectively in one component. Impedance spectroscopy in combination with frequency dependent orientation experiments enable a quantitative analysis of ionic polarization and a direct demonstration of its aligning effect on the interfaces. The transition time from the fast dielectric to the slow ionic interfacial polarization is much longer than expected from classical Maxwell-Wagner-Sillars theory and attributed to the formation of diffuse double layers at the internal interfaces. The much stronger orientation effect of ionic as compared to dielectric polarization offers a new route to align microdomains and therewith the ion conducting paths of the polymer.

CPP 11: POSTERS Amphiphilic Systems

Time: Tuesday 14:00–16:30

Location: P3

CPP 11.1 Tue 14:00 P3

Micellization of PAO-PEO Diblock Copolymers — MICHAEL STRÖBL, ●GERALD JOHANNES SCHNEIDER, JÖRG STELLBRINK, JÜRGEN ALLGAIER, and DIETER RICHTER — Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich

If amphiphilic diblock copolymers are dissolved in aqueous solutions micelles may be formed. The dependency of the shape from the interfacial tension between micelle and solvent has not been understood to any great extent and thus the investigation is of great importance for basic research. Existing applications further enhance the interest. For example active pharmaceutical ingredients which can be imbedded within the micelles and then selectively released at a particular place in a human body open a broad field of applications.

In order to investigate the dependency of the shape from the surface tension poly(alkyleneoxide)-poly(ethyleneoxide)-blockcopolymers, which were only recently synthesized [1], are very suitable. In aqueous solutions these samples form micelles whereas the geometry depends on the surface tension, and therefore on the length of the hydrophobic alkyleneoxide-block. In our contribution findings of SANS experiments are presented. The results of the surface tension measurements are compared to existing theories.

[1] J. Allgaier, S. Willbold, T. H. Chang, *Macromolecules*, 40, 518-525, 2007.

CPP 11.2 Tue 14:00 P3

Multilamellare Vesikel untersucht mit Neutronenkleinwinkelstreuung — ●HENRICH FRIELINGHAUS — Jülich Centre for Neutron Science, Forschungszentrum Jülich GmbH, 85747 Garching, Germany

Es wurde ein Modell entwickelt, um die Kleinwinkelstreuung von Multilamellaren Vesikeln zu beschreiben. Bei den größten Längenskalen beschreibt das Guinier-Verhalten die Streuung. Ein erstes Potenzgesetz ist mit der Kompaktheit der Vesikel verknüpft. Für viele Schalen erscheint das Vesikel kompakter und ein Porod-Verhalten wird vorhergesagt, während für wenige Schalen die 2-dimensionale Struktur der Schalen dominiert. Alle Exponenten zwischen 2 und 4 sind im Prinzip möglich, so daß damit die Schalenzahl durch die Kompaktheit bestimmt werden kann. Bei noch kleineren Längenskalen wird ein Korrelationspeak vorhergesagt, der die regelmäßigen Abstände der Schalen beschreibt. Bei noch kleineren Längenskalen dominiert die 2-dimensionale Struktur der individuellen Schalen. Zudem wurden Fluktuationen der Schalenzentren betrachtet. Hierdurch wird der Korrelationspeak in Schärfe und Position verändert, und die Kompaktheit (bzw. deren Exponent) verringert. Dies liegt daran, daß mit diesen Fluktuationen die Struktur offener erscheint und der dominierende Schalenabstand wächst. Erste Ergebnisse zu Polymer-basierten Vesikeln werden vorgestellt.

CPP 11.3 Tue 14:00 P3

Structure, dynamics and kinetics of thermoresponsive block-copolymer gels — ●JOSEPH ADELSBERGER¹, ANDREAS MEIER-KOLL¹, WEINAN WANG¹, THOMAS HELLWEG², ACHILLE M. BIVIGOU KOUMBA³, ANDRÉ LASCHEWSKY³, PETER MÜLLER-BUSCHBAUM¹, and CHRISTINE M. PAPADAKIS¹ — ¹TU München, Physik-Department E13, Garching — ²Universität Bayreuth, Physikalische Chemie I — ³Universität Potsdam, Institut für Chemie

Thermoresponsive polymer gels display strong changes in volume when heated above the lower critical solution temperature (LCST). We investigate triblock copolymers consisting of two hydrophobic polystyrene (PS) end blocks and a hydrophilic poly-(N-isopropyl-acrylamide) (PNIPAM) middle block. In aqueous solution they form core-shell-micelles or micellar networks. The structure of the micelles and their correlation is determined using SANS and dynamic light scattering [1]. The micellar radius shows a sudden decrease at the LCST. Above the LCST the collapsed micelles form clusters. Water is released and the formerly hydrophilic shell shrinks. The results are compared to the ones of diblock copolymers [2]. Neutron spin-echo spectroscopy is used to study the segmental dynamics of the hydrophilic block. Below the LCST the averaged diffusion coefficient of the PNIPAM block is unchanged. Time resolved SANS allowed us to investigate the kinetics of structural changes induced by fast heating above the LCST.

[1] A. Jain, C. M. Papadakis et al., *Macromol. Symp.*, submitted

[2] K. Troll, C. M. Papadakis et al., *Colloid Polym. Sci.*, 286 (2008),

1079-1092

CPP 11.4 Tue 14:00 P3

Phase Separation Kinetics under Continuous Cooling: Shape matters — ●DORIS VOLLMER, MIKA KOBAYASHI, GUENTER AUERNHAMMER, and YUMINO HAYASE — MPI for Polymer Research, Mainz

The dynamics of phase separation strongly depends on the thermal protocol, for example, whether phase separation is induced by a single quench from a one-phase to a two-phase region, or slow continuous ramping. In the latter case, qualitatively new features can arise, like oscillations in the turbidity and the apparent heat capacity. Oscillatory phase separation has been observed in several systems, as different as microemulsions, polymer solutions, and even in binary mixtures of olive oil and methanol. Material exchange is achieved through the macroscopic interface between both coexisting phases. To investigate the effect of the interfacial area on the phase transition kinetics we modified the area per unit volume using samples of different geometry, i.e. cylindrical and dog-bone shaped cells. As a model system we studied the phase separation of microemulsions and methanol and hexane under continuous cooling. In the dog-bone shaped cells the oscillation period exceeds those in cylindrical ones at cooling rates of a few K/h. The different dependence on the cooling rate indicates that the phase separation kinetics is either determined by volume dominated nucleation (fast cooling) or interface induced droplet formation (slow cooling).

CPP 11.5 Tue 14:00 P3

Phase Separation Dynamics in (Pseudo)Binary Mixtures — ●EBIE M. SAM, GUENTER K. AUERNHAMMER, YUMINO HAYASE, and DORIS VOLLMER — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

We investigated the phase separation dynamics in a pseudo-binary mixture of C4E1 and water, doped with a few percent of decane. The system phase separates under heating, as it crosses the binodal. Cooling rates of 1-20 K/h were used. We used sample cells with a diameter of 15cm and a height of around 1 cm, resulting in an aspect ratio of approx 15. Video microscopy of scattered light was utilized to track the dynamics of the phase separation. A temperature gradient was induced, with the upper side hotter. Patterns, whose sizes are comparable to the cell-thickness, were observed just after the initial clouding. Due to the sign of the temperature gradient their origin cannot be attributed to the Rayleigh-Benard convection. Possibly these patterns could be formed by the latent heat during the droplet-formation in the system. This is sufficient to induce a convective flow. A similar explanation could be given to the patterns we observed in the methanol-hexane binary system, which phase separates under cooling.

CPP 11.6 Tue 14:00 P3

Collapse behavior of thermosensitive poly(2-oxazoline) copolymers — STEPHAN SALZINGER¹, STEPHAN HUBER¹, RAINER JORDAN¹, and ●CHRISTINE M. PAPADAKIS² — ¹TU München, Department Chemie, Garching — ²TU München, Physikdepartment E13, Garching

The poly(2-oxazoline) (POx) system offers the possibility to tune the water-solubility in a wide range. Moreover, using 2-isopropyl (iPr) or n-propyl (nPr) as a side group results in a thermo-sensitive polymer with a lower critical solution temperature (LCST). Along with a number of architectures (homo-, gradient or block copolymers), a large variety of polysoaps can be created [1].

We have investigated the LCST behavior of iPrOx or nPrOx homopolymers as well as their gradient copolymers with n-nonyl-2-oxazoline (NOx) in aqueous solution. The LCST and the molecular aggregation behavior were investigated using single molecule as well as ensemble characterization techniques (fluorescence correlation spectroscopy (FCS), turbidimetry and scattering techniques).

[1] R. Jordan, C. M. Papadakis, et al., *Colloid Polym. Sci.* **282**, 833 (2004); *Macromol. Chem. Phys.* **208**, 1402 (2007); *Colloid Polym. Sci.* **285**, 491 (2007); *Macromol. Chem. Phys.* **209**, 2248, (2008).

CPP 11.7 Tue 14:00 P3

Circular Dichroisms und Energietransfer bei molekularen Aggregaten — JAN RODEN¹, ●ALEXANDER EISFELD¹ und JOHN BRIGGS²

— ¹MPI-PKS Dresden, Finite Systems — ²Uni Freiburg, Theoretische Quantendynamik

Amphiphile Cyanin Farbstoffe können supramolekulare Aggregate bilden [1]. Unter Verwendung der CES-Näherung (Coherent Exciton Scattering [2]), können experimentelle Aggregat-Spektren mit sehr guter Übereinstimmung direkt aus dem gemessenen Monomer-Spektrum berechnet werden [3]. Es lassen sich die verschiedenen Linienformen des blauen verschobenen H-Bandes und des extrem schmalen, rot verschobenen J-Bandes auf einfache Weise erklären. Insbesondere erhalten wir den exponentiellen Abfall der langwelligen Flanke des J-Bandes (Urbach-Martienssen Regel) analytisch aus der Form des Monomer-Spektrums in diesem Energie-Bereich [4].

Neben der Absorption zeigt sich auch beim Circular Dichroismus eine gute Übereinstimmung zwischen Theorie und Experiment [4]. Des weiteren untersuchen wir den Einfluss von Vibrationen auf den Energietransfer in molekularen Aggregaten im Rahmen der CES Näherung. [1] S. Kirstein and S. Dähne, *Int. J. of Photoenergy* (2006), Article ID 20363

[2] J.S. Briggs, A. Herzenberg *J. Phys. B* 3, 1663 (1970)

[3] A. Eisfeld and J.S. Briggs, *Chem. Phys.* 324, 376 (2006)

[4] A. Eisfeld and J.S. Briggs, *Chem. Phys. Lett.* 446, 354 (2007)

[5] A. Eisfeld, R. Kniprath and J.S. Briggs, *J. Chem. Phys.* 126, 104904 (2007)

CPP 11.8 Tue 14:00 P3

Aggregation of cationic surfactants with different counterions in the presence of poly(methacrylic acid) — ●ALINA IOVESCU, DAN-FLORIN ANGHEL, SHUJI SAITO, ADRIANA BARAN, and GABRIELA STÎNGA — Department of Colloids, *Ilie Murgulescu* Institute of Physical Chemistry, Spl. Independentei 202, Bucharest, Romania

Counterions effect of a cationic surfactant upon its interaction with poly(methacrylic acid) (PMA) was investigated and compared with the analogous in poly(acrylic acid) (PAA) systems. Decylammonium (DeA+) with different counterions (Cl-, SCN-, acetate (Ac-) and butyrate (Bu-) were employed. The interaction critical concentrations, determined from surface tension measurements, were the critical aggregation concentration (cac or T1) at which the surfactants are abruptly

bound to the polymer chain in a micellar form (the primary aggregates), T2' at which the isolated primary aggregates on the polymer chain begin to contact with each other forming secondary aggregates, and T2 at which free micelles appear in equilibrium. For each counterion, T1 with PMA was higher than the respective T1 with PAA. In aqueous solution, PMA was compactly coiled up forming hydrophobic microdomains (HMD) in the chain. The surfactants were first bound to the HMD, and at T1 the free ones cooperatively formed primary aggregates on the other parts of PMA. Different from PAA systems, T1 with PMA was the sum of the surfactant amount bound to HMD and the ordinary cac. For both polymers, T1 raised in the order DeA-Ac < DeA-Bu < DeA-Cl < DeA-SCN, which was opposite to the order of the respective critical micellar concentration (cmc).

CPP 11.9 Tue 14:00 P3

Wetting and surface tension dynamics of aqueous anionic surfactant/cationic polyelectrolyte mixture — ●V. DUTSCHK¹, R. SLAVCHOV^{1,2}, B. RADOEV², G. PETZOLD¹, and B. BREITZKE³ — ¹Leibniz Institute of Polymer Research Dresden, Germany — ²Faculty of Chemistry, University of Sofia, Bulgaria — ³Sasol Germany GmbH

It is well-known that the interaction between polyelectrolyte and surfactant starts at very low concentrations, therefore basic research is often carried out for low concentrations of surfactant solutions below the cmc.

Differences in the wetting kinetics depend on adsorption mechanisms. Modifying the highly hydrophobic polymer surfaces with solutions and mixtures allowed the conclusion that hydrophilisation of highly hydrophobic polymer surfaces occurs if modifying them with positively charged surfactant-polyelectrolyte mixtures (depending on the concentration of the both components). If the surfaces were modified with negatively charged mixtures, no change in the wettability of the Parafilm surface were observed. An essential conclusion is that the degree of wettability of a highly hydrophobic polymer surface with aqueous surfactant solutions and their mixtures can be assessed from the measurements of dynamic surface tensions. The corresponding isotherms of the surface tension and the contact angle show almost the same shape if the measuring points are recorded in non-equilibrium state at the same time.

CPP 12: POSTERS Magnetic Soft Matter

Time: Tuesday 14:00–16:30

Location: P3

CPP 12.1 Tue 14:00 P3

Interaction between rotating anisotropic paramagnetic doublets at Oil-Water Interface and in the bulk — ●NEBOJŠA ČASIĆ¹, PIETRO TIERNÒ², and THOMAS FISCHER³ — ¹Institut für Experimentalphysik V, Universität Bayreuth, Bayreuth, Germany — ²Department de Química Física, Universitat de Barcelona, Barcelona, Spain — ³Institut für Experimentalphysik V, Universität Bayreuth, Bayreuth, Germany

Optical microscopy is employed for studying hydrodynamic interactions between rotating anisotropic paramagnetic doublets in the bulk and at the oil-water interface. Anisotropic rotors are formed by linking two paramagnetic colloidal particles with two complementary sequences of single stranded DNA. An external precessing magnetic field induces rotation of the doublet.

CPP 12.2 Tue 14:00 P3

Experiments on dynamics of transients in magnetic colloids — ●DMITRY BORIN and STEFAN ODENBACH — Technische Universität Dresden, Institute of Fluid Mechanics, Chair of Magnetofluidynamics, 01062 Dresden, Germany

The detailed understanding of the internal physical nature of slow relaxation phenomena in disordered materials is still not reached. Therefore the study of relaxation phenomena in magnetic suspensions of single-domain Brownian nanoparticles (ferrofluids) is highly interesting for the general theory of dynamical phenomena in complex and soft systems. As it is known from previous studies, some ferrofluids show a long time reaction to a stepwise change of shear stress at constant magnetic field strength, as well as to a stepwise change of magnetic field strength at constant shear rate. The goal of this work was to shed some light on this temporal behavior. We performed experiments on magnetite based ferrofluids with a small particle-particle

interaction parameter, as well as on cobalt based ferrofluids, containing particles which are large enough to form chain-like structures. The obtained results are compared with measurements performed on magnetorheological suspensions consisting of non-Brownian particles. This comparison enables a study of the fundamental role of the Brownian effects for the macroscopic rheological properties of such suspensions.

CPP 12.3 Tue 14:00 P3

Dynamics of rolling ferrofluidic drops propelled by a rotating magnetic field — ●FABIAN RITTEWEG, REINHARD RICHTER, and INGO REHBERG — Experimentalphysik V, Universität Bayreuth, D-95440 Bayreuth

We report on the controlled transport of drops of magnetic liquid, which are swimming on top of a non-magnetic liquid layer. A magnetic field which is rotating in a vertical plane creates a torque on the drop. Due to surface stresses within the immiscible liquid beneath, the drop is propelled forward. We measure the drop speed for different field amplitudes, field frequencies and drop volumes. The results are compared with simplifying theoretical models proposed by V. Sterr, *et al.*, *New J. Phys.*, 10, 063029 (2008), where also our first measurements can be found.

CPP 12.4 Tue 14:00 P3

Cross-calibration of MRX and micro-CT for analysis of tissue samples after magnetic drug targeting — ●HELENE RAHN¹, INGRID HILGER², LUTZ TRAHMS³, and STEFAN ODENBACH¹ — ¹Institute of Fluid Mechanics, TU Dresden — ²University Hospital Jena — ³Physikalisches Technische Bundesanstalt, Berlin

Magnetic Drug Targeting (MDT) and Magnetic Hyperthermia, using the strong influence of a magnetic field on ferrofluids, are being considered as local cancer treatments with the aim of reducing the side

effects occurring during conventional cancer methods. The success of MDT and MHT depends on the correct distribution of the iron oxide nanoparticles within the tumour. This distribution can be analyzed by the non-invasive methods X-Ray microcomputed tomography (micro-CT) and magnetorelaxometry (MRX). To enable semi-quantitative analysis of these samples, a calibration with phantoms consisting of magnetic nanoparticles embedded in agarose-gel has been performed. The iron concentrations have been determined by MRX and vary from 2,88 E-5 mg/ml for a dilution of 1:300000 to 8,51 mg/ml for a dilution of 1:3. The same samples have been analysed by micro-CT and the minimum concentrations of these iron particles that can be detected by both methods have been determined and represented in a calibration curve. Based on this cross-calibration of micro-CT and MRX any biological sample with an iron oxide concentration within the range from 0.864 mg/ml to 8.64 mg/ml can be analysed by both methods. From both techniques, that is, the concentration and the volume distribution of these nanoparticles will be presented.

CPP 12.5 Tue 14:00 P3

Column formation in magnetic granular matter — ●SEBASTIAN LEHMANN, INGO REHBERG, THOMAS FISCHER, and REINHARD RICHTER — Experimentalphysik V, Universität Bayreuth,

Inspired by the Rosensweig Instability occurring in magnetic fluids, we are investigating a related pattern forming mechanism in magnetic granular matter. A monolayer of magnetizable spheres rearranges itself to columns of spheres under increase of the magnetic field. The latter is created by a Helmholtz pair of coils. We measure the heights of the columns as a function of the applied field and compare it with different models, using the energy of the different configurations as a basis of the computation.

CPP 12.6 Tue 14:00 P3

COLLOIDAL MICROMOTORS — ●LARYSA BARABAN, CHRISTIAN KREIDLER, DENYS MAKAROV, PAUL LEIDERER, and ARTUR ERBE — Department of Physics, University of Konstanz, Universitätstrasse 10, Konstanz, D-78457, Germany

The interest in investigations of colloidal systems has been growing during the last years. This is mainly related to the flexibility of properties of the colloidal particles which allows their usage in life science, for instance, as drug delivery vehicles. Here we demonstrate that the system of magnetic capped colloids is the appropriate tool to realize the concept of the synthetic nano- and micro-engines. A long -range controlled movement of capped colloids, which is induced by a local catalytic reaction, is demonstrated. The application of a weak homogeneous magnetic field blocks processes of rotational diffusion, causing random changes of the direction of the driving force; it thus allows achieving directed motion of the particle on long scales. Therefore, these fully controlled artificial motors can be further developed to be used, for example, for the targeted delivery of micro-objects to the relevant places.

CPP 12.7 Tue 14:00 P3

Time-resolved X-ray microscopy of nanoparticle aggregates under oscillatory shear — ●GÜNTER K. AUERNHAMMER¹, KAI FAUTH^{2,3}, JINYU ZHAO¹, MARKUS WEIGAND², and DORIS VOLLMER¹ — ¹Max-Planck-Institut für Polymerforschung, Ackermannweg 10, 55128 Mainz — ²Max-Planck-Institut für Metallforschung, Heisenbergstrasse 3, 70569 Stuttgart — ³Experimentelle Physik 4, Physikalisches Institut, Am Hubland, 97074 Würzburg

X-ray microscopy is an imaging technique which allows for a spatial resolution below 35 nm. We used it to investigate shear-induced structural dynamics by inserting a piezo actuator-driven shear cell into the focal plane of a scanning transmission x-ray microscope (STXM). We investigate shear-induced reorganization of aggregates of 50 nm sized magnetite particles embedded in a polymer melt. Depending on the amplitude of the applied oscillatory shear, either the aggregates strongly move and reorganize (large amplitudes) or just slightly deform (low amplitudes). We correlated the deformations of the aggregates with their structure (as visible in the STXM) and the amplitude of the applied shear. Comparison of our results to experiments with nonmagnetic colloids is made.

CPP 12.8 Tue 14:00 P3

Structure formation in ferrofluid monolayers: theory and computer simulations — ●CHRISTIAN HOLM^{1,2,3}, JUAN CERDA^{1,2}, and SOFIA KANTOROVICH^{3,4} — ¹Universität Stuttgart, Institut für Computerphysik, 70569 Stuttgart, Germany — ²FIAS, Goethe-

University Frankfurt, Germany — ³MPI for Polymer Research, Mainz, Germany — ⁴Department of Mathematical Physics, Urals State University, Ekaterinburg, Russia

Ferrofluid particles are known to self-assemble into a variety of magnetic equilibrium structures which depend on several factors such as: system geometry, magnetic interactions, particle polydispersity, presence or absence of external fields, etc. The phase behaviour and microstructure of ferrofluid systems in reduced dimensions is not necessarily equivalent to that of 3D systems. In order to investigate the peculiarities brought by the 2D geometry into the aggregation processes in ferrofluids, a combination of density functional theory, and molecular dynamics (MD) simulations is presented. Long-range dipolar interactions in our monolayer simulations are computed using a recently developed dipolar-P3M-layer correction algorithm. In comparison to the traditional Ewald sum methods, this approach allows to handle larger systems. The microstructure formation and the behaviour of monodisperse and bidisperse ferrofluid monolayers are studied thoroughly, and a comparison between numerical simulations and DFT is presented.

CPP 12.9 Tue 14:00 P3

Effects of magnetic fields on ferrofluids in a Taylor Couette System — ●REINDE MATTHIAS — George Bähr Str. 3, 01062 Dresden

The magnetization of a ferrofluid in rest is describable by equations for the equilibrium magnetization. A flowing ferrofluid, yielding, due to shear gradients, a vorticity with directions perpendicular to a magnetic field, turns the magnetic dipoles out of magnetic field direction. The magnetization is now also dependent on the flow field. Hence, equations to describe the magnetization out of equilibrium are necessary. Since the different models for this purpose differ more or less, the adequate one has yet to be distinguished. By comparing experimental and simulation data of a model system, this goal might get achieved. As a model system, a Taylor-Couette apparatus with the fluid cell exposed to magnetic fields was chosen. Measurement data obtained by capturing the transition from circular Couette flow to Taylor vortex flow at different magnetic fields is compared to simulation data and presented.

CPP 12.10 Tue 14:00 P3

Thermomagnetic convection influenced by a parametric modulated magnetic field — ●HARALD ENGLER and STEFAN ODENBACH — Lehrstuhl für Magnetofluidynamik, Technische Universität Dresden, 01062 Dresden

Previous theoretical investigations on thermal convection have shown that the behaviour of the onset of convection where the characteristic of the heat flux changes from a conductive to a convective state depends on the frequency of the driving force. The implementation of an experimental setup to review the theoretical predictions fails due to the immense technical effort to provide a time-modulated driving force. A way out of these technical difficulties affords the fact that by applying an external magnetic field a magnetic force in ferrofluids arises which is able to drive a convective flow. The external magnetic field can thus be arranged to provide a time-dependent progress of the field strength leading to a time-modulated magnetic force. This kind of convection which is driven by the magnetic force is called thermomagnetic convection. The experiments have shown a shift in the onset of convection that means for certain ranges of the frequencies of the magnetic force the convection is stabilized or destabilized. The results of the experimental investigations as well as the experimental setup to indicate the onset of convection will be presented at the talk.

CPP 12.11 Tue 14:00 P3

Structure factor of the ferrofluid with chain aggregates. — ●ELENA PYANZINA¹, SOFIA KANTOROVICH^{1,2}, JUAN CERDA², and CHRISTIAN HOLM² — ¹Ural State University, Ekaterinburg, Russia — ²University of Stuttgart, Stuttgart, Germany

We analyze the structure factor of a ferrofluid with strong interparticle magnetic dipole-dipole interaction. Results on bidisperse model systems in the absence of an external magnetic field are presented. The theoretical calculations are based on the explicit construction of radial distribution functions from the chain distributions obtained via density functional minimization. Data obtained via molecular dynamics simulations for the same model are provided for the verification of our analytical calculations. The results of our study are compared to the experimental data from [L.M. Pop, S. Odenbach, J. Phys.: Cond. Mat. (2006)].

CPP 12.12 Tue 14:00 P3

Traveling-stripe forcing of a ferrofluid — ●THOMAS FRIEDRICH, REINHARD RICHTER, and INGO REHBERG — Experimentalphysik V, Universität Bayreuth, D-95440 Bayreuth

Transport of a ferrofluid has been achieved by rotating magnetic fields [1]. In contrast, we apply a smooth periodic spatiotemporal modulation of the magnetic induction to a shallow layer of magnetic liquid. In the subcritical regime of the Rosensweig instability [2], driven surface waves [3] occur. These surface waves cause a transport of ferrofluid, which is analysed by means of radioscopes. For supercritical magnetic field strengths, a frequency dependent pattern formation can be observed. The effect of locomotion and the structural transitions in the subcritical and the supercritical regime are studied. The results are compared to Refs.[4,5].

[1] R. Krauss, M. Liu, B. Reimann, R. Richter, I. Rehberg, Appl. Phys. Lett. **86** 024102-1 (2005)

[2] M. D. Cowley and R. E. Rosensweig, J. Fluid Mech. **30** 671 (1967)

[3] A. Beetz, C. Gollwitzer, R. Richter, I. Rehberg, J. Phys.: Condens. Matter **20** 204109 (2008)

[4] S. Rüdiger, E. M. Nicola, J. Casademunt, L. Kramer, Physics Reports **447** 73-111 (2007)

[5] K. Zimmermann, I. Zeidis, V.A. Naletova, V.A. Turkov, J. Magn. Mater. **268** 227 (2004)

CPP 12.13 Tue 14:00 P3

Locoregional Polymerization from Nano-Object Surfaces: A Kinetic Study — CELIN GÜRLER¹, ALEX BIAN², and ●ANNETTE SCHMIDT¹ — ¹Institut für Organische Chemie und Makromolekulare Chemie, Heinrich-Heine-Universität, Universitätsstr. 1, 40225 Düsseldorf, Germany — ²Department of Chemistry, University of Calgary, Alberta, Canada

The possibility to activate a chemical reaction locally in a confined environment by selective heating is of great potential and interest for the design of complex nanostructures. Our approach is to use the ability of dipolar nanoparticles to transform electromagnetic energy into thermal energy in order to activate a (surface-initiated) polymerization process predominantly on the particle-medium interface.[1] The particles investigated are cobalt-based nanoparticles, known to undergo heat dissipation by Brownian rotation upon irradiation in an AC field in the kHz range. In our work we directly compare kinetic data obtained by magnetic heating and conventional heating. Both data sets indicate a reaction rate of pseudo first order, while a significant faster conversion is obtained by using magnetic heating when compared to conventional heating at the same bulk temperature. We found significant differences in the architectures of the particles that suggest an impact of the heating mode on the morphology of the resulting materials and a reasonable control on the shell thickness by the field parameters in magnetically heated experiments.

CPP 13: POSTERS Polymer Physics

Time: Tuesday 14:00–16:30

Location: P3

CPP 13.1 Tue 14:00 P3

Automatic mapping of WAXS fiber patterns and its application: Crystallization mechanisms in polypropylene — ●NORBERT STRIBECK¹, ULRICH NÖCHEL¹, and SÉRGIO S. FUNARI² — ¹Universität Hamburg, Institut TMC, 20146 Hamburg, Germany — ²HASYLAB c/o DESY, 22603 Hamburg, Germany

In time-resolved WAXS studies thousands of patterns are recorded that must be mapped into reciprocal space and evaluated for structure evolution analysis. Crystallographers refine an approximation, but this takes time. The exact solution [1] for fiber orientation with respect to the detector plane is found. Then an automatic mapping and evaluation algorithm [2] is devised. For oriented polypropylene it returns weight crystallinities and crystallite sizes for two sets of crystallites that are differently oriented (c , a^*). The method is applied in a study of crystallization mechanisms by WAXS [3] and SAXS [4]. At shallow quench we observe (1) decomposition of the amorphous melt, (2) a nucleation regime of several minutes in which crystallinity stays below 1% (latency period), (3) a growth regime with rapid growth of crystallinity. Begin and length of the latency period are different for c - and a^* -set and vary as a function of undercooling.

[1] Stribeck Acta Cryst. (2009), doi:10.1107/S0108767308029772

[2] Stribeck *et al.* J. Appl. Cryst., submitted Sept 2008

[3] Stribeck *et al.*, Macromolecules, submitted Nov 2008

[4] Stribeck *et al.*, Macromolecules (2007), 40(13), 4535-4545

CPP 13.2 Tue 14:00 P3

Dipole moment dependent investigation of Surface Relief Grating formation on azobenzene polymer thin films — ●PADMANABH VEER¹, ULLRICH PIETSCH¹, PAUL ROCHON², and MARINA SAPHIANNIKOVA³ — ¹Department of Solid State Physics, University of Siegen, ENC, 57068, Siegen, Germany — ²Department of Physics, Royal Military College, Kingston, Ontario, Canada K7K5L0 — ³Leibniz Institute of Polymer Research, 01069, Dresden, Germany

The formation mechanism of surface relief gratings (SRGs) was studied in the context of dipole moment of the azobenzene material with respect to time and temperature dependent measurements. The orientation mechanism of chromophore as an initiative to the grating formation was studied insitu using continuous and pulse like exposure techniques at various temperatures upto the glass transition temperature (TG) of the respective polymer material. The results obtained for high dipole moment pDR1M and low dipole moment pMEA were compared in terms of the rate of the grating formation and related to the quantities as relaxation of the chromophores in the absence of

the inscribing light and induced stress due to the chromophore orientation. The parameters obtained from the simulation data can be well explained in the frame of the viscoplastic approach. The deformation caused by the light induced movement of the azopolymer chains has found to alter the mechanical properties of the polymer material.

CPP 13.3 Tue 14:00 P3

Dielectric Spectroscopy and Rheology on Different Poly(alkylene oxide)s — ●CHRISTINE GERSTL¹, GERALD JOHANNES SCHNEIDER¹, WIM PYCKHOUT-HINTZEN¹, JÜRGEN ALLGAIER¹, ANGEL ALEGRIA², JUAN COLMENERO^{2,3}, and DIETER RICHTER¹ — ¹Institut für Festkörperforschung, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — ²Centro de Fisica de Materiales, Apartado 1072, 20080 San Sebastian, Spain — ³Donostia International Physics Center, Apartado 1072, 20080 San Sebastian, Spain

Poly(alkylene oxide)s (PAOs) form a homologous series of type-A polymers with side groups of varying length. Since the PAOs poly(ethylene oxide) and poly(propylene oxide) are known for a long time and have been studied extensively, the higher homologues are ideally suited to probe the influence of side chains on the dynamics of a polymer.

We will present the results of dielectric and rheologic measurements on poly(butylene oxide), poly(hexylene oxide) and poly(octylene oxide), having side groups of $(\text{CH}_2)\text{CH}_3$, $(\text{CH}_2)_3\text{CH}_3$, and $(\text{CH}_2)_5\text{CH}_3$ respectively. The relaxation of the whole polymer chain as well as the segmental dynamics will be discussed in terms of different models and compared to existing results.

CPP 13.4 Tue 14:00 P3

Synthesis and characterization of metallopolymer nanocomposites based on PAN — ●MARAT BULATOV¹, ULLRICH PIETSCH², and TOBIAS PANZNER² — ¹Astrakhan State University, 414056 Astrakhan, Russia — ²Universität Siegen, 57072 Siegen, Germany

Conductive polymers are widely used in manufacturing of electrodes of various technical application and for use in micro- and nanoelectronics. Also the application of conductive polymers for data storage and photoconversion is very challenging. The aim of the present work is investigation and optimization of the preparation technology for composites based on polyacrylonitrile (PAN). In particular we have prepared nanocomposites of iron (Fe/PAN) and nickel (Ni/PAN). The samples have been produced by means of the infrared heating method with various Fe and Ni concentrations. Structural characterisation was performed by X-ray powder diffraction, X-ray fluorescence analysis, IR and Raman spectroscopy, as well as by synchrotron scattering and EXAFS techniques. It was observed that after synthesis the nickel

atoms have formed crystallized nanoclusters with a size smaller than 30 nm. After analysis of the IR-spectra and literature data we can assume that the iron atoms are distributed within the polymer matrix and most likely form iron polyacrylate (FePAcr). Finally the structure of nanocomposites is correlated to the magnetic properties of the obtained samples. Acknowledgement: M.Bulatov thanks DAAD for financial support.

CPP 13.5 Tue 14:00 P3

Light induced lattice expansion in azopolymer films — ●SEBASTIAN KRAMER, PADMANABH VEER, and ULLRICH PIETSCH — Department of Solid State Physics, University of Siegen, ENC, 57068, Siegen, Germany

Light induced lattice expansion of azopolymer films was observed under homogeneous illumination with polarized light of 514nm of about 1W. The polymer film made from pDR1M was irradiated parallel to the surface normal. The light induced deformation effects were probed using a low power He-Ne laser of wavelength ($\lambda=633\text{nm}$) at a fixed reflection angle of about 63 degree and recorded using a pair of photodiodes. Straight after switching the actinic light on the intensity of the probe laser shows a sudden jump followed by an oscillation behavior damped out as function of time. Evaluated in terms of Fresnel equations the sudden increase and the oscillations can be related to the change in the refractive index and an increase of film thickness under light illumination. Considering the Gaussian profile of the laser beam the evaluated increase in film thickness reaches a value of several 100nm in centre and decreases respectively towards the borders. The behavior can be explained in terms of light-induced visco-elastic flow.

CPP 13.6 Tue 14:00 P3

Quantitative analysis of block copolymer microdomain dynamics — ●CHRISTIAN RIESCH, EIKE-CHRISTIAN SPITZNER, and ROBERT MAGERLE — Chemische Physik, TU Chemnitz, D-09107 Chemnitz

Microdomain ordering in a thin film of a cylinder-forming diblock copolymer is observed during vapour annealing by in situ atomic force microscopy. The ordering process is observed with high temporal resolution of ~ 60 s/frame over several hours. The domain coarsening in the resulting image series is analysed using local and global measures of order. We compute orientation maps, local curvature and correlation lengths; furthermore the temporal evolution of individual defects is tracked. The experimental results are compared with the microdomain dynamics observed in cell dynamics simulations of a similar system. We investigate the influence of film thickness and polymer-substrate interactions.

CPP 13.7 Tue 14:00 P3

Micromechanics of thin films of elastomeric polypropylene — ●MECHTHILD FRANKE and ROBERT MAGERLE — Chemische Physik, TU Chemnitz, Chemnitz

Elastomeric polypropylene consists of lamellar crystals embedded in an amorphous matrix. The arrangement, distribution, and connectivity of these crystals are important factors which determine the mechanical properties of the polymer. We stretch $\sim 1 \mu\text{m}$ thick films stepwise up to 100% and observe the changes in shape, orientation, and morphology of crystalline regions in situ with scanning force microscopy. We find heterogeneous deformations on length scales smaller than $2 \mu\text{m}$. On larger length scales the deformation is homogeneous. Branching points of epitaxial grown branches on mother lamellae are very rigid and do not deform up to strains of $\sim 40\%$. Reversible bending of single lamellae is also observed. On stretching, some lamellae break into fragments which upon further stretching break into smaller, only 10 nm large, blocks. Less frequently, we observe strain induced melting and crystallization. Our setup allows for a number of novel experiments. For instance, cyclic loading could reveal processes on the nanometer scale leading to fatigue behavior of the specimen.

CPP 13.8 Tue 14:00 P3

Investigation of Laser Heating Effects on Polymerfilms — ●RALF ST. KAPPES^{1,2} and JOCHEN S. GUTMANN^{1,2} — ¹Joh.-Gutenberg University, Mainz, Germany — ²Max-Planck-Institute for Polymer Research, Mainz, Germany

With Laser heating it is possible to deposit large amounts of energy in short time scales to a small region and by that create far from equilibrium conditions. In that context, we applied a NIR-laser pulse of microsecond duration to a thin PS-Film, doped with a dye for energy

conversion, observing the spectrum of the thermal radiation. Therefore we built up an optical detection system using interference filters and a microsecond-gated camera as detector. By then fitting Planck law to the spectral curve we were able to obtain the temperature and could show that the peak temperature is in the order of 1000 K, with a non-linear dependence of the dye concentration. Furthermore with this approach it was possible to obtain a temperature-time-profile and investigate the behaviour of the thin film system under such extreme conditions.

CPP 13.9 Tue 14:00 P3

Dynamical properties of chain molecules in confinements and in variation of system properties: model of DNA segregation — ●RON DOCKHORN^{1,2} and JENS-UWE SOMMER^{1,2} — ¹Leibniz Institute of Polymer Research Dresden, D-01069 Dresden, Germany — ²Technische Universität Dresden, Institute for Theoretical Physics, D-01069 Dresden, Germany

Large chain molecules are studied and simulated in various conditions such as restricted geometries, interaction potential and solvent quality using the bond fluctuation method. How relaxation time, diffusion and segregation time are related due to strong confinements is analyzed and compared to scaling approaches. The investigations are also focused on the influence of topological constraints such as linear and circular polymers and excluded volume effect in confinements compared with theoretical predictions. The process of duplicating and segregating of chain molecules in cylindrical confinements is examined as a model of prokaryotic DNA during replication. Furthermore the model can be extended to study the influence of condensin, cohesin and topoisomerases in DNA condensation and segregation in eukaryotes.

CPP 13.10 Tue 14:00 P3

Mobility of single polymer chains in thin films by widefield fluorescence microscopy — ●BENTE MARID INGEBORG FLIER and ANDREAS ZUMBUSCH — Fachbereich Chemie, Universität Konstanz, D-78457 Konstanz

Thin polymer films with a thickness of several tens of nanometers are of high interest both for scientific and industrial applications. The adhesion and interdiffusion properties of such films are affected by the mobility of the polymer chains. In order to probe bulk-obscured heterogeneities in the chain mobility we use single molecule fluorescence techniques. For this purpose, single fluorescent molecules are covalently attached as labels to the end of a polymer chain and their motion is observed via fluorescence wide-field microscopy. We use two different approaches to investigate dynamical processes. Rotational diffusion of a fluorophor is observed by defocused imaging. Defocussing the sample under investigation leads to patterns in spatial distribution of the emitted photons which are specific for each orientation of the emission dipole. Analysing the orientational dynamics allows the analysis of rotational diffusion. Translational diffusion, by contrast, can be observed by determining the position of the fluorophors and analysing the trajectories by single particle tracking. We present results of investigations of the dependence of polymer chain mobility on chain length and temperature using both approaches.

CPP 13.11 Tue 14:00 P3

Quantitative analysis of energy dissipation processes during tapping mode atomic force microscopy of soft materials. — ●EIKE-CHRISTIAN SPITZNER, CHRISTIAN RIESCH, CHRISTIAN DIETZ, and ROBERT MAGERLE — Chemische Physik, TU Chemnitz, D-09107 Chemnitz

We aim for a better understanding of the energy dissipation processes during tapping mode atomic force microscopy of soft materials. As model systems we investigate thin films of polystyrene homopolymer and polystyrene-*block*-polybutadiene diblock copolymers. The mechanical properties of the specimen are varied by controlled swelling in chloroform vapor. With an atomic force microscope operated in tapping mode, the energy dissipated between tip and sample, as well as the tip indentation into the polymer film, are determined. Polystyrene and polybutadiene differ in the amount of dissipated energy as well as in the detailed shape of energy dissipation curves as function of amplitude set point. Possible energy dissipation processes causing these differences are discussed.

CPP 13.12 Tue 14:00 P3

Ion transport mechanisms in polymer electrolytes - a molecular dynamics simulation study — ●DIDDO DIDDENS^{1,2}, ANDREAS HEUER^{1,2}, and OLEG BORODIN³ — ¹Institut für physikalische Chemie,

Westfälische Wilhelms-Universität Münster, Corrensstraße 30, 48149 Münster, Germany — ²NRW Graduate School of Chemistry, Corrensstraße 36, 48149 Münster, Germany — ³Department of Materials Science and Engineering, 122 S. Central Campus Dr, Rm 304, University of Utah, Salt Lake City, Utah 84112-0560

Solid state polymer electrolytes based on poly(ethylene oxide) (PEO) and lithium salts have been intensely studied both experimentally and theoretically and are thus a prototype for technical applications such as batteries or fuel cells. The motion of the ions in such electrolytes is complex due to the amorphous polymer matrix and has not yet been fully understood. In contrast to ceramic ion conductors the host network is not immobile and also contributes to the net transport. We studied both intramolecular and intermolecular ion transport mechanisms by MD simulations of an electrolyte composed of PEO and LiTFSI. Special emphasis was placed on the transfer of ions between different PEO molecules, which is of fundamental relevance for the resulting macroscopic conductivity.

CPP 13.13 Tue 14:00 P3

Polymer phase diagram in ionic liquids — ●DANIELA FELL^{1,2} and JOCHEN S. GUTMANN^{1,2} — ¹University of Mainz, Germany — ²Max Planck Institute for Polymer Research, Mainz, Germany

We have developed a new, fast and simple method for recording polymer phase diagrams using a normal flatbed scanner. The synchronization of the scanner and a temperature control unit allows us to automatically heat our setup in well-defined steps and then automatically scan. In one measurement series we are able to examine up to 80 different polymer concentrations. With this setup we are detecting the change of the cloudiness of a polymer in an ionic liquid. The obtained pictures are automatically analysed and the results are transferred to a single phase diagram.

With the help of this fast and automated method we have recorded phase diagrams of polymethylmethacrylate (PMMA) of different molecular weights in the room-temperature ionic liquid 1-butyl-3-methylimidazolium hexafluorophosphate ([bmim][PF6]).

CPP 13.14 Tue 14:00 P3

Patterning of surface immobilized ATRP starter — ●SEBASTIAN G.J. EMMERLING and JOCHEN S. GUTMANN — Max Planck Institute for Polymer Research, Ackermannweg 10, D-55128 Mainz, Germany

Patterning of silanes on silicon surfaces by photolithography or electron beam lithography has become a routine technique. Photolithography however involves several steps and therefore can be time-consuming, as it is the case in electron beam lithography. In contrast to this, we have developed a method to pattern an ATRP-starter that is immobilized on a silicon surface via a silane group with the use of an inject-printer. Since the ATRP-starter (4-(Chlorodimethylsilyl)-2-methylbutan-2-yl 2-bromo-2-methylpropanoate) contains a hydrolytically labile bromoester functionality, we printed sulphuric acid to cleave the molecule at this point. The remains on the surface then contain no longer a bromo-functionality and thus are inactive in ATRP. Subsequently PMMA brushes grew then selectively in the areas, which had not been in contact with sulphuric acid. Imaging ellipsometry allowed to measure site specific the film thickness. Depending on the concentration of the plotted sulphuric acid, we were able to tune the density of starter molecules in the plotted region. Given that in ATRP all chains grow to the same length, the density determines the thickness of the produced polymer film, which we were able to observe. The advantage of this technique is that large areas can be patterned quickly in just one step, while the smallest features generated thus far were single droplets the size of 100 to 200 micrometer.

CPP 13.15 Tue 14:00 P3

Quantum dot synthesis on thin polymer films — ●JANNIS OCHSMANN^{1,2} and JOCHEN GUTMANN^{1,2} — ¹Max-Planck Institute für Polymerforschung, 55128 Mainz, Germany — ²Universität Mainz, 55099 Mainz, Deutschland

Thin polymer films of asymmetric diblock copolymer of polystyrene and poly(ethylene oxide), PS-b-PEO, were spin-coated on glass substrate. The conditions were optimised to obtain cylindrical PEO microdomains normal to the surface. The obtained PEO domains were swollen by immersing the copolymer film in an acidic thioacetamide solution. Heating the film induces a hydrolysis reaction of the thioacetamide and S²⁻ ions were obtained inside the PEO microdomains. By this means, we created a localized S²⁻ ions source in the film. Immersing the swollen film into a solution of CdCl₂, leads to an reaction

between the S²⁻ ions and the Cd²⁺ ions at the film/water interface to form CdS quantum dots. The effect of the concentration of thioacetamide, CdCl₂, the temperature and pH is investigated with AFM, X-ray reflectivity and UV/Vis spectroscopy.

1Kim, D. H., S. H. Kim, et al. (2004) Nano Letters 4(10): 1841-1844

CPP 13.16 Tue 14:00 P3

Structure-property relationship in minor ampullate spider silk as studied by combined mechanical and time-resolved polarized FTIR spectroscopy — ●ROXANA-GIORGIANA ENE, PERIKLIS PAPADOPOULOS, and FRIEDRICH KREMER — Institut für Experimentelle Physik I, Leipzig, Germany

Simultaneous FTIR and mechanical measurements are employed in order to explore the relation between macroscopic and microscopic properties, in spider silk[1]. Minor ampullate has been studied because although its chemical structure is similar with major ampullate, their mechanical properties differ considerably[2]. The way the different nanocrystalline building blocks are interconnected is investigated by stretching the sample. Mechanical studies on minor ampullate silk show that the stiff crystalline domains are connected in series with the amorphous chains and that the mechanical field inside the fiber is uniform[3]. The results reveal oriented crystals interconnected by prestrained chains. It is shown that minor ampullate can be described by the same model[2] as for major. The prestress is significantly lower, explaining the lower modulus, while the toughness is similar. References: [1]P.Papadopoulos, J.Sölter, F.Kremer;Eur.Phys.J.E:Soft Matter 24,193(2007) [2]P.Papadopoulos, J.Sölter, F.Kremer;in press Colloid Polym.Sci(2008) [3]P.Papadopoulos, R.G.Ene, I.Weidner, F.Kremer (in preparation)

CPP 13.17 Tue 14:00 P3

Polymer blends and diblock copolymer melts in external electric fields — ●ILJA GUNKEL¹ and SEMJON STEPANOW² — ¹Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle, Germany — ²Martin-Luther-Universität Halle-Wittenberg, Institut für Physik, 06099 Halle, Germany

We generalize the statistical mechanical description of low molecular liquid systems in external electric fields in the E-ensemble at constant potential [1] to polymer blends and diblock copolymer melts. The anisotropic part of the segment polarizability results in a change of the polymer shape from a Gaussian coil to an ellipsoid. The effective binary interactions between the segments, which we have calculated to the quadratic order in the segment polarizabilities, are attractive in the ensemble at fixed potential, and result in an upward shift of the critical temperature in phase transitions in these systems. We have generalized the Flory-Huggins free energy for polymer blends in an electric field in both the E- and the E0-ensembles (constant charges). The collective structure factor for diblock copolymer melts is computed by taking into account the anisotropic parts of the segment polarizabilities as well as the effective binary interactions. We also computed the dielectric permittivity of the diblock copolymer melt in the vicinity of the order-disorder transition. The results of the statistical mechanical treatment of diblock copolymer melts are compared with the existing phenomenological approaches for these systems.

[1] S. Stepanow and T. Thurn-Albrecht, submitted, preprint <http://arxiv.org/abs/0810.1881>

CPP 13.18 Tue 14:00 P3

Adsorption of nano-particles on polymer brushes — ●HUILAN ZHANG¹, HOLGER MERLITZ², and JENS-UWE SOMMER¹ — ¹Leibniz-Instituts für Polymerforschung Dresden, Germany — ²Department of Physics, Xiamen University, Xiamen, PRC

We investigate the interaction of nano-particles with polymer brush using molecular dynamics simulations. The adsorption properties of particles and the equilibrium structure of the polymer brush (thickness, monomer density profile, distribution of end monomers) are studied at different grafting densities and temperatures. A stretch-collapse transition is found for the particle-brush complex at a threshold temperature T_0 , depending on the particle size and grafting density. At high temperatures, above T_0 , due to the dominant excluded volume effect the brush will stretch out and increase the coverage of the particles inside the brush by decreasing the temperature. For temperatures lower than T_0 , the increasing contacts between the particles and monomers will drive the brush into a compact brush-particle complex. We found a maximum particle number trapped in the brush and a maximum loading capacity of the brush for a given brush-particle configuration. Additionally, the influence of particle size and chain length of polymer

on the behavior of the brush-particle complex has been studied.

CPP 13.19 Tue 14:00 P3

Infrared Transition Moment Orientational Analysis on Liquid Single Crystal Nematic Elastomers — ●WILHELM KOSSACK¹, PERIKLIS PAPADOPOULOS¹, FELICITAS BRÖMMEL², HEINO FINKELMANN², and FRIEDRICH KREMER¹ — ¹Universität Leipzig, Institut für Experimentelle Physik I, Linnéstr. 5, 04103 Leipzig — ²Albert-Ludwigs-Universität Freiburg, Institute for Makromolecular Chemistry, Stefan Meier-Str. 31, 79104 Freiburg

Liquid *Single* Crystal Nematic Elastomers (LSCNE) form a novel class of materials combining the properties of liquid crystals with elastomeric networks and in which the crystalline order is extended to and stabilized on a macroscopic scale ($\sim\text{cm}^2$). In order to determine mean orientation and molecular order parameter of the different molecular moieties (mesogen, polymer backbone, etc.) IR-Transition Moment Orientational Analysis (IR-TMOA) is employed. This technique takes advantage from the specificity of the IR spectral range. Based on the measurements of the transmission dependence of polarization and an intentionally adjusted inclination of the sample numerical analysis of Fresnel-equations enables one to determine separately real *and* imaginary part of the refractive index n^* . From that mean orientation and molecular order parameter of the molecular moieties, represented by different absorption bands, are deduced. As further refinement the sample can be mechanically stretched during the IR measurements. By that the microscopic response to macroscopic excitation can be unraveled and phenomena like elastic memory effects and the phase relationships in reorientation of the molecular units can be traced.

CPP 13.20 Tue 14:00 P3

Temperature-resolved structures and kinetics of deswelling in PNIPAM hydrogels and solutions — ●ANDREAS MEIER-KOLL¹, ANASTASIA GOLOSOVA¹, JOSEPH ADELSBERGER¹, WEINAN WANG¹, PETER BUSCH², VITALIY PIPICH², CHRISTINE M. PAPADAKIS¹, and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik-Department E13, Garching — ²JCMS at FRM II, Garching

The deswelling behavior as well as its kinetics of highly concentrated aqueous poly(N-isopropylacrylamide) (PNIPAM) solutions are investigated with small angle neutron scattering (SANS) and are discussed in terms of spinodal decomposition. The phase transition is shown to be of second order. After a temperature jump from the swollen to the deswollen state, three different time regimes of the decomposition process are observed: In the early stage, small fluctuations of the density are reinforced by the negative curvature of the Gibbs free energy, which lead to a negative diffusion coefficient and an exponential increase of the scattering intensity. Within this time, well-defined interfaces between both species are formed. The corresponding strong forward scattering can be described by a Porod behavior. The coarsening in the intermediate and late stage manifests itself in a decrease of the forward scattering intensity which follows a power law behavior with an exponent below 1 in the intermediate, whereas an unusual exponent above 1 is observed in the late stage.

CPP 13.21 Tue 14:00 P3

ESPresSo++ - Extensible Simulation Package for Research on Soft Matter Systems — ●AXEL ARNOLD¹, THOMAS BRANDES¹, DIRK REITH¹, ANTON SCHÜLLER¹, JONATHAN HALVERSON², OLAF LENZ², and TORSTEN STÜHN² — ¹Fraunhofer institute SCAI, St. Augustin, Germany — ²MPI for polymer research, Mainz, Germany

We present the simulation package ESPresSo and its successor, ESPresSo++, which is currently under development. ESPresSo is designed to be an extensible and flexible tool to perform Molecular dynamics studies on coarse grained soft matter models in a parallel environment. Being developed by the MPI for polymer research in collaboration with the Fraunhofer institute SCAI, the software is particularly suited for polymer systems, but has also been successfully applied to other systems such as colloids or lipid membranes.

Its particular strengths are a flexible script interface, state-of-art algorithms for the calculation of interactions and an extensive set of more than 30 analysis routines. Included algorithms are e.g. RATTLE for constraints, P3M, ELC, MMM1/2D for electrostatics in partially periodic boundary conditions, or Lattice-Boltzmann for hydrodynamics. New interactions can be easily added even by unexperienced users due to simple interfaces, providing an easy to use platform to implement and test new algorithms. Nevertheless, the code is parallelized and has been shown to run on up to 1024 processors.

ESPresSo is maintained as an open-source project, and is

used by many users world-wide. For further information, see <http://www.espresso.mpg.de>.

CPP 13.22 Tue 14:00 P3

MD Simulations of Sheared Polymer Brushes with Explicit Solvent — ●ANDRE GALUSCHKO, TORSTEN KREER, and JÖRG BASCHNAGEL — Institut Charles Sadron CNRS, 23, rue du Loess, 67034 Strasbourg Cedex 2, France

Polymer brushes play an important role as lubricants in many technical applications, e.g. in hard disk drives or artificial joints[1]. They are furthermore believed to be crucial for minimizing friction between synovial joints[2], such as human knees or hips.

Using Molecular Dynamics simulations of a standard coarse grained model we study the lubrication properties of short chain polymer brushes. We extend further approaches (see, e.g.[3,4,5]), which have been performed without explicit solvent, to new simulations, where we now account for hydrodynamic interactions via including solvent molecules. We investigate the static properties of compressed brushes, and study the response of these systems to stationary and non-stationary external shear. This is done under variation of the molecular parameters, i.e. grafting density and chain length.

We compare our simulation results with the same model without explicit solvent. [1] T. Moro, Y. Takatori, K. Ishihara, et al., *Nat. Mater.* **3**, 829 (2004). [2] J. Klein, *Proc. IMechE J* **220**, 691 (2006). [3] G.S. Grest, *Phys. Rev. Lett.* **76**, 4979 (1996). [4] P.S. Doyle, E.S.G. Shaqfeh, A.P. Gast, *Phys. Rev. Lett.* **78**, 1182 (1997). [5] T. Kreer, M.H. Müser, K. Binder, J. Klein, *Langmuir* **17**, 7804 (2001).

CPP 13.23 Tue 14:00 P3

Polymer-grafted silica nanoparticles: a structural characterization in solution and bulk — ●MATHIAS MEYER¹, EIKE HÜBNER¹, WIM PYCKHOUT-HINTZEN¹, JÜRGEN ALLGAIER¹, JÖRG STELLBRINK¹, AUREL RADULESCU², DIETER RICHTER^{1,2}, and HORST WEISS³ — ¹Institut für Festkörperforschung, Forschungszentrum Jülich GmbH — ²Jülich Centre for Neutron Science, Forschungszentrum Jülich GmbH — ³BASF AG Ludwigshafen

In the framework of an EU FP7 propals with coordination by BASF, nanoparticles basing on organo-modified commercial silica particles of definite size are chemically grafted with PS and PB chains of different length and graft density. They serve as model filler and viscosity modifier if blended with linear matrices. In a combination of SANS, SAXS, DLS and rheology measurements we have characterized the silica nanoparticles with and without grafted polybutadiene and polystyrene in solution and in the blend. The focus of the investigation is on the radial density profile in the various combinations of graft density, chain length and type of the graft as well as the matrix being ideally short-chained i.e. solvent or of intermediate length compared to the grafts. The experiments take profit from the different scattering contrasts and partial labeling. Methods of synthesis i.e. grafting from and grafting to are compared.

CPP 13.24 Tue 14:00 P3

Surface plasmon assisted reversal switching nanolithography — ●TOBIAS KÖNIG and SVETLANA SANTER — Department of Microsystems Engineering (IMTEK), University of Freiburg

We have recently suggested that it should be possible to move or reposition strongly adsorbed nano-objects with relative ease, in large number and simultaneously. The essential idea is not to put more effort in fighting against the prevailing surface forces but rather to utilize them - in clear contrast to current techniques of nano-manipulation with atomic force microscopy (AFM) [S. Santer et. al, *Advanced Materials* **18**, (2006) 2359-2362]. Here we present photosensitive polymer thin films [T. Seki, *Chemical Society of Japan* **80**, (2007) 2084-2109] with integrated optically active elements which are supposed to support and steer the response of polymer films to external UV-illumination by acting as nano-scale antennas. For this, we are going to exploit the properties of surface plasmons excited within metal gratings during UV irradiation at a certain wavelength. The resulting intensity distribution leads to a corresponding change in topography that can be changed back to its initial state by irradiating with a different wavelength. In contrast to direct illumination with UV-interference patterns, the use of plasmon interference from metal gratings will allow to generate intensity variation and thus topographical structures below the diffraction limit. This opens up several new possibilities in the field of nano-manipulation discussed in this work.

CPP 13.25 Tue 14:00 P3

Multistage switching in bent-core smectic liquid crystal: Experiment and theory — ●STEPHAN STERN, ALEXEY EREMIN, and RALF STANNARIUS — Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, D-39106 Magdeburg

We describe a novel type of switching behavior in a series of homologous bent-core liquid crystal compounds in external dc electric fields. This kind of switching is distinguished by the occurrence of an intermediate field-induced ferroelectric state between an antiferroelectric ground state (off-state) and a ferroelectric on-state. Here we present the results of Second-Harmonic-Generation (SHG) experiments on those compounds, propose a structure for the ground state and the field induced states and develop a simple Ising-type model which can account for the unusual switching behaviour.

S. Findeisen et al., EPJ (2008)

CPP 13.26 Tue 14:00 P3

Toroidal Microcavities Produced by Self-Rolling of Strained Polymer Bilayer — ●KAMLESH KUMAR¹, VALERIY LUCHNIKOV², and MANFRED STAMM STAMM¹ — ¹Leibniz Institute of Polymer Research Dresden, Hohe Str. 6, 01069 Dresden, Germany — ²Institute de Chimie des Surfaces et Interfaces, rue Jean Starcky 15, 68057 Mulhouse, France.

We have demonstrated the fabrication of microtoroids by self-rolling of crosslinked thin strained bilayer polymer films, composed of polystyrene (PS)/poly (4-vinyl pyridine) (P4VP) and released in controllable manner from a solid substrate. The toroids formation proceeds from a circular opening in the film made by photolithography or by mechanical scratching followed by immersion of patterned sample in 2 wt % dodecylbenzene sulfonic acid solution (DBSA). DBSA forms supramolecular complexes with pyridine rings of P4VP and increases the specific volume of the polymer. Since the PS layer is neutral in this solution, bilayer film develops strain due to unequal swelling of polymers in solution of DBSA and hence the film bends and scrolls in order to minimize its free energy. The increasing radius of the toroid causes lateral strain in the film, such that the strain isolines are closed concentric circles centered at the middle of the lithographic window. Furthermore, the kinetics of toroid formation is also studied. The toroids with metallic inner surface are promising for the future research as IR-frequency range resonators.

[1] V. Luchnikov, K. Kumar, M. Stamm, J. Micromech. Microeng. 2008, 18, 035041

CPP 13.27 Tue 14:00 P3

Improving Long Range Order in Block Copolymer based Nanotemplates — ●MARCUS BÖHME, BHANU NANDAN, and MANFRED STAMM — Leibniz-Institut für Polymerforschung Dresden, Hohe Str. 6, 01069 Dresden

Thin films of block copolymers and block copolymer based supramolecular assemblies (SMA) are promising candidates for the generation of self assembled templates. One of the biggest challenges in such soft matter systems is the creation of nanostructures which are uniformly ordered on a large scale. In most cases the long range ordering in block copolymer based thin films is either not sufficient for possible applications e.g. in storage technology or can only be achieved with expensive and time-consuming pre-patterning methods (guided self assembly).

It has been shown, that an appropriate treatment with solvent vapours can improve the ordering in thin films of block copolymers[1] or SMA[2] at least on a scale of a few micrometers. We would like to present our recent results on the improvement of the solvent annealing process and the resulting effects on the long range order in thin films of Poly(styrene-*b*-4-vinyl pyridine) (PS-P4VP) as an example for block copolymer templates and thin films of PS-P4VP with 2-(4-Hydroxyphenylazo)benzoic acid (HABA) as an example of SMA templates. [1]G. Krausch et al., *Macromolecules* **33** (3), 947-953, 2000 [2]M. Stamm et al., *JACS* **125** (40), 12211-12216, 2003

CPP 13.28 Tue 14:00 P3

Molecular Dynamics Simulations of Bottle-Brush Copolymers with a Rigid Backbone under Poor Solvent Conditions — ●PANAGIOTIS E THEODORAKIS, WOLFGANG PAUL, and KURT BINDER — Institute for Physics, Johannes-Gutenberg University, Mainz, Germany

We have performed extensive Molecular Dynamics simulations for a bead-spring off-lattice model of flexible side chains tethered to a rigid backbone under poor solvent conditions. In particular, we study the static conformational properties of bottle-brush macromolecules by

varying parameters specific to this molecular architecture, i.e. the grafting density of the side chains and the backbone length. We also compute structure factors describing the scattering from a single side chain and the total bottle-brush polymer. These results are used for the interpretation of experimental scattering data for bottle-brush macromolecules. Furthermore, we examine the structure formation in co-polymer bottle-brushes under marginal to poor solvent conditions for the side chains.

CPP 13.29 Tue 14:00 P3

Structural relaxation process in epoxy nanocomposites as seen by mechanical and dielectric spectroscopy — ●MATTHIEU THOMASSEY, JÖRG BALLER, MARKUS ZIEHMER, BARTOSZ ZIELINSKI, MARTINE PHILIPP, ULRICH MÜLLER, JAN KRISTIAN KRÜGER, and ROLAND SANCTUARY — Université du Luxembourg, Laboratory of Physics of Condensed Matter and Advanced Materials (LPM), 162a, avenue de la Faïencerie, L-1511 Luxembourg

Epoxy resins based on diglycidyl ether of bisphenol A (DGEBA) are thermal glass formers with glass transition temperatures of about 250 K. Incorporation of inorganic nanoparticles into these oligomer matrices take influence on their thermal glass transition behaviour. Depending on the interaction between epoxy resin oligomers and nanoparticles the structural relaxation process which is made responsible for the glass transition can be changed. Mechanical and dielectric spectroscopy is used to study the structural relaxation process in two types of nanocomposites: DGEBA filled with silica and alumina nanoparticles. These investigations which are also supported by measurements of the complex specific heat capacity indirectly elucidate the molecular interaction between nanoparticles and oligomer matrix.

CPP 13.30 Tue 14:00 P3

Analysing dielectric interphases in composites containing nano- and micro- particles — ●BÉATRICE HALLOUET¹, PAULINE DESCLAUX¹, BERND WETZEL², ALOIS SCHLAR², and ROLF PELSTER¹ — ¹Universität des Saarlandes, FR 7.2 Experimentalphysik, D-66123 Saarbrücken, Germany — ²Institut für Verbundwerkstoffe GmbH (IVW), Erwin-Schrödinger-Straße Geb.58, D 67663 Kaiserslautern, Germany

We have investigated a molecular relaxation process in a solid polymer filled with dispersed magnetite particles. Especially, we compare systems containing nano-particles with diameters between 20 and 30 nm and micro-particles with diameters between 0.5 and 5 μm . Temperature-dependent broadband dielectric spectroscopy in a frequency range between 50 Hz and 1 GHz reveals that the presence of nano- or micro-particles does not affect the molecular dynamics. However, there is a marked difference in the polymers relaxation strength reflecting both the polarizability and the number of relaxing units. While in the micro-composites the polymer matrix behaves bulk-like, its relaxation strength increases in the nano-composites, the deviation from the bulk value being proportional to the volume fraction of particles. We discuss the results in terms of interphases of thickness δ around particles and agglomerates, the volume fraction of which increases with increasing particle concentration and decreasing particle size. Additional IR and DSC measurements are used to check whether the chemical properties or the amorphous state of the polymer matrix have been altered by the addition of particles.

CPP 13.31 Tue 14:00 P3

The influence of silica nano fillers on the structure and dynamics of linear polymer melts — KLAUS NUSSER^{1,2}, ●GERALD JOHANNES SCHNEIDER^{1,2}, WIM PYCKHOUT-HINTZEN¹, LUTZ WILLNER¹, and DIETER RICHTER¹ — ¹IFF, Forschungszentrum Jülich GmbH, Leo-Brandt-Str., 52425 Jülich — ²Jülich Centre for Neutron Science at FRM2, Lichtenbergstr. 1, 85747 Garching bei München

Elastomer-filler composite materials are technically very important and widely used. In particular, the reinforcing effect achieved by the addition of fillers like silica into a polymer matrix is commonly used to tune macroscopic properties like the elastic modulus of the composite material. In order to get new insight into the microscopic mechanisms of reinforcement, a blend material consisting of a linear polymer (Polyethylene-propylene, polyisoprene and polydimethylsiloxane) and hydrophobized silica was investigated. A study of the rheology of the material in dependence of the filler volume percentage was performed. Moreover Small Angle Neutron Scattering and Neutron Spin Echo experiments were performed in order to get insight into the microscopic structure and dynamics of the systems. In particular, the constraints on the polymer dynamics imposed by the presence of the silica particles

were investigated for different filler degrees.

CPP 13.32 Tue 14:00 P3

Nano two-point Microrheology: Structure and Dynamics of Polymer-melts near T_g — ●MARKUS SELMKE, SUBHASIS ADHIKARI, and FRANK CICHOS — Molecular Nanophotonics Group, University Leipzig

The structure of glassy polymer melts near their glass transition point has been controversially debated for a long time, and so are the numerous partly successful models suggested for such complex systems. A qualitatively proposed one, the view that cage-like structures form, i.e. soft cavities in-between interlocked stiff polymer-backbone arches, is one among others. To investigate the structure, molecular dynamics in the low M_w glass former glycerol have been studied by Orrit et. al. (2006), and rheological data has been found to agree with SM rotational relaxation times. Our group has not only extended this comparison to the complex high- M_w glass-former PMA, where such a match is far from being evident, but also compared the SM experiments to dielectric data that yields information on local flexibility and reorientation of the matrix the molecules are embedded in, confirming the expected difference in timescales due to different observable physical phenomena underlying the methods (Ngai, 1988). To further study polymer networks, the cross-correlated thermal motion of suitably chosen fluorescent tracer-dyes attached to the ends of bi-functionalized polymer strands is to be explored in the system with FRET on a nm-scale with the method of 2-point microrheology as introduced by (Crocker, 2000). This way, a 1/r-strain-field consistent correlation, or any deviation, is expected to shed light on the cage structure.

CPP 13.33 Tue 14:00 P3

Shapes of two dimensional star polymers — ●CHRISTIAN VON FERBER^{1,2}, YATES MONTEITH³, and MARVIN BISHOP³ —

CPP 14: POSTERS Nanoparticles

Time: Tuesday 14:00–16:30

Location: P3

CPP 14.1 Tue 14:00 P3

Energy Transfer on Molecular Aggregates — ●JAN RODEN¹, ALEXANDER EISFELD¹, and WALTER STRUNZ² — ¹MPI-PKS Dresden, Finite Systems — ²TU Dresden, Theoretische Quantenoptik

Since the discovery in the 1930's, molecular aggregates have attracted experimental and theoretical research, due to their unique linear and non-linear optical properties [1]. Furthermore they are possible candidates for artificial light harvesting units.

The properties of such molecular aggregates are strongly affected not only by static disorder, but also by internal vibrations of the constituting monomers, which couple strongly to electronic excitation [2]. To understand the optical properties and the energy transfer dynamics of molecular aggregates a theory has to properly take into account these effects.

Using a new approach based on a non Markovian Schrödinger equation [3] allows the non-perturbative treatment of internal vibrational modes of the monomers which are coupled to the surrounding. The comparison with results obtained by direct diagonalization of a model Hamiltonian containing one vibrational mode per monomer shows good agreement. The influence of vibrations to the energy transfer is discussed.

[1] T. Kobayashi, (ed.) J-Aggregates, World Scientific, 1996

[2] A. Eisfeld, J. S. Briggs, Chem. Phys. 324, (2006) 376

[3] T. Yu, L. Diosi, N. Gisin, W. Strunz, Phys. Rev. A. 60, (1999) 91

CPP 14.2 Tue 14:00 P3

About the active role of aluminum oxide nanoparticles on network formation in epoxy nanocomposite system: Influence of mixing sequence. — ●BARTOSZ ZIELINSKI, MARTINE PHILIPP, ULRICH MÜLLER, PIERRE-COLIN GERVAIS, ROLAND SANCTUARY, JÖRG BALLER, and JAN KRISTIAN KRÜGER — LPM, University of Luxembourg, Luxembourg

Many properties of polymer nanocomposites can be significantly improved by adding appropriate fillers like nanoparticles. The desired features of the polymer nanocomposites can be achieved by the properties of the nanoparticles themselves and/or by interactions between the polymer matrix and the particles. Due to chemical and/or physi-

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We explore the shapes of excluded volume, two dimensional star polymers by both renormalization group methods and Monte Carlo computer simulation of a tangent hard disk model. The mean-square radius of gyration, the g-ratio and the asphericity of linear and star polymers are examined. The standard expansion for the g-ratio is modified to use the known exact value of the radius of gyration exponent $\nu = 3/4$ rather than only the first order ϵ -expansion value. Good agreement is obtained with the current Monte Carlo Pivot algorithm results and previous simulations of other polymer models. Our approach also improves the predictions of the g-ratio in three dimensions significantly enhancing the accuracy of the renormalization group results for calculating shape properties.

CPP 13.34 Tue 14:00 P3

Characterization of flexible dendrimers by small-angle scattering — ●SABINE ROSENFELDT¹, MATTHIAS BALLAUFF¹, and LUDGER HARNAU² — ¹Physikalische Chemie I, Universität Bayreuth, Germany — ²MPI für Metallforschung, Universität Stuttgart, Germany

Solutions of flexible dendrimers are investigated up to volume fractions of 0.23, which is a value slightly over the overlap concentration of the dendrimers. Small-angle neutron scattering and contrast variation were used to determine the radial structure and the interparticular interactions. The experimental structure factors will be used to test the validity of the decoupling approximation of the total scattering intensity. The data were interpreted using the PRISM integral equation formalism. It is shown that the decoupling approach using the form factor of an undisturbed dendrimer is a good approximation, even for the data in the range of the overlap concentration.

cal interactions between the nanoparticles and the polymer matrix the properties of the composite are often more affected than predicted, as such interactions lead to the creation of an additional morphology called interphase. The formation of interphases is often in concurrence with the bulk polymerization process. In consequence the mixing sequence of the nanoparticles and the other constituents of the nanocomposite can already have a strong impact on the final properties.

It will be shown that by optical investigations already in the primary suspensions (resin/nanoparticles and hardener/nanoparticles) significantly different properties and therefore different interactions are present. As a matter of fact the different optical properties do not vanish but even increase in the course of polymerization. Accordingly the network formation has to be influenced by the interactions, too.

Refractometry was chosen as experimental technique.

CPP 14.3 Tue 14:00 P3

Photophysical studies of zinc porphyrin oligomers — ●ĘDRZEJ SZMYTKOWSKI^{1,2}, JONAS CONRADT¹, WOLFGANG LÖFFLER¹, TEODOR SILVIU BALABAN^{2,3}, MATTHIEU KOEPF⁴, JENNIFER WYTKO⁴, JEAN WEISS⁴, and HEINZ KALT^{1,2} — ¹Karlsruhe Institute of Technology (KIT), Universität Karlsruhe (TH), Institute of Applied Physics, Karlsruhe, Germany — ²Center for Functional Nanostructures (CFN), Karlsruhe, Germany — ³Karlsruhe Institute of Technology (KIT), Forschungszentrum Karlsruhe, Institute for Nanotechnology, Karlsruhe, Germany — ⁴Institut de Chimie, UMR 7177, Université Louis Pasteur, Strasbourg, France

The fabrication of novel multiporphyrinic arrays is important for the progress of molecular electronics and to mimic self-assembling chromophores in artificial light harvesting devices. We report on the time resolved photoluminescence studies of two novel phenanthroline strapped Zn-porphyrins having an imidazole pendant arm and C₁₂ or C₁₈ alkyl chains. The luminescence dynamics have been analyzed using decay associated spectra (DAS). The obtained results show the formation of well-ordered J-aggregates. Such self-assembled species have been recently directly observed for these porphyrins deposited on the mica surface by various nanoscopic techniques. No evidence of energy transfer from the phenanthroline strap to the zinc porphyrin has been found, a fact which can be explained by unfavourable Förster-

and Dexter-type energy transfer processes.

CPP 14.4 Tue 14:00 P3

Time resolved luminescence spectroscopy of self-assembling magnesium porphyrins — ●JĘDRZEJ SZMYTKOWSKI^{1,2}, JONAS CONRADT¹, CHILLA MALLA REDDY³, TEODOR SILVIU BALABAN^{2,3}, and HEINZ KALT^{1,2} — ¹Karlsruhe Institute of Technology (KIT), Universität Karlsruhe (TH), Institute of Applied Physics, Karlsruhe, Germany — ²Center for Functional Nanostructures (CFN), Karlsruhe, Germany — ³Karlsruhe Institute of Technology (KIT), Forschungszentrum Karlsruhe, Institute for Nanotechnology, Karlsruhe, Germany

Self-assembled porphyrins are promising materials to mimic natural bacteriochlorophylls (BChl) *c*, *d* or *e* encountered in the chlorosomes of photosynthetic bacteria. Such large assemblies of porphyrin metal complexes can be also used in hybrid solar cells as light harvesting antennas. In order to address their suitability we have studied the time resolved luminescence of novel magnesium diacetyl porphyrins. The decays of luminescence have been analyzed by a fitting procedure, which produces decay associated spectra (DAS). The analysis shows a short-lived component associated with the supramolecular architecture. This has implications for optimizing device geometries where the exciton diffusion lengths are not surpassed.

CPP 14.5 Tue 14:00 P3

Magnetische Eigenschaften Mn-dotierter CdSe/CdS-Halbleiternanopartikel bei thermischer Behandlung — ●ANDREAS HOFMANN¹, SHIH-HAO KUNG¹, CHRISTINA GRAF¹, KRISCHAN JELTSCH¹, CHRISTINE BOEGLIN² und ECKART RÜHL¹ — ¹Inst. f. Chemie u. Biochemie, Freie Universität Berlin, 14195 Berlin — ²Inst. de Physique et Chimie d. Matériaux de Strasbourg, 67034 Strasbourg

Mn-dotierte CdSe/CdS-Nanomischkristalle mit variabler Mn-Konzentration und einem Durchmesser von 2.9-3.8 nm wurden mit chemischen Hochtemperaturverfahren synthetisiert. Im Anschluss daran wurden die Partikel bei 210 °C für 48-72 h in Hexadecylamin getempert. Um die elektronische Struktur und die magnetischen Eigenschaften der Mn-Atome während dieser Erhitzungsphase näher zu untersuchen, wurden an den Partikeln magnetische Röntgenzirkulardichroismus-Messungen durchgeführt.[1] Dabei wurde untersucht, inwieweit hierbei eine Änderung des paramagnetischen Verhaltens erfolgt und ob eine lokale Mn-Se-Mn-Clusterbildung auftritt.[2] Die durchgeführten Messungen zeigen eine Änderung des Spinmoments nach dem Tempern infolge der veränderten lokalen Umgebung des Mn. Dabei konnte gezeigt werden, dass der Syntheseprozess den Temper-Effekt deutlich beeinflusst. Ein in Ref. [2] diskutierter Übergang des Mn vom paramagnetischen hin zum superparamagnetischen Verhalten konnte jedoch für diese Systeme ausgeschlossen werden, da keine oder nur eine unvollständige Clusterbildung stattfindet. [1] A. Hofmann et al. Chem. Phys. Chem. 8, 2008 (2007). [2] D. Magana et al. J. Am. Chem. Soc. 128, 293 (2006).

CPP 14.6 Tue 14:00 P3

Spectroscopic fingerprints of photodegrading CdSe/ZnS quantum dots — ●DANNY KOWERKO, JÖRG SCHUSTER, and CHRISTIAN VON BORCZYKOWSKI — Center of nanostructured materials and analytics, TU-Chemnitz, 09107 Chemnitz

Colloidal semiconductor nanocrystals have been under investigation for more than a decade with a growing field of applications in science and industry. However, photophysics and chemistry are still not fully understood, since crystal structure of core and shell as well as ligands may vary slightly between different charges, thus yielding individual optical properties even of single quantum dots from the same stock. We will discuss the role of surface (states) and its defined modification (e.g. by functionalized dye molecules) with special regard to nanocrystal degradation processes which are obviously accompanied by distinct spectral shifts and lifetime alterations. Besides time resolved ensemble studies in solution, we have chosen a multiparameter single particle approach, giving insight to spectral and luminescence lifetime fluctuations of individual quantum dots. Comparison of individual - on SiO₂ immobilized - untreated and modified species will provide a deeper insight towards the underlying mechanisms of surface manipulation induced photodegradation and thus allow for a correlation with the ensemble results.

CPP 14.7 Tue 14:00 P3

Sidewall functionalization of carbon nanotubes for preparation of nanocomposites — ●ANASTASIA GOLOSOVA^{1,2}, GERHARD RICHTER², ANDREAS TIMMANN³, RAINER JORDAN², and CHRISTINE

PAPADAKIS¹ — ¹TU München, Physikdepartment, Garching — ²TU München, Department Chemie, Garching — ³HASYLAB at DESY, Hamburg

In polymer nanocomposites, the nanometer size active fillers can change the material properties of polymer matrices within a wide range. Among others, carbon nanotubes (CNTs) are some of the most intriguing additives due to their unique mechanical, thermal, and electrical properties. However, until now the challenge of efficient incorporation and compatibilization of the CNTs with the surrounding matrix, which is crucial for the anticipated improved properties of the composite, is still unsolved.

To tune the surface properties of CNTs we extended a recently developed modification to form well-defined self-assembled monolayers from (bi)phenyl diazonium salt derivatives on carbon-based substrates to the sidewall modification of CNTs. Successful covalent functionalization of the nanotubes was confirmed by Raman spectroscopy and thermo-gravimetric analysis.

In order to investigate the dispersion ability of modified samples, we performed SAXS experiments (HASYLAB at DESY). Intensive scattering from big agglomerates of raw carbon nanotubes in deionized water was observed, while the dispersions of modified CNTs were homogeneous, which confirms better solubility of functionalized samples.

CPP 14.8 Tue 14:00 P3

Characterization of optical active nanostructures on silicon — ●THOMAS BAUMGÄRTEL, HARALD GRAAF, and CHRISTIAN VON BORCZYKOWSKI — Center of Nanostructured Materials and Analytics, TU Chemnitz, 09107 Chemnitz, Germany

Anchoring optically active molecules on nanostructured surfaces is a promising step towards building complex structures with variable properties and functions. Recently we could demonstrate that nanostructures on silicon surfaces can be functionalized in a neat way through selective binding of dye molecules and nanoparticles [1]. Here we report on the characterization of nanostructures on silicon that have been optically functionalized by binding of cationic dye molecules. The nanostructures were created by AFM-induced local anodic oxidation of dodecyl-terminated silicon. The two cationic dyes rhodamine 6G and cresyl violet have been selectively attached to nanostructures via electrostatic interactions and were studied using wide-field and confocal microscopy. The spectrum of the bound dyes indicates the existence of two different species of molecules: some of the molecules show the same spectral emission compared to dye molecules in solution, for other molecules there is a clear blue-shift of the emission wavelength. The bleaching behaviour of the dyes on to the structure follows a biexponential decrease pointing also towards two different species of bound dyes.

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

CPP 14.9 Tue 14:00 P3

Mechanical properties of self-assembled mesoscale fibers investigated by AFM bending experiments — ●DANIEL KLUGE¹, FRANK ABRAHAM², STEPHAN SCHMIDT¹, HANS-WERNER SCHMIDT², and ANDREAS FERY¹ — ¹Department of Physical Chemistry II, University of Bayreuth, Universitätsstraße 30, 95440 Bayreuth, Germany — ²Department of Macromolecular Chemistry I, University of Bayreuth, Universitätsstraße 30, 95440 Bayreuth, Germany

Fibers with diameters in the range of nm to μm have a large field of applications, mainly for tissue engineering and in composite materials. However, little is known about the mechanical properties of individual fibers on the mesoscale. We used AFM (atomic force microscopy) for force measurements in analogy to a macroscopic 3 point bending test to investigate self-assembled fiber-like structures of aromatic benzene trisamides. These had the ability to form remarkable hexagonal hollow cylinder morphologies. Our results suggest that their elastic modulus is comparable to semi-crystalline polymers. One special feature of our measurements was the usage of the force mapping mode of the AFM. This was a facile way to enhance the reliability of the measurements and collect significant amounts of data at the same time. The extensive data collection of our method marks a good starting point for future modeling and a thorough understanding of single-fiber deformation on the mesoscale.

CPP 14.10 Tue 14:00 P3

Molecular dynamics simulations of nucleation and growth of mixed FeCl₂/NaCl nanoparticles from supercritical water — ●NORBERT LÜMMEN and BJØRN KVAMME — University in Bergen, De-

partment of Physics and Technology, Allégaten 55, 5007 Bergen, Norway

Nanoparticle formation from single $\text{Fe}^{2+}/\text{Na}^+/\text{Cl}^-$ ions in water at supercritical conditions was investigated by molecular dynamics (MD) simulations [1]. Systems with 2048 H_2O rigid SPC/E water molecules and 120 Fe^{2+} ions, 240 Cl^- ions and additional either 24 or 72 Na^+/Cl^- ion pairs were simulated at various state points. The water-ion and ion-ion interaction was treated by a combination of Coulomb and Lennard-Jones potentials. The temperature was controlled by a heat bath thermostat using the Nosé-Hoover mechanism on the water molecules.

The method of Yasuoka and Matsumoto [2] and the Mean First Passage Time method [3] were compared for obtaining nucleation rates and critical cluster sizes from the simulation data. We found good agreement between these methods. The nucleation rates increased with increasing NaCl amount while the critical cluster sizes decreased. We also investigated properties of the growing clusters like size, composition, structure and shape and their dependence on the state conditions.

- [1] Lümmen, Kvamme, Phys. Chem. Chem. Phys. 10, 6405 (2008)
- [2] Yasuoka, Matsumoto, J. Chem. Phys. 109, 8451 (1998)
- [3] Wedekind et al., J. Chem. Phys. 126, 134103 (2007)

CPP 14.11 Tue 14:00 P3

Optically Detected Cyclic Voltammetry on Single Semiconductor Quantum Dots — ●ANGEL TOPALOV, NICOLE AMECKE, and FRANK CICHOS — Molecular Nanophotonics Group, Institute of Experimental Physics I, University Leipzig, Linnéstraße 5, 04103 Leipzig

An interesting and promising class of materials studied over the last years are semiconductor nanocrystals. Many applications seek to make use of their favorable fluorescence characteristics, like tunable emission wavelength, high quantum yield and photon statistics (antibunching). Additionally they show certain peculiarities like power-law blinking, lifetime-fluctuations and spectral diffusion which can be explained by charges close to or in the dot center leading to Auger processes (non-radiative energy transfer to those charges) and the quantum confined Stark effect. Those charges can arise from ejection of electron or hole via tunneling leaving behind the counterpart and additionally changing the matrix charge constellation. One of the main ideas is, thus, the development of an experimental method and setup for controlling those charges on the single particle level, starting with a determination of the specific ionization energy and electron affinity of different sizes of quantum dots. We then use confocal microscopy and cyclic voltammetry (CV) together, which gives us remarkable opportunities for experimental observations on the influences of charges on single crystal fluorescence.

CPP 14.12 Tue 14:00 P3

Absorption and energy transfer of quantum aggregates — ●JAN RODEN¹, WALTER STRUNZ², JOHN BRIGGS³, and ALEXANDER EISFELD¹ — ¹MPIPKS Dresden — ²TU Dresden, Theoretische Quantenoptik — ³Uni Freiburg, Theoretische Quantendynamik

The coupling of electronic excitation to vibrational degrees of freedom strongly influences characteristic properties of quantum aggregates (e.g. optical properties and energy transfer dynamics). We treat this exciton-phonon coupling using a non-Markovian stochastic Schrödinger equation [1]. Solving a Holstein-type model, we determine optical and transfer properties for exciton dynamics coupled to a realistic, complex phonon bath such that energy dissipation to the phonons is fully included. Our approach captures uniformly the transition from fully coherent to incoherent excitation transfer. As a specific

example demonstrating the capability of this approach, we investigate J-band and H-band spectra and energy transfer dynamics of mesoscopic molecular aggregates. The results are compared with that of the well established CES approximation (Coherent Exciton Scattering [2]) and the exact solution for the extreme case when the complex spectral density is replaced by that of a single harmonic oscillator.

- [1] T. Yu, L. Diosi, N. Gisin, W. Strunz, Phys. Rev. A. 60, (1999) 91
- [2] J.S. Briggs, A. Herzenberg J. Phys. B 3, 1663 (1970)

CPP 14.13 Tue 14:00 P3

Raman Spectroscopic Study of Plasma Functionalized Carbon Nanotubes (CNTs) — ●VERENA KATZENMAIER^{1,2}, JAKOB P. BARZ¹, NICOLAS P. ZSCHOERPER^{1,2}, MICHAEL HAUPT¹, UWE VOHRER¹, CHRISTIAN OEHR¹, and THOMAS HIRTH^{1,2} — ¹Fraunhoferinstitut Grenzflächen- und Bioverfahrenstechnik, 70569 Stuttgart — ²Institut Grenzflächenverfahrenstechnik, Universität Stuttgart

Raman spectroscopy is well known as a powerful tool for the characterization of carbon structures. In the case of CNTs, Raman spectroscopy provides a deep insight into their physical properties as well as the material quality. In resonance conditions, the Raman scattering process is strongly influenced by the electronic states of the system: in the case of single walled nanotubes, this is seen by e.g. the van Hove singularities.

In order to get a fundamental insight in structural properties and effects of chemical functionalization via low pressure plasma treatment, measurement conditions were varied in different ways: bulk material in the form of bucky papers was probed by a confocal system with three different excitation energies (e.g. 488 nm, 632.8 nm, 785 nm). In addition, the CNTs were measured with a tunable laser system in order to probe resonant scattering processes.

We focused on the low-frequency radial breathing mode for studying the nanotube diameter distribution of our samples as well as the conducting properties of the tubes.

CPP 14.14 Tue 14:00 P3

A universal relationship concerning the mechanical properties of amorphous materials: the generalized Cauchy relation — ●MARTINE PHILIPP¹, ULRICH MÜLLER¹, ROLAND SANCTUARY¹, PATRICK ALNOT², and JAN KRÜGER¹ — ¹LPM, University of Luxembourg, Luxembourg, Luxembourg — ²LPMIA, University of Nancy, Nancy, France

Classical Cauchy relations (CR) are known for crystals from solid state physics. They reduce the number of independent elastic moduli compared to that given by point symmetry. From the theoretical viewpoint such CR are not expected for amorphous materials. However, a linear relationship between the longitudinal and shear elastic moduli $c_{11}(x)$ and $c_{44}(x)$, called generalized CR (gCR) $c_{11}(x) = 3c_{44}(x) + A$ (x : driving parameter), was observed for many amorphous materials at high probe frequencies. The Cauchy parameter A is a constant for a given material. Recently it has been shown that the gCR with the same parameter A holds even true when varying consecutively different parameters x (like temperature, chemical conversion). This implies that the independency of the elastic moduli is strongly reduced for a given material.

In this presentation the combination of the two parameters chemical conversion and different amount of nanoparticles will be discussed for a reactive epoxy/silica nanocomposite. A new interpretation of the gCR and its parameter A will be given in terms of the local morphology of the considered material. All investigations were performed by Brillouin spectroscopy.

CPP 15: POSTERS Dynamics and Diffusion

Time: Tuesday 14:00–16:30

Location: P3

CPP 15.1 Tue 14:00 P3

Monte Carlo simulations of chain dynamics in crosslinked polymer networks — SORIN NEDELUCU and ●JENS-UWE SOMMER — Leibniz Institute of Polymer Research Dresden, Germany

We consider the reptation dynamics of freely diffusive long chains in monomodal, crosslinked polymer networks in a dry state, and then in a swollen state. The chain terminal relaxation time shows an increase with the network degree of swelling (Q), with an exponent of about

$0.37+/-0.1$, while the center of mass diffusion coefficient remains almost constant with Q . The monomer friction coefficient decreases with Q vary rapidly, with a coefficient of approximately -1.3, and this Q -dependence explains why the diffusion coefficient does not change. We also present a dynamical scaling theory to compare with our simulation results, and comparisons with de Gennes predictions for semi-dilute solutions. An important finding is that the number of entanglements that a chain can form seems to vary very little with the network de-

gree of swelling, which is explained by a nonaffine deformation of the network by swelling. The case of unentangled, short chains diffusing in the polymer network, and a comparison with long chain dynamics is briefly reviewed.

CPP 15.2 Tue 14:00 P3

On the diffusion of circular domains on a spherical vesicle — PIETRO TIERNO¹, PRAJNAPARAMITA DHAR², ZIAD KHATTARI³, ●SAEEDAH ALIASKARISOHI⁴, and THOMAS FISCHER⁴ — ¹Universitat de Barcelona — ²University of California Santa Barbara — ³Hashemite University, Zarqa, Jordan — ⁴University of Bayreuth

Tracking the motion of single, two or more lipid domains on a vesicle is a rheological technique allowing to measure surface shear viscosities of vesicular lipid phases. The ratio of surface to bulk viscosity defines a viscous length scale. Hydrodynamic interactions split the motion of the domains into different modes of diffusion. The measurability of surface shear viscosities from any mode of diffusion is limited to viscous length scales between the radius of the domains and the radius of the vesicle. The measurability of the surface shear viscosity results from the sensitivity of the diffusion to surface shear viscosities and from sufficient spatial resolution to resolve the diffusive motion. Switching between the various modes of diffusion is a trade between sensitivity gained and resolution lost by the hydrodynamic interactions leaving the measurability unchanged. Measurability drops with the number of domains making single-domain rheology the best technique to measure surface shear viscosities. Ultimately confinement of the domains to small vesicles renders measurements of surface rheological properties with domain tracking rheology impossible. Our results suggest that recent experiments on the diffusion of domains on liquid ordered vesicles need to be reanalyzed.

CPP 15.3 Tue 14:00 P3

Precise determination of the mutual diffusion and Soret coefficient by a laser beam deflection technique — ●ANDREAS KÖNIGER, BÖRN MEIER, and WERNER KÖHLER — Physikalisches Institut, Universität Bayreuth

We have built a diffusion cell with optical beam deflection readout to measure the mutual diffusion and Soret coefficients in binary liquid mixtures, following a design suggested by Piazza [1]. Utilizing a fiber coupled laser with a very short coherence length, a particularly precise determination of the transport coefficients is possible by comparing the measured beam deflection signal to a numerical solution of the coupled heat and mass transport equations. The onset of convection can be suppressed both for heating from above and from below at least up to temperature differences of 2°C for ethanol-water mixtures.

We performed numerous tests to validate the measurement method and the procedure for data analysis. Measurements of three organic benchmark systems [2] consisting of tetralin, dodecane and isobutylbenzene and the system water-ethanol demonstrate compliance with existing literature values. In the case of ethanol-water, the concentration and temperature range could be expanded in comparison with data available in literature [3].

[1] Piazza R., *Phil. Mag.* 83, (2003) 2067

[2] Platten J., Bou-Ali M., Costesèque P., Dutrieux J., Köhler W., Leppla C., Wiegand S., Wittko G., *Phil. Mag.* 83, (2003) 1965

[3] Kolodner P., Williams H., Moe C., *J. Chem. Phys.* 88, (1988) 6512

CPP 15.4 Tue 14:00 P3

Study of order/disorder transitions in β -hydroquinone clathrates with ²H-NMR and dielectric spectroscopy — ●ANDRE NOWACZYK, CATALIN GAINARU, SEBASTIAN SCHILDMANN, BURKHARD GEIL, and ROLAND BÖHMER — Experimentelle Physik III, Fakultät für Physik, Technische Universität Dortmund

We are studying the behavior of the guest molecules in partly filled β -hydroquinone clathrates. If the cage occupation x is higher than a critical value x_c , these substances undergo an order/disorder transition at a composition dependent temperature. The advantage of these binary mixtures, when compared for example with plastic crystals, is their stable and well-defined crystal structure into which the guest molecules are embedded. We have grown crystals with acetonitrile or methanol as guest molecules for different occupation factors x . By applying a combination of deuterium nuclear magnetic resonance and dielectric spectroscopy we study the guest-guest interactions in dependence on the occupation factor x . Several ²H-NMR techniques were applied, comprising relaxation experiments as well as stimulated-echo measurements to gain information on different timescales.

CPP 15.5 Tue 14:00 P3

Water dynamics on the hydrate lattice of a tetra-butyl ammonium bromide semi-clathrate — ●SEBASTIAN SCHILDMANN, ANDRE NOWACZYK, BURKHARD GEIL, CATALIN GAINARU, and ROLAND BÖHMER — Experimentelle Physik III, Fakultät für Physik, Technische Universität Dortmund

Deuteron nuclear magnetic resonance (NMR) and dielectric spectroscopy are utilized to investigate the dynamics of the water molecules in the tetra-*n*-butyl ammonium bromide semi-clathrate (TBAB · 26H₂O). Semi-clathrates are nano-porous structures suitable for the encapsulation of small guest molecules which here are part of the water lattice. Stimulated-echo spectroscopy and dielectric measurements were employed and yielded the same distribution of correlation times corresponding to a mean activation energy of about 5165 K. Solid-echo spectra were acquired over a broad temperature range and compared with random-walk simulations. They exhibit an apparent two-phase character which is discussed in terms of various scenarios. Two-dimensional NMR spectra and four-time stimulated echoes were recorded, but an exchange between slow and fast reorienting molecules could not be detected. Spin-lattice relaxation does not directly reflect the local reorientational motion and its non-exponentiality is interpreted with reference to the translational dynamics of the water molecules. Estimated diffusion coefficients suggest that a translational step takes place after every 10th reorientational step. Replacing the bromide anion by fluoride the semi-clathrate TBAF · 32H₂O is investigated and compared with the former results.

CPP 15.6 Tue 14:00 P3

Para-hydrogen induced nuclear spin polarization at variable magnetic field — ●SERGEY KORCHAK¹, KONSTANTIN IVANOV², ALEXANDRA YURKOVSKAYA^{1,2}, and HANS-MARTIN VIETH¹ — ¹Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin — ²International Tomography Center, Institutskaya 3a, Novosibirsk, Russia

A way of boosting the sensitivity of NMR is exploiting hyperpolarization resulting from non-thermal population of the spin energy levels. A very efficient method is enriching the para-spin isomer of H₂ (PHIP) and subsequent transferring the polarization to target spins of choice. This has been applied in magnetic resonance imaging in biological studies. Both the PHIP effect and the polarization transfer vary strongly with an external magnetic field B . We will report a detailed experimental and theoretical study of this magnetic field dependence. As a model system polarized ethylbenzene formed by catalytical attachment of the para-H₂ molecule to styrene was measured at fields ranging from 0.1mT to 7T by use of a fast field-cycling technique. Theoretical simulations of the polarization pattern as a function of B assuming scalar spin-spin coupling to be responsible for the change reproduce the experimental data for this 5-spin system. Polarization transfer across several bonds from the primarily polarized aliphatic protons to the aromatic moiety of ethylbenzene was also observed. The optimal conditions for forming polarization and manipulating its transfer as well as the influence of spin-lattice relaxation will be discussed.

CPP 15.7 Tue 14:00 P3

From Monomers to Polymers: Correlated Segments in Diffusive Transport — ●DOMINIK STADELMAIER and WERNER KÖHLER — Universität Bayreuth, Physikalisches Institut

We have performed measurements on dilute polymer and alkane solutions to investigate the influence of the polymer stiffness on the Soret effect. The Soret effect (thermal diffusion) describes the mass flow in a binary system with a temperature gradient. In the high polymer limit the thermal diffusion coefficient is - contrary to the long-range hydrodynamic coupling in case of isothermal diffusion - independent of the polymer chain length. For polystyrene, thermal diffusion mainly depends on a factor proportional to the correlated segment size and on the solvent viscosity [1]. Measurements with the flexible polymers PDMS and polyethylen-oligomers however show that the solvent viscosity is no longer the only relevant solvent parameter for the Soret effect. Even a sign change is possible if the solvent viscosity is increased. For the measured alkane solutions D_T is always negative thus the alkane molecules are more thermophilic than the solvent. But the crossover from a small molecule to a molecule with polymer properties always takes place at a chain length that is approximately of the size of the Kuhn segment.

[1] Stadelmaier D., Köhler W., *Macromolecules* 41, (2008), 6205

CPP 15.8 Tue 14:00 P3

Brownian Motion of Colloid Particles in Thin Liquid Films — ●INES TRENKMANN, JÖRG SCHUSTER, and CHRISTIAN VON BORCZYKOWSKI — Chemnitz University of Technology, Institute of Physics, 09107 Chemnitz

The growing field of micro- and nanofluids requires an understanding of the role of solid liquid interactions in hydrodynamics.

It is well-known since some years that thin liquid films form layering structures near smooth surfaces and free interfaces [1]. Thereby it is apparent that the dynamical properties of these films differ from those of bulk liquids. Besides the altered film structure, interfaces enter into the hydrodynamics via the hydrodynamic boundary conditions (HBC). To investigate the alteration of the hydrodynamical features of the liquid films by reduction of the film thickness single-particle tracking is an sensitive method to observe chances in the individual diffusion motion of tracers [2].

We want to show recent measurements of the influence of film thickness on the diffusion behavior of colloid particles as tracers in thin films of a silicon grease. By variation of the tracer size or film thickness the influence of the HBC will be studied down to molecular thin films [3].

- [1] G. Evmenenko, et al.: *Langmuir* 17(2001) 4021
- [2] J. Schuster, et al.: *Eur. Polymer J.* 40(2004) 993
- [3] M. J. Saxton: *Biophys J.* 72 (1997) 1744

CPP 15.9 Tue 14:00 P3

Low Field NMR for Analysis of Heterogeneous Mixtures and Polymers under Stress — ●UTE BÖHME and ULRICH SCHELER — Leibniz-Institut für Polymerforschung Dresden, Hohe Str. 6, 01069 Dresden

Small and low-cost NMR systems based on permanent magnets provide an interesting alternative for NMR in materials characterization. They are used as fast, non-destructive tools for the routine analysis of food-stuffs, cosmetics and chemicals. They are of particular interest, when shift information is not required, i.e., when there is a priori knowledge about the system. NMR relaxation times provide a wealth of information on molecular mobility, they are influenced by the composition and treatment of the sample. Impacts like stress, heating or cooling change the molecular mobility. Extending the relaxation time measurements to two-dimensions significantly enhances the resolution of the components of the sample despite lack of chemical shift resolution. For our investigations we use an in-house built portable NMR system with Halbach magnets arrangement and a proton Larmor frequency of 32 MHz. Examples shown include the determination of the principal components of water- in- oil- emulsion and stretched polypropylene using T1-T2 correlation experiments at low field. Comparison to results obtained with high-field measurements confirm the results obtained.

CPP 15.10 Tue 14:00 P3

Charge transport and dynamic glass transition in imidazole-based liquids — ●CIPRIAN IACOB¹, JOSHUA RUME SANGORO¹, ANATOLI SERGHEI¹, SERGEJ NAUMOV¹, YASMIN KORTH², JÖRG KÄRGER¹, CHRISTIAN FRIEDRICH², and FRIEDERICH KREMER¹ — ¹Institute of Experimental Physics I, University of Leipzig, Linnéstr. 5, 04103 Leipzig, Germany — ²Freiburger Materialforschungszentrum (FMF) und Institute für Makromolekulare Chemie der Albert-Ludwigs Universität Freiburg i. Br., Germany

Broadband Dielectric Spectroscopy (BDS), differential scanning calorimetry, rheology and Pulsed Field Gradient - Nuclear Magnetic Resonance (PFG - NMR) are combined to study glassy dynamics and charge transport in a homologous series of imidazole-based liquids with systematic variation of the alkyl chain length. The dielectric spectra are interpreted in terms of dipolar relaxation and conductivity contribution. By applying Einstein, Einstein-Smoluchowski and Stokes-Einstein relations, translational diffusion coefficients - in quantitative agreement with PFG NMR measurements are obtained. With increasing alkyl chain length, it is observed that the viscosity increases whereas the structural α -relaxation rate decreases in accordance with Maxwell's relation. Between the rate of electrical relaxation and the rate w_a of the structural α -relaxation scaling is observed over more than 6 decades with a decoupling index of about 2.

References: C. Iacob et al., : *J. Chem.Phys.*, 2008, In press; J. Sangoro et al., *J. Chem.Phys.* 128, 214509, 2008; J. Sangoro et al., *Phys. Rev. E*, 051202, 2008; F. Kremer et al., *Phys. Rev. E*, 54, 1996

CPP 15.11 Tue 14:00 P3

Diffusion in polymer networks of hydrogels — ●FATEMEH TABATABAEI¹, OLAF LENZ², and CHRISTIAN HOLM¹ — ¹Institute für Computationalphysik, Universität Stuttgart, 70569 Stuttgart, Ger-

many — ²Max-Planck-Institut für Polymerforschung, 55021 Mainz, Germany

In this work we consider the diffusion behavior of a simple spherical tracer particle in polymer networks of hydrogels. There have been hints obtained via Fluorescence Correlation Spectroscopy on FCS tracer particles in a hydrogel. We investigate, by means of MD simulation, the diffusion properties of a tracer particle in a confined geometry of a polymer network. We present single model that shows anomalous diffusion, namely if the tracer particle is confined to follow the coiled polymer contour length. As an extension we investigate the diffusion property of a single tracer particle interacting with the polymer via simple Lennard-Jones potential.

CPP 15.12 Tue 14:00 P3

Fourier-series approach for analytical treatment of diffusion in periodic systems (Floquet method) — ●GÜNTER HEMPEL — Martin-Luther-Universität, Institut für Physik, D-06099 Halle, Germany

The data evaluation of diffusion experiments in periodic systems is often performed (i) at numerical way, (ii) at the basis of an approximately exponential behaviour, or (iii) by means of an analytical solution in terms of rather complicated analytical expressions. Here a simplification is proposed: The diffusion equation is expanded in Fourier series with respect to space coordinates (Floquet method) which results in a system of ordinary differential equations. Solving the latter we obtain the time evolution of the Fourier coefficients of the concentration distribution. They decrease exponentially; the higher the order of the Fourier coefficient is the faster is the decay. At this way the concentration-time dependency can be estimated.

Depending on the experiment, the term concentration might be replaced by temperature, magnetization, spin polarization, or others. Moreover, sometimes not this generalized concentration is of interest but its integral, here denoted as intensity. (In the case of concentration as particle density, the intensity will be the total amount of particles in a certain volume.) This procedure was applied to the data evaluation of a nuclear-spin diffusion experiment in lamellae of a lactide macromonomer. The local magnetization density plays the role of the generalized concentration, and the magnetization of a lamellae that of the intensity.

CPP 15.13 Tue 14:00 P3

Thermal trapping of single molecules in liquids — ●ROMY RADÜNZ¹, FRANK CICHOS¹, and ALOIS WÜRGER² — ¹Molecular Photonics Group, Institute of Experimental Physics I, University Leipzig, Linnéstr. 5, 04103 Leipzig, Germany — ²CPMOH, Université Bordeaux 1, 351 Cours de la Libération, 33405 Talence, France

Brownian motion prevents an extended optical observation of single molecules in solution as it drives molecular species out of the observation volume. To overcome this drawback surface chemistry is applied to immobilize molecular entities for detailed optical studies. But the presence of a surface may change the electrical, optical and conformational properties of molecules considerably. Thus contact-free methods are needed to confine single molecules or nanoparticles to an observation volume appropriate for optical investigation. Such a trapping in liquids paired with manipulative tools could open a completely new route for single molecule chemistry in solution. Here we propose a thermal trap, which is based on highly localized temperature gradients. Such gradients exert forces on molecules, known as thermophoretic forces. Localized temperature gradients in the fluid are realized by single gold nanoparticles of a diameter of approximately 50 nm, which are immobilized on glass cover slips and selectively excited by a focussed laser beam. Due to the fact that gold nanoparticle exhibit a large absorption cross section near the plasmon resonance they represent very efficient nano heat-sources. In this contribution detailed theoretical considerations on the thermophoretic trap are presented. First experimental results on the trapping of polystyrene beads will be shown.

CPP 15.14 Tue 14:00 P3

Photothermal fluctuation spectroscopy on gold nanoparticle dimers — ●MIRIAM WÄHNERT, NILS NEUBAUER, ROMY RADÜNZ, and FRANK CICHOS — Molecular Nanophotonics Group, University of Leipzig, Linnéstraße 5, 04103 Leipzig

To measure distance changes on the nanoscale, FRET (Fluorescence resonance energy transfer) is a heavily applied technique in biophysical studies. The upper limit of distance fluctuations being measured with this method is about 10 nm. Furthermore it suffers from photochemi-

cal degradation mechanisms like blinking and bleaching of the energy transferring dye molecules.

We report on recent experiments using pairs of gold nanoparticles as absorbing markers replacing dye molecules. Gold particles are strongly interacting with light, if they are excited near the plasmon resonance. The resulting dipoles of two closely spaced gold nanoparticles can couple to form a new resonance, which appears in the absorption as a distinct feature. The strength of this absorption depends on the distance of the two particles and is visible up to a few 10 nm, which clearly exceeds the lengthscale of FRET. The gold nanoparticles are detected by photothermal heterodyne detection, using the release of heat from the absorbing particles to create a local refractive index change around them, which can be probed with a confocal laser scanning setup. Due to the plasmon coupling a fluctuating distance will result in a fluctuating photothermal signal. Numerical analyses of the spectra together with first experimental results will be presented.

CPP 15.15 Tue 14:00 P3

Convection at the isotropic-nematic interface under slow

continuous cooling — ●BEATE ULLRICH, DORIS VOLLMER, and GÜNTER K. AUERNHAMMER — Max-Planck-Institut für Polymerforschung, Mainz, Germany

Small amounts of added alkane alter the kinetics of the isotropic-nematic phase transition of cyanobiphenyls such that isotropic and nematic domains coexist within a defined temperature interval. Under continuous cooling, redistribution of alkane between the domains can be limiting and local inhomogeneities may arise. Tracking hydrophobic PMMA tracer colloids close to growing nematic droplets revealed convection-like motion within a range of some 10 μm . This motion pattern seems to require interaction with alkane, as it does not occur in silica colloids. It follows initial colloid attraction towards the interface, and is associated with slow but steady droplet growth at cooling rates below 0.05 K/min. Once developed, it even outlasts coalescence events, but is abolished when the temperature ramp is interrupted and droplet growth ceases. We discuss local alkane concentration gradients as well as alkane effects on the isotropic-nematic interfacial tension as possible driving mechanisms of this small-scale convection.

CPP 16: POSTERS Polyelectrolytes and Biological Systems

Time: Tuesday 14:00–16:30

Location: P3

CPP 16.1 Tue 14:00 P3

Temperature dependence of positron annihilation in high permeability polymers: Teflons AF — ●KLAUS RÄTZKE¹, JAN KRUSE¹, FRANZ FAUPEL¹, YURI YAMPOLSKII², VICTOR SHANTAROVICH³, and GÜNTER DLUBEK⁴ — ¹Faculty of Engineering, University of Kiel, Germany — ²A.V. Topchiev Institute of Petrochemical Synthesis, Moscow, Russia — ³N.N.Semenov Institute of Chemical Physics, Moscow, Russia — ⁴Institute for Innovative Technologies, Köthen/Halle, Germany

The performance of polymeric membranes for gas separation is given by the free volume. Positron annihilation lifetime spectroscopy (PALS) is an accepted technique for investigation of free volume; the ortho-Positronium (o-Ps) lifetime is directly related to the mean hole size. PALS was done on amorphous Teflon AF 1600 and AF 2400. (copolymers of tetrafluoroethylene and 2,2-bis(trifluoromethyl)-4,5-difluoro-1,3-dioxole units). From the data mean hole size and width were calculated. Both polymers show large o-Ps lifetimes (\Rightarrow large hole sizes) and glass transition near the expected values. AF 2400 shows a non-linear temperature dependence of the ortho-positronium lifetime, extraordinarily large mean values of o-Ps lifetimes and the widths of the lifetime distributions. Explanations will be discussed in relation to the microstructure of the copolymer.

M. Rudel, J. Kruse, K. Rätzke, F. Faupel, Y. P. Yampolskii, V. P. Shantarovich, G. Dlubek, *Macromolecules*, 41 (2008) 788.

G. Dlubek, J. Pionteck, K. Rätzke, J. Kruse, F. Faupel, *Macromolecules* (2008); 41; 6125.

CPP 16.2 Tue 14:00 P3

Allocation of crystalline and amorphous minerals in calcified tissues: A confocal Raman study — ●SABINE HILD^{1,2}, HELGE FABRITIUS², TORSTEN FISCHER², and DIERK RAABE² — ¹Institut für Polymerwissenschaften, JKU Linz, Linz, Austria — ²Max-Planck-Institut fuer Eisenforschung, Duesseldorf

The mineralized exoskeleton formed by the cuticle of crustaceans is an excellent model to study biological nano-composite materials. In spite of the diversity of crustacean species they share a similar structural principle for their cuticle: An organic matrix composed of chitin-protein fibers associated with variable amounts of biominerals. The most widespread mineral is crystalline and amorphous calcium carbonate and to lower amounts calcium phosphate. In contrast to calcium carbonate, only little is known about the modification, the distribution and the function of the latter. Using the combination of electron microscopy, Energy-Dispersive X-Ray Analysis, Raman spectroscopy and atomic force microscopy we studied the mineral distribution within the claw cuticle of the american lobster *Homarus americanus*. Similar to other crustaceans, in the lobster cuticle crystalline calcium carbonate is restricted to the exocuticle forming a continuous calcite layer only close to the surface. Further inside the crystalline phase forms a post-like structure. Amorphous calcium carbonate (ACC) is localized in between the crystalline domains and appears homogeneously distributed within the endocuticle. It is accompanied by amorphous calcium car-

bonate (ACP). Selective dissolution and SFM nano-indentation experiments will provide further information about the function of ACC and ACP.

CPP 16.3 Tue 14:00 P3

Fluorescence Lifetime Measurements of Molecular Crystals and Giant Unilamellar Vesicles — ●MAREK BLASZCZYNSKI and LOTHAR KADOR — University of Bayreuth, Institute of Physics and BIMF, D-95440 Bayreuth, Germany

Fluorescence lifetime imaging microscopy in the frequency domain is applied to mixed molecular crystals and giant unilamellar vesicles (GUVs). The custom-built set-up is based on a confocal microscope and uses a cw laser which is amplitude-modulated in the MHz regime with an acousto-optic modulator (AOM). The phase shift and modulation amplitude of the fluorescence signal with respect to the excitation yield information about the fluorescence lifetime(s). The fluorescence decay of pentacene in *p*-terphenyl host crystals shows a bi-exponential behavior, which is ascribed to the presence of pentacene monomers and dimers. Spatially resolved studies on GUVs of binary mixtures (DOPC/DPPC) and ternary mixtures (DOPC/DPPC/cholesterol) with the head-labelled phospholipid Rhod-DMPE as a fluorescent probe were performed, and preliminary results of their phase behavior are presented.

CPP 16.4 Tue 14:00 P3

Controlling Protein Interfacial Affinities by Ionic and Non-Ionic Cosolvents — FLORIAN EVERS¹, JUNY KOO², THOMAS GUTBERLET³, ROLAND STEITZ⁴, ●METIN TOLAN¹, and CLAUS CZESLIK² — ¹Fakultät Physik, TU Dortmund, 44221 Dortmund — ²Fakultät Chemie, TU Dortmund, 44221 Dortmund — ³Paul-Scherrer-Institut, CH-5232 Villigen — ⁴Helmholtz-Zentrum Berlin, 14109 Berlin

In a biological cell, proteins perform their functions in a highly complex environment comprising crowding and confinement effects as well as interactions with interfaces and cosolvents. Cosolvents can stabilize or destabilize proteins in solution. Here, we present recent studies on how ionic and non-ionic cosolvents affect the interfacial affinity and structure of proteins at hydrophilic and hydrophobic solid surfaces. RNase A at a silica-water and a polystyrene-water interface were used as model systems and studied by neutron and optical reflectometry. The degree of protein adsorption and the density profile of the adsorbed protein films were determined in the absence and the presence of cosolvents. In the case of the hydrophilic silica-water interface, both the protein stabilizing glycerol and the destabilizing urea cause a distinct reduction in the interfacial affinity of RNase A. At the hydrophobic polystyrene surface, two trends become apparent: The kosmotropic SO_4^{2-} ion lowers the amount of adsorbed protein when it is present at sub-molar concentrations, whereas the chaotropic SCN^- ion significantly enhances the degree of protein adsorption at concentrations of a few moles per liter. The obtained results will be discussed in terms of the underlying effects of the cosolvents on the adsorption mechanisms.

CPP 16.5 Tue 14:00 P3

Optical Bloch equations of light harvesting nanostructures — ALEXANDER CARMELE¹, ●MARTEN RICHTER¹, THOMAS RENGER², and ANDREAS KNORR¹ — ¹Institut für Theoretische Physik, AG Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — ²Institut für Chemie und Biochemie, Freie Universität Berlin, Takustr. 3, 14195 Berlin, Germany

Within a Bloch equation approach [1], we calculate linear and pump-test spectra of Coulomb-coupled nanostructures (like pigments in pigment-protein complexes in LHC-II or the Fenna-Matthews-Olson (FMO) complex). The theory includes Förster-coupling induced excitation transfer between the nanostructures, electron-vibrational coupling between the nanosystems and their environment as well as the interaction with external optical fields and is based on many particle Liouville and cluster-expansion techniques. Hereby, we include self-consistently the structural data for the optical transition energies of pigments in protein environments and the spectral density of exciton-vibrational coupling [3].

[1]M. Richter, Th. Renger, G. Renger, A. Knorr, J. Chem. Phys. 127, 075105 (2007)

[2]M. Richter, Th. Renger, A. Knorr, Photosyn. Res. 95, 2-3, 119 - 127 (2008)

[3]J. Adolphs, F. Müh, M. El-Amine Madjet, Th. Renger, Photosyn. Res. 95, 2-3, 197-209 (2008)

CPP 16.6 Tue 14:00 P3

X-Ray Reflection Study on Block Copolymer Langmuir Films — ●VOLKER SCHÖN and PATRICK HUBER — Saarland University, 66123 Saarbrücken, Germany

We present X-ray measurements on Langmuir films of amphiphilic block copolymers of variable length at various surface pressures corresponding to different phases in their compression isotherms.

The measurements were taken on a home made butterfly X-ray reflectometer with an accessibility of up to 9 orders of magnitude in reflected intensity while the films were prepared and controlled in a Langmuir trough.

The obtained reflectivities give hints to distinct conformational changes within the films investigated.

CPP 16.7 Tue 14:00 P3

Photothermal imaging of gold particles in living cells — ●NILS NEUBAUER¹, CARSTEN STÜBER², JOSEF KÄS², and FRANK CICHOS¹ — ¹Molecular Nanophotonics Group, University of Leipzig, Linnéstraße 5, 04103 Leipzig — ²Soft Matter Physics Group, University of Leipzig, Linnéstraße 5, 04103 Leipzig

Many biochemical processes in living cells depend strongly on temperature. Local heating might provide a versatile tool for manipulating such processes. Nevertheless a strongly localized heat generation is required for this purpose. This can be achieved by optical heating of single nanometer sized gold particles. Optical excitation of the plasmon resonance of the gold nanoparticle allows precise control of heat release. Furthermore the thermal field around a single particle is strongly localized. Here we present a study on the following two questions: How do the particles distribute within a cell and secondly, how do they affect the cell metabolism? Gold nanoparticles have been visualized in living cells by photothermal heterodyne detection. By absorbing laser light and the subsequent conversion into heat, these particles locally induce a change in refractive index of the surrounding media, which can be probed with a confocal laser scanning setup. This technique offers both imaging and studying the local effect of heat release by the gold nanoparticles. In the first experiments fibroblasts were used to study the distribution of gold nanoparticles with 40 nm down to 10 nm in size. While the 40 nm particles do not penetrate the membrane and adhere around the cell, the 10 nm particles enter and accumulate inside the cell.

CPP 16.8 Tue 14:00 P3

Two-dimensional Lamellar Phase of Poly(styrene) — JENS-UWE GÜNTHER, ●HEIKO AHRENS, and CHRISTIANE A. HELM — Institut für Physik, Uni Greifswald, Felix-Hausdorff-Str. 6, 17487 Greifswald

Polystyrene sulfonate (PSS) adsorbed onto oppositely charged dodecyltrimethylammonium bromide (DODA) monolayers at the air/water interface is investigated with X-ray reflectivity and grazing incidence diffraction. DODA in the condensed phase is in an oblique lattice. At low PSS bulk concentrations (0.001 * 0.1 mmol/L) the surface pressure corresponding to the fluid/condensed phase transition and the DODA molecular area in the condensed phase are decreased,

the latter due to a reduced tilt angle. Both findings are attributed to PSS shielding the electrostatic repulsion between the DODA molecules. Bragg peaks caused by flatly adsorbed, aligned PSS chains are observed, with DODA in the fluid or the condensed phase. The two-dimensional lamellar phase is only found at intermediate PSS bulk concentrations (0.001 * 1 mmol/L). In this phase, the PSS coverage can be varied by a factor three, depending on DODA molecular area and polymer bulk concentration. Charge compensation in the lamellar phase is almost achieved at 1 mmol/L. At larger bulk concentrations, PSS adsorbs flatly yet without chain alignment. Presumably, a necessary condition for a two-dimensional lamellar phase is a pronounced electrostatic force which causes a large persistence length as well as repulsion between the aligned chains.

CPP 16.9 Tue 14:00 P3

Solvation structure of ice-binding antifreeze proteins — ●HENDRIK HANSEN-GOOS and JOHN WETTLAUER — Department of Geology and Geophysics, Yale University, New Haven, CT 06520, USA

Antifreeze proteins (AFPs) can be found in organisms which survive at subzero temperatures. They were first discovered in polar fishes since the 1950's [1] and have been isolated meanwhile also from insects, plants, and bacteria. While AFPs shift the freezing point of water (and hence the bulk melting point and hence can prevent recrystallization; the effect is non-colligative) and there is a pronounced hysteresis between freezing and melting. For many AFPs it is generally accepted that they function through an irreversible binding to the ice-water interface which leads to a piecewise convex growth front with a lower nonequilibrium freezing point due to the Kelvin effect.

Recent molecular dynamics simulations of the AFP from *Choristoneura fumiferana* reveal that the solvation structures of water at ice-binding and non-ice-binding faces of the protein are crucial for understanding how the AFP binds to the ice surface and how it is protected from being overgrown [2]. We use density functional theory of classical fluids in order to assess the microscopic solvent structure in the vicinity of protein faces with different surface properties. With our method, binding energies of different protein faces to the water-ice-interface can be computed efficiently in a simplified model.

[1] Y. Yeh and R.E. Feeney, Chem. Rev. **96**, 601 (1996).[2] D.R. Nutt and J.C. Smith, J. Am. Chem. Soc. **130**, 13066 (2008).

CPP 16.10 Tue 14:00 P3

Assessing different mapping schemes for coarse grained simulations of peptide systems. — ●OLGA BEZKOROVAYNAYA and CHRISTINE PETER — Max Planck Institute for Polymer Research

The study of organic/inorganic interfaces using theoretical methods became in the last years of central importance in many fields of condensed matter, material science and chemistry due to the large number of applications in current technology.

The aim of the present project is to explore the ability and the limitation of a coarse-grained (CG) model to reproduce structural and conformational properties of a peptide.

At first, it is necessary to devise a CG model and the corresponding potentials. Important aspects of the CG model are the mapping scheme, i. e. the relationship between the CG particles and the underlying atomistic coordinates; the intramolecular interaction potentials and the non-bonded potentials between CG particles. At this moment we are testing several CG mapping schemes for a short peptide (poly-alanine) with 24 atoms. We determined bonded potentials for the different CG models using Boltzmann inversion. We compared their ability to reproduce structural properties of the molecule that had been previously determined by atomistic simulation.

At a later stage we will extend this work to other peptides and peptides in proximity to a surface.

CPP 16.11 Tue 14:00 P3

Silk - as seen by X-ray microdiffraction and small angle X-ray scattering with *in situ* tensile tests — ●IGOR KRASNOV¹, IMKE DIDDENS², CHRISTINA KRYWKA¹, FLORIAN KUNZE¹, and MARTIN MÜLLER³ — ¹Christian-Albrechts-Universität zu Kiel, Institut für Experimentelle und Angewandte Physik, Leibnizstraße 19, D-24098 Kiel — ²University of Oxford, Dept. of Zoology, South Parks Road, OX1 3PS United Kingdom — ³GKSS Forschungszentrum Geesthacht, Max-Planck-Straße 1, D-21502 Geesthacht

Silkworm silk is a natural composite material produced by the silkworm *bombyx mori* and is known to have a high tensile strength comparable to that of steel. Unlike steel however, it is extremely stretchable with

an extreme elongation before breaking and a high degree of toughness. It would be highly desirable to mimic nature's spinning process to produce artificial fibres with optimized mechanical performance either from silkworm or recombinant spider silk spinning dope. Using a combination of in situ tensile tests and X-ray microdiffraction [1] as well as small angle X-ray scattering, we have determined the mechanical properties of both the crystalline and the disordered phase of the biological nanocomposite silk by adapting a model from linear viscoelastic theory to the semicrystalline morphology of silk. We have observed a strong interplay between the morphology of silk and the fibers' mechanical properties. It is apparent, that the high extensibility of silk results mainly from the disordered phase, however, we have observed that the crystals are also elastically deformed.

[1] I. Krasnov et al. *Phys. Rev. Lett.* **100**, 048104 (2008)

CPP 16.12 Tue 14:00 P3

The Nanostructure of the Tracheid Wood Cell Wall — ●MALTE OGURRECK^{1,2}, PEKKA SARANPÄÄ³, MANFRED BURGHAMMER⁴, SEBASTIAN SCHOEDER⁴, CHRISTINA KRYWKA¹, WIEBKE KNOLL¹, and MARTIN MÜLLER² — ¹IEAP, University Kiel — ²GKSS, Geesthacht — ³METLA, Vantaa (Finland) — ⁴ESRF, Grenoble (France)

Tracheid wood cell walls are mainly composed of cellulose nanocrystals (microfibrils) embedded in an amorphous matrix. These microfibrils are helically wound around the cell axis and are arranged in several layers.

While the structure of tracheid wood cells has been a research topic for many decades now and the structure on the biological and molecular level are well known, the detailed structure on intermediate length scales is still largely unknown. Here, we present results of a nanodiffraction experiment carried out at the microfocus beamline ID13, ESRF.

Tracheid cross sections have been scanned with a position resolution of 200 nm. A novel mathematical description of the scattering geometry for tracheid wood cells allows for the calculation of the crystal orientation from the scattering data. Thus, it is possible to determine the cellulose crystal orientation on a length scale of 200 nm and refine tracheid cell wall models.

CPP 16.13 Tue 14:00 P3

Crystallization and melting of fibrous silk — ●ANDREAS WURM, DANIELA ARBEITER, and CHRISTOPH SCHICK — University of Rostock, Institute of Physics, Polymerphysics, 18051 Rostock, Germany

The fundamental thermodynamic properties of materials based on fibrous proteins are important parameters, which are needed in order fully to understand the behavior of these materials in vitro and as structural elements in vivo.

Often these proteins exist in nature as semi-crystalline material. As for semi-crystalline polymers, differential scanning calorimetry (DSC) would be the easiest tool for determination of thermal properties like heat capacity, temperatures of transitions, melting enthalpy, crystallinity etc.

For fibers from the bombyx mori silk worm it arises the difficulty, that thermal decomposition during a DSC scan with common heating rate of about 10 K/min starts about 30 K above glass transition temperature, already before melting. To overcome this problem we applied faster calorimetric methods, like HyperDSC and ultra fast chip calorimetry with heating rates up to 500 K/min and 1 MK/min, respectively. These methods are suitable to prevent thermal decomposition on heating into the melt because of the short exposition time at high temperatures. We will present results from several crystallization-melting experiments of silk, using these fast calorimetric methods.

CPP 16.14 Tue 14:00 P3

CIDNP as a tool for determining the structure and magnetic resonance parameters of transient radicals of biomolecules — ●TALEA KÖCHLING¹, GERALD HÖRNER², SERGEY KORCHAK¹, ALEXANDRA YURKOVSKAYA^{1,3}, and HANS-MARTIN VIETH¹ — ¹Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin — ²Chemical Physics Department, Faculty of Chemistry, Adam Mickiewicz University Poznan — ³International Tomography Center, Institutskaya 3a, Novosibirsk, Russia

Combining NMR spectroscopy with the effect of spin hyperpolarization opens new ways to get information about structure of transient radicals and their pathways. A way for creating transient non-thermal signal amplitudes in proteins is Chemically Induced Dynamic Nuclear Polarization (CIDNP) resulting from the formation of a radical pair of a photo-excited dye molecule and an amino acid residue. Field de-

pendence of CIDNP allows to determine structure and magnetic resonance parameters (hyperfine coupling constants and g-factor) of elusive radicals. Furthermore, from time dependence with microsecond resolution it is possible to differentiate geminate and bulk processes, so that reaction pathways and rate constants of dynamic processes can be extracted.

In present study, CIDNP results for free amino acids and different peptides containing combination of methionine, glycine and tyrosine in aqueous solution at ambient temperature are obtained. Dependence of intramolecular electron transfer in the peptides on pH and its pathways are discussed.

CPP 16.15 Tue 14:00 P3

The influence of substrates on protein adsorption: adsorption kinetics studies and structural investigations. — ●HENDRIK HÄHL, HUBERT MANTZ, and KARIN JACOBS — Saarland University, Experimental Physics, D-66041 Saarbruecken, Germany

Surfaces that come into contact with an aqueous solution of proteins will be immediately covered with a thin protein layer. We seek to better understand the driving forces of this process. Concentrating on the influence of the substrate on the adsorption, the surface chemistry has been the focus of many studies. Recent studies have shown that, next to the chemical composition of the uppermost surface layer, also the substrate's composition influences the adsorption kinetics of proteins such as α -amylase and BSA [1, 2]. The experimental findings are corroborated by simulations assuming conformational or orientational changes of the protein molecules upon adsorption.

Thus, one also assumes different structures of the formed protein layers. To experimentally observe such differences, high resolution measurements of film thickness and density are needed. Therefore, we used surface plasmon resonance enhanced ellipsometry as well as neutron and X-ray reflectivity measurements for better film thickness and density data.

[1] A. Quinn et al., *EPL*, 2008, **81**, 56003.

[2] M. Bellion et al., *J.Phys.: Condens. Matter*, 2008, **20**, 404226.

CPP 16.16 Tue 14:00 P3

Investigation of Hofmeister effects in the swelling behaviour of polyelectrolyte microgels — ●MICHAEL ZEISER, YVONNE HERTLE, and THOMAS HELLWEG — Universität Bayreuth, Physikalische Chemie I, Universitätsstr. 30, 95447 Bayreuth, Germany

The present contribution describes the swelling behaviour of different poly(N-isopropylacrylamide) copolymer microgels with charged comonomers as a function of counterion type and concentration. To our knowledge Hofmeister effects were not yet studied for these responsive polymer colloids. The swelling behaviour is studied by means of photon correlation spectroscopy and small angle neutron scattering. Also influences with respect to the lower critical solution temperature are reported.

CPP 16.17 Tue 14:00 P3

Formation of necklace structures for intermediates of a Ca²⁺ induced shrinking of dilute anionic polyacrylate chains — ●PRASHANT SINHA¹, SEBASTIAN LAGES², ANTON KIRIY¹, MANFRED STAMM¹, and KLAUS HUBER² — ¹Leibniz-Institut für Polymerforschung Dresden e.V., Hohe Strasse 6, 01069 Dresden, Germany — ²Chemistry Department, Universität Paderborn, Warburger Str.100, D-33098 Paderborn, Germany

Sodium polyacrylate coils in dilute aqueous solutions shrink drastically upon addition of stoichiometric amounts of Ca²⁺ ions. An essential feature of this shrinking mechanism is its enhancement upon increase of temperature. The conformational changes in response to the addition of Ca²⁺ cations and upon an increase of temperature are investigated by means of light and neutron scattering and by AFM on the same samples. To this end, partially collapsed coils at 15°C were further shrunken and modified in shape by increasing the temperature to 30°C. The scattering curves at 30°C could only be interpreted with a model, which included the feature of a dumbbell, a reflection of necklace-like shape. Supplementary AFM imaging supports the drastic changes inferred to the system upon addition of the Ca²⁺ cations and upon a temperature increase by 15°C. AFM images have been analysed for radius of gyration of single molecules and evaluation of a 2D form factor curve. The information obtained is compared with scattering data. The results are considered to be one of the rare direct evidences for a pearl necklace-like intermediate along the coil-to-globule transition of polyacrylate chains.

CPP 16.18 Tue 14:00 P3

Calculation of the helical interaction parameters and groove binding potentials for DNA like charged cylinders.

— ●DOMINIC LEE — Max-Planck Institut für Physik Komplexer Systeme, Nöthnitzer Str. 38, D-01187, Dresden, Germany

An effective (KL) theory was developed to calculate the interaction between helically charged macro-ions [1]. Helical effects, resulting from this theory, may be important in cholesteric phases and in columnar assemblies [1]. It relies upon a "linearized" PB equation; but nonlinearities in the electrostatic potential, bound counter-ions, finite sizes of ions, and some correlation effects can be included in effective KL parameters. These define the strength of the helical contributions to the interaction, which have so far been treated as phenomenological. However, the KL parameters can be calculated if one knows the counter-ion charge and fixed charge distributions about a single macro-ion [1]. We briefly review the KL theory. Then, we calculate these parameters utilizing a model of a charged cylinder with DNA like surface distributions, taking into account counter-ions adsorbed within the grooves of DNA. We use two methods: the non-linear PB equation and a modified PB equation that incorporates some correlation and finite size effects that adjust the counter ion atmosphere. The distributions of groove-adsorbed counter-ions are related to groove binding potentials, by calculation of an adsorption isotherm.

[1]A.A Kornyshev, D. J. Lee, S. Leikin, A. Wynveen, Rev. Mod. Phys. 79, 943 (2007); and references contained therein.; EPAPS Document No. E-RMPHAT-79-010702

CPP 16.19 Tue 14:00 P3

Correlation between swelling and internal mobility of polyelectrolyte multilayers — ●SAMUEL DODOO and REGINE VON KLITZING — Stranski-Laboratorium für Physikalische & Theoretische Chemie, Institut für Chemie, TU Berlin, Strasse des 17. Juni 124, D-10623 Berlin

Polyelectrolyte multilayers (PEM) have emerged as a method to build up well-defined coatings for several kinds of surface modifications, ranging from photonics to biomaterials, membrane and sensor applications. Their preparation is via the layer-by-layer adsorption method. In this work the real-time monitoring of the layers adsorption and build-up in situ was performed by Quartz Crystal Microbalance (QCM). In addition, the lateral mobility of polyelectrolyte multilayers was investigated by means of the fluorescence recovery after photobleaching (FRAP) technique. The QCM results showed the successive build-up process of two-component multilayer and structural information such as swelling. From the FRAP measurements the results emerged that at high charge density, more complexes are formed, and the diffusion coefficient decreases. Further more the lateral mobility increases with increasing ionic strength and with decreasing hydration shell of the added anion in the polyelectrolyte solution.

[1] G. Decher Science 1997, 277, 1232. [2] P. Nazaran, V. Bosio, W. Jaeger, D. F. Anghel, R. v. Klitzing J. Phys. Chem B 2007, 111,

CPP 16.20 Tue 14:00 P3

Structuring of Polyelectrolyte Solutions Under Confinement of Solid-Solid and Air-Air Interfaces — ●CAGRI ÜZÜM¹, JÉROME DELACOTTE², DOMINIQUE LANGEVIN², and REGINE V. KLITZING¹ — ¹Stranski-Laboratorium für Physikalische und Theoretische Chemie - Institut für Chemie TU Berlin, Sekr. TC 9 Strasse des 17. Juni 124 D-10623 Berlin, Germany — ²Laboratoire de Physique des Solides, UMR 8502 Université Paris-Sud, Bât. 510 91405 Orsay cedex, France

The presented work focuses on the structuring of polyelectrolyte solutions (PAMPS) which are confined either between two fluid interfaces in a free-standing foam film or between two solid interfaces. The forces

between the opposing interfaces depend on the composition of the film interfaces and characteristics (e.g. type of charged and neutral groups, charge fraction, concentration) of the film fluid [1]. The confinement leads to oscillatory forces in a Colloidal Probe AFM and to a stepwise thinning in foam films. The oscillatory pressure curves are then compared to small angle scattering (SANS or SAXS, which give information about bulk structuring) spectra. Solutions of linear polyelectrolytes show a structure peak scaling with the polyelectrolyte concentration c as $q[\text{max}] \sim c^{1/2}$. The scaling law is predicted by theoretical models [2, 3]. The effect of the molecular architecture, e.g. linear, comb-like and branched polyelectrolytes on the structuring will be shown. [1] R. v. Klitzing, Adv. Coll. Interf. Sci. 2005, 114/115, 253. [2] R. v. Klitzing, B. Kolaric, W. Jaeger, A. Brandt. Phys. Chem. Chem. Phys. 2002, 4, 1907. [3] D. Qu, J.S. Pedersen, S. Garnier, A. Laschewsky, H. Möhwald, R. v. Klitzing. Macromolecules. 2006, 39, 7364.

CPP 16.21 Tue 14:00 P3

Ultrafast dynamics in polyelectrolyte/ gold multilayer structures studied by femtosecond pump-probe spectroscopy— ●MAREIKE KIEL^{1,2}, MARC HERZOG², DIRK KURTH¹, WOLFRAM LEITENBERGER², THORSTEN SIEVERS¹, HELMUTH MÖHWALD¹, and MATIAS BARGHEER^{1,2} — ¹Max Planck Institute of Colloids and Interfaces, Research Campus Golm, 14476 Potsdam, Germany — ²Institute of Physics, University of Potsdam, 14476 Potsdam, Germany

The dynamic response of hybrid nanolayer systems composed of polyelectrolytes and gold colloids upon optical excitation is studied by ultrafast pump-probe spectroscopy. Relative intensity changes of transient absorption and reflection spectra are measured with light in the visible and near infrared region, providing information on the photoinduced dynamics within the structure. We investigate multilayer structures of gold colloid strata that are separated by several polyelectrolyte layers. The well pronounced Bragg peaks and Kiessig fringes from x-ray reflectivity measurements prove the excellent structural quality of the samples with clear separation of the gold particle layers. We observe intensity modulations due to coherently excited breathing modes in 10nm and 20nm gold particles. From the monitored transmission and reflection data we deduce the time-dependant values of the imaginary and real part of the dielectric function.

CPP 16.22 Tue 14:00 P3

Silicon Rubber as Support for PEM Films: Rubber Surface Properties at Different Preparation Procedures— ●JOHANNES FRÜH¹, RUMEN KRASSTEV², and RALF KÖHLER^{3,1} — ¹MPI of Colloids and Interfaces, Dept. Interfaces, Potsdam, Germany — ²NMI, WB Bioanalytik, Tübingen, Germany — ³Helmholtz Centre Berlin for Materials and Energy, Dept. SF1, Berlin, Germany

Silicon rubber (polydimethyl siloxane [PDMS]) shall serve as support for polyelectrolyte multilayers (PEM) an organic material made from oppositely charged organic polyions. Both materials were intensively investigated in the past, but little is known about their conjoint behaviour and interactions.

Since the reproducible generation of compound PDMS-PEM systems demand for defined interfaces, the surface properties of PDMS have to be determined, and to be tuned in the end. Different techniques, as AFM, contact angle measurements, and X-ray reflectometry were used for surface characterisation. It turned out, that a gentle mixing process during the cross-linking of PDMS can supply microscopically flat rubber surfaces with roughnesses in nanometre range. Additional chemical surface treatment allows for tuning of adsorption behaviour (i.e. wetting/ dewetting) of PDMS-substrate. With it, a preparation techniques could be established which can provide molecularly flat soft-matter substrates with tunable surface properties.

CPP 17: Confined Fluids

Time: Tuesday 9:30–12:15

Location: ZEU 160

CPP 17.1 Tue 9:30 ZEU 160

Solid-liquid phase transitions in hard spheres and colloid-polymer mixtures — ●TATYANA ZKOVA-TIMAN¹, JÜRGEN HORBACH², and KURT BINDER¹ — ¹Institut für Physik, Johannes Gutenberg-Universität Mainz, Staudinger Weg 7, 5509 Mainz — ²Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln, Germany

We present the results of Monte Carlo (MC) simulations of liquid-to-crystal phase transitions in hard spheres and colloid-polymer mixtures, the latter modeled by the Asakura-Oosawa potential. In the traditional approaches such as thermodynamic integration or phase-switch MC, the coexistence point is computed from the estimates of bulk solid and liquid free energies. These methods are computationally demanding and do not provide any information about crystal growth kinetics.

On the contrary, we considered a direct simulation of solid-liquid coexistence in a slab geometry and obtained the melting point from an analysis of the interface velocity. Using Monte Carlo in the *NPT* ensemble we determined the coexistence pressures and kinetic growth coefficients. Their dependence on system size is investigated and compared to results reported in the literature. Moreover, the solid-liquid interface properties are studied including a careful analysis of finite size effects in the capillary wave spectrum.

CPP 17.2 Tue 9:45 ZEU 160

Lennard Jones Fluid in the Slit Pore. How Does It Nucleate? A Simulation Study. — ●NADEZHDA GRIBOVA^{1,2}, HAMED MALEKI³, AXEL ARNOLD⁴, TANJA SCHILLING³, and CHRISTIAN HOLM¹ — ¹Institute for Computational Physics, Stuttgart, Germany — ²Institute for High Pressure Physics, RAS, Troitsk, Moscow Region, Russia — ³Institute of Physics, Johannes Gutenberg-University, Mainz, Germany — ⁴Fraunhofer SCAI, Bonn, Germany

A study of heterogeneous nucleation has practical reasons because it occurs more often in nature than homogeneous. The existing theories describe heterogeneous nucleation mostly phenomenological and are the extensions of classical nucleation theory. When fluids are confined in the pore their properties differ significantly from the bulk. In this work we report a study of one of the simplest models that is still capable to reproduce the thermodynamic behaviour of classical fluids, the Lennard-Jones system. Confining it between the structureless walls and observing layering in the system we ask ourselves: do walls induce heterogeneous nucleation? Does it start from the layers? Is the crystallization a 3D or 2D process? The talk will summarise our current answers to the above questions.

CPP 17.3 Tue 10:00 ZEU 160

Phase transitions of charged colloidal suspensions in slit pores — ●STEFAN GRANDNER and SABINE H. L. KLAPP — Institut für theoretische Physik, Freie Universität Berlin, D-14195 Berlin, Germany

Employing Monte Carlo simulations in grandcanonical and isobaric ensembles we investigate freezing phenomena in a charged colloidal suspension confined to narrow slit-pores [1]. The macroion interactions are described by the Derjaguin-Landau-Verwey-Overbeek (DLVO) potential, which involves the counter- and salt ions implicitly, supplemented by a repulsive soft-sphere potential. Corresponding to experiments [2] we focus on moderately charged silica particles in solvents of low ionic strengths. The considered densities are too small to drive bulk freezing transitions. However, confining the suspension to sufficiently small pore widths does not only yield the well-known layering but also the formation of crystalline in-plane structures. This capillary freezing is consistent with ground-state calculations [3]. Furthermore, varying the parallel pressure at given surface separation we found a solid-solid transition from two-layer to three-layer systems with different in-plane order as found for uncharged spheres [4]. Finally, we consider the influence of wall charges including the possibility of charge-induced freezing.

[1] S. Grandner and S. H. L. Klapp, *J. Chem. Phys.*, *accepted*.

[2] S. H. L. Klapp, D. Qu, and R. v. Klitzing, *J. Phys. Chem. B* **111**, 1296 (2007); S. H. L. Klapp, Y. Zeng, D. Qu, and R. v. Klitzing, *Phys. Rev. Lett.* **100**, 118303 (2008).

[3] R. Messina and H. Löwen, *Phys. Rev. Lett.* **91**, 146101 (2003).

[4] A. Fortini and M. Dijkstra, *J. Phys.: Cond. Matter* **18**, L371 (2006).

CPP 17.4 Tue 10:15 ZEU 160

Molecular dynamics simulation of evaporation processes of fluid bridges confined in slit-like pore — ●KATARZYNA BUCIOR, LEONID YELASH, and KURT BINDER — Institute of Physics, Johannes-Gutenberg University of Mainz, Mainz, Germany

We study a simple fluid, described by point-like particles interacting via the Lennard-Jones potential, under confinement in a slit geometry between two walls at distance L_z apart for densities inside the vapor-liquid coexistence curve. Equilibrium then requires the coexistence of a liquid "bridge" between the two walls, and vapor in the remaining pore volume. We study this equilibrium for several choices of the wall-fluid interaction (corresponding to the full range from complete wetting to complete drying, for a macroscopically thick film), and consider also the kinetics of state changes in such a system. In particular, we study how this equilibrium is established by diffusion processes, when a liquid is inserted into an initially empty capillary (partial or complete evaporation into vacuum), or when the volume available for the vapor phase increases. We compare the diffusion constants describing the rates of these processes in such inhomogeneous systems to the

diffusion constants in the corresponding bulk liquid and vapor phases.

CPP 17.5 Tue 10:30 ZEU 160

Condensation of single drops. — ●MORDECHAI SOKULER, GÜNTER K. AUERNHAMMER, and HANS-JÜRGEN BUTT — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz

Water condensation on surfaces, or growth of breath figures, is an important and common natural process with applications ranging from heat transfer to dew collection. Many works have detailed the growth of breath figures and their simulation. However, what has yet to be addressed comprehensively is the growth of individual, isolated droplets. Existing theory predicts drop volume increases linearly with time, between nucleation and the merging stage. We show the volumetric growth of isolated drops is much faster than predicted. Thus, the spacing of the drops becomes an important factor. And the distinction needs to be made between the growth of individual drops compared to tightly packed groups of drops. We use calculation of the concentration profiles of the two cases to predict the packing density required for each type of behaviour.

15 min. break

CPP 17.6 Tue 11:00 ZEU 160

Critical Casimir Forces in the presence of varying surface fields — ●URSULA NELLEN, LAURENT HELDEN, and CLEMENS BECHINGER — 2. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart

In 1978 Fisher and de Gennes predicted that the confinement of critical fluctuations in a binary liquid leads to so-called Critical Casimir Forces. Direct experimental measurements of such forces has been only obtained recently. The amplitude of the Critical Casimir Force has been demonstrated to scale with the reduced temperature whereas a variation of the surface field from symmetric to antisymmetric boundary conditions changes the sign of the interaction from attraction to repulsion. Here we report first measurements where the amplitude of the surface field is systematically varied by controlling the surface properties of the confining surfaces. The Critical Casimir Forces are measured with total internal reflection microscopy between a single colloidal particle and a flat surface in a water - 2,6-lutidine mixture.

CPP 17.7 Tue 11:15 ZEU 160

Crystallization of soft crystals — ●MAX WOLFF^{1,2,3}, ANDREAS MAGERL⁴, and HARTMUT ZABEL¹ — ¹Institute for Solid State Physics/EP IV, Ruhr-University Bochum, Germany. — ²Institute Laue-Langevin, Grenoble, France. — ³Materials Physics, Uppsala University, Sweden. — ⁴Crystallography and Structural Physics, University Erlangen-Nürnberg, Erlangen, Germany

The crystallization of metals or ionic crystals either propagates throughout the melt starting from a single seed or small grains grow and develop simultaneously at different locations. In the first case, a single crystal is formed, and the second case results in a polycrystal, which may show pronounced texture. The driving force is the ionic or metallic interaction with binding energies on the order of 100 kBT at room temperature. Inert gas crystals form as a result of much weaker van der Waals forces, and regarding the spherical shape of atoms, in most cases an fcc structure. Soft matter is also characterized by relatively weak binding energies of hydrogen bonds, entropic forces, or hydrophobic interaction.

The crystallization of micelles formed by surfactant F127 solvated by 20 % in water was investigated in the vicinity of a hydrophilic interface. Upon entering the crystalline phase from low temperature, a large correlation length develops without preferential texture. Upon heating, the correlation length decreases and Oswald ripening is observed with crystallites orienting with respect to each other while retaining long-range and textured correlation [1].

[1] M. Wolff et al.: *Langmuir* (Letter) doi: 10.1021/la803015t.

CPP 17.8 Tue 11:30 ZEU 160

Deformation of nanoporous materials during the sorption process — ●GERRIT GÜNTHER and MARTIN SCHOEN — Stranski-Laboratorium für Physikalische und Theoretische Chemie, Sekretariat C7, Technische Universität Berlin, Straße des 17. Juni 135, D-10623 Berlin, Germany

Several experiments point at deformations of nanopores due to the sorption of confined fluids. To investigate such strains and their influence on phase behavior of the confined fluid we use the grand canonical

ensemble Monte Carlo method (GCEMC). We consider a simple fluid between two plane parallel walls which themselves consist of single wall particles. Wall and fluid particles are of the same type and are interacting via Lennard-Jones(12,6) potentials. The wall particles are not fixed to their lattice sites but bound to them by harmonic potentials. Thus we are able to control the softness of the wall via the force constant of this harmonic potential from an almost rigid structure to more flexible walls. Flexible means that the wall atoms can move from their equilibrium positions to react to the fluid. Despite a shift of fluid phase transition flexible pores reveal a typical sequence of pore deformations during the sorption process even in the critical regime. It is remarkable that strains of our slit pore model are in good agreement with experimental results of cylindrical pores. [1] This suggests that dispersion forces rather than curvature effects are responsible for pore deformation.

[1] G. Günther, J. Prass, O. Paris, and M. Schoen, Phys. Rev. Lett. 101 (2008), 086104.

CPP 17.9 Tue 11:45 ZEU 160

Modelling pore lattice deformations during sorption and capillary condensation of fluids in ordered mesoporous silica — ●DIRK MÜTER, JOHANNES PRASS, and OSKAR PARIS — Max Planck Institute of Colloids and Interfaces, 14476 Potsdam, Germany

Sorption and capillary condensation of fluids in nanoporous silica materials like SBA-15 and MCM-41 can cause considerable deformations on the pore lattice[1]. Since these materials are promising candidates for a wide range of applications (e.g. catalysts and filters) their deformation behaviour and mechanical stability are important fields of current interest. While the fundamental physical effects can be understood and modelled with simple pore models using Monte Carlo[1] or Molecular Dynamics simulations, the complex mechanical response of the whole pore lattice is not covered by these models. In this talk, the deformations of model crystallites under external and internal loads

are calculated using the Finite-Elements-Method and their dependence on the porosity is analysed. The Finite-Element results are used to produce scattering curves which are compared to small angle x-ray scattering data from in-situ sorption experiments.

[1] Günther et al., Phys. Rev. Lett., 101 (2008)

CPP 17.10 Tue 12:00 ZEU 160

Analysis of sorption strains in ordered mesoporous materials by in-situ x-ray diffraction — ●JOHANNES PRASS, DIRK MÜTER, and OSKAR PARIS — Department of Biomaterials, Max Planck Institute of Colloids and Interfaces, D - 14424 Potsdam, Germany

Sorption and condensation of fluids create stresses in nanoporous materials. These induce strains in the porous matrix. The details of the solid matrix deformation, and how far in turn a strained matrix affects the sorption process are not well understood. In order to elucidate the extend of these interactions, we apply in-situ x-ray diffraction in ordered mesoporous materials during fluid sorption and condensation. Diffraction data provide not only valuable information on the pore structure and the fluid sorption behaviour [1]. Also "strain isotherms" - i.e. the strain of the pore lattice as a function of the fluid vapour pressure - are extractable from these experiments [2]. We investigated several different materials with 2D hexagonal pore ordering, and thereby varied the material, the porosity and the pore size. In addition we varied the fluid-solid interactions by using different fluids. We demonstrate that an "elastic modulus" can be extracted from the strain isotherms. This modulus cannot be directly related to the Young's modulus or the Bulk modulus due to the peculiar loading conditions which act within the porous body. We use simple analytical considerations and finite element analysis to better understand the relationship between measured strains and elastic properties of the porous solid.

[1] G. A. Zickler et al. (2006). Phys. Rev. B 73, 184109

[2] G. Günther et al. (2008). Phys. Rev. Lett. 101, 086104

CPP 18: Polyelectrolytes

Time: Tuesday 9:30–12:30

Location: ZEU 114

CPP 18.1 Tue 9:30 ZEU 114

Small-angle x-ray scattering of lignosulfonate in aqueous methanol solutions — ●ULLA VAINIO¹, ROLF ANDREAS LAUTEN², SYLVIO HAAS³, KIRSI LEPPÄNEN⁴, LARISSA VEIGA¹, RITVA SERIMAA⁴, ARMIN HOELL³, and RAINER GEHRKE¹ — ¹HASYLAB at DESY, Hamburg, Germany — ²Borregaard Lignotech, Sarpsborg, Norway — ³Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany — ⁴Department of Physics, University of Helsinki, Helsinki, Finland

Lignosulfonate is a binder, dispersant, and emulsion stabilizer. It may be used as a component in plastics and low-cost methanol fuel cell membranes. We studied the structure and aggregation of sodium and rubidium lignosulfonate particles in water-methanol mixtures by small-angle x-ray scattering (SAXS). Volume fraction of lignosulfonate in solution ranged from 0.01 to 0.17, covering the semi-dilute regime. Interestingly, rubidium lignosulfonate particles self-associated more than sodium lignosulfonate particles even though both ions have valence +1. The effect was most pronounced in 1:1 methanol-water mixtures. Measurements were made also for 1:3 methanol-water solution and aqueous solution. We conclude that the heavier rubidium ions associate to the sulfonate groups more readily than sodium ions. Methanol enhanced the self-association tendency for both rubidium and sodium lignosulfonate. A contrast variation method, anomalous small-angle x-ray scattering (ASAXS), was used to study how rubidium is distributed in the lignosulfonate solutions. The measurements were made at the 7T MPW SAXS beamline at BESSY in Berlin.

CPP 18.2 Tue 9:45 ZEU 114

Reentrant Condensation of Proteins in Solution Induced by Multivalent Ions — ●LUCA IANESELLI¹, FAJUN ZHANG¹, ROBERT M. J. JACOBS², MAXIMILIAN W. A. SKODA³, CHRISTOPHER C. MARTIN⁴, SYLVAIN PRÉVOST⁵, and FRANK SCHREIBER¹ — ¹Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen, Germany — ²CRL, University of Oxford, UK — ³ISIS Rutherford Appleton Laboratory, UK — ⁴SRS, Daresbury, UK — ⁵Helmholtz Center Berlin

Proteins in aqueous solution in the presence of multivalent salt ions can

exhibit reentrant condensation [1]. In order to address the dependencies of the phenomenon on protein structure and surface charge density we examined systematically different proteins and multivalent ions systems using UV-Vis spectroscopy and small angle scattering (SAS). Phase diagrams with similar features at the two critical concentrations as expected by the charge inversion theory [2] were determined for wide protein and salt concentration ranges. Positively charged proteins at neutral pH like lysozyme do not show reentrant behavior by using Y3+ as salt ions whereas negative proteins like BSA, OV or HSA do. Al3+ and the organic salt Spermine4+ do not induce reentrant condensation because of their too high and too low charge density respectively. Y3+ however induces reentrant condensation for 5 of the 6 analyzed proteins. Selected samples with fixed protein concentration were studied by SAS. The data analysis provides evidence of the changes in protein-protein interactions, from repulsive to attractive as a function of salt concentration. [1] F. Zhang, et al. Phys. Rev. Lett. 2008,101,148101 [2] A.Y. Grosberg, et al. Rev. Mod. Phys. 2002, 74, 329

CPP 18.3 Tue 10:00 ZEU 114

Counterion condensation on compact molecules — UTE BÖHME and ●ULRICH SCHELER — Leibniz-Institut für Polymerforschung Dresden, Hohe Str. 6, 01069 Dresden

Condensation of counterions reduces the effective charge of macromolecules. Electrophoresis NMR provides a versatile tool for the experimental determination of the effective charge [1, 2]. The detection in both diffusion and electrophoresis NMR is performed with chemical shift resolution, enabling the identification of the moving species. Condensation of organic counterions is thus monitored directly [3]. Stiff, rod-like molecules, flexible polymers and globular molecules like proteins [4] have been investigated, proving the concept of counterion condensation. Dendrimers are studied as model systems for nearly spherical polyelectrolytes. Inspection of the proton NMR spectra yields information on the degree of protonation of amino groups and thus the nominal charge of dendrimers. The effective charge of these small globular molecules is a fraction of their nominal charge. The effective charge does not reach the maximal nominal charge even for a small

molecule like citric acid.

[1] U. Böhme, U. Scheler, *Colloids and Surfaces A*, 222, (2003), 35 [2] K. Grass, U. Böhme, U. Scheler, H. Cottet, C. Holm, *Physical Review Letters* 100, (2008) 096104 [3] U. Böhme, C. Vogel, J. Meier-Haack, U. Scheler, *J. Phys. Chem. B* 111, (2007), 8344 [4] Ute Böhme, Ulrich Scheler *Chemical Physics Letters* 435, (2007), 342

CPP 18.4 Tue 10:15 ZEU 114

Optimizing end-labeled free-solution electrophoresis by increasing the hydrodynamic friction of the drag-tag — ●KAI GRASS¹, CHRISTIAN HOLM², and GARY SLATER³ — ¹FIAS, Goethe-University Frankfurt, Ruth-Moufang-Strasse 1, 60438 Frankfurt, Germany — ²ICP, University of Stuttgart, Pfaffenwaldring 27, 70569 Stuttgart, Germany — ³University of Ottawa, 150 Louis-Pasteur, Ottawa, Ontario K1N 6N5, Canada

We study the electrophoretic separation of polyelectrolytes of varying length in free-solution by means of end-labeled free-solution electrophoresis (ELFSE). A coarse-grained molecular dynamics simulation model, using full electrostatic interactions and a mesoscopic Lattice Boltzmann fluid to account for hydrodynamic interactions, is used to characterize the drag coefficients of different label types: linear and branched polymeric labels, as well as transiently bound micelles.

It is specifically shown that the label's drag coefficient is determined by its hydrodynamic size, and that the drag per label monomer is largest for linear labels. However, the addition of side chains to a linear label offers the possibility to increase the hydrodynamic size, without having to increase the linear length of the label, thereby simplifying synthesis. The third class of labels investigated, transiently bound micelles, seems very promising for the usage in ELFSE, as they provide a significant higher hydrodynamic drag than the other label types.

The results are compared to recent experimental results, as well as to theoretical predictions, and it is analyzed how the efficiency of the ELFSE method can be improved by using smartly designed drag-tags.

CPP 18.5 Tue 10:30 ZEU 114

Intermediate states in the coil to globule transition of polyacrylate chains: Single chain structures in dilute aqueous solutions and on surfaces — ●PRASHANT SINHA¹, SEBASTIAN LAGES², ANTON KIRIY¹, MANFRED STAMM¹, and KLAUS HUBER² — ¹Leibniz-Institut für Polymerforschung Dresden e.V., Hohe Strasse 6, 01069 Dresden, Germany — ²Chemistry Department, Universität Paderborn, Warburger Str.100, D-33098 Paderborn, Germany

A cascade of intermediate states appear along the coil to globule transition of polyacrylate chains in dilute aqueous solutions during interactions with specifically binding ions. Conformational changes of these chains induced by Sr²⁺, Pb²⁺ and Ca²⁺ ions have been studied. In the last case, temperature has been introduced as a secondary parameter to substantiate recent findings that the binding of carboxylate groups with calcium ions may be entropic in nature. The samples were characterized using combined static and dynamic light scattering. Intermediate states which exhibited a drastic reduction of coil dimensions upon addition of stoichiometric amounts of specifically binding ions were then investigated for single chain structures using SAXS, ASAXS and SANS, as suitable. The very same samples were also investigated on mica surfaces using Atomic Force Microscopy. Various characteristics of the single chain structures of intermediate states, primarily radius of gyration, have been compared for dilute solution behavior and surface behavior. We believe that the results provide one of the rare direct visual evidences of the coil to globule transition in a regime investigated also through scattering.

CPP 18.6 Tue 10:45 ZEU 114

Self-stretching of DNA-amphiphile complexes on pre-coated graphite surfaces — ●HUA LIANG, WEI ZHUANG, NIKOLAI SEVERIN, and JÜRGEN P. RABE — Department of Physics, Humboldt University Berlin, Newtonstr.15, D-12489 Berlin, Germany

Stretching single DNA molecules on a surface is important, for instance for the purpose of direct DNA sequencing with scanning probe techniques and for studies of enzyme activities [1]. Micrometer-long single DNA molecules have been deposited and aligned on a poly-L-lysine modified mica surface [2]. However this method does not allow to stretch the molecules perfectly, which makes sequencing a difficult task. Here we report a method which allows us to stretch both single- and double-stranded DNA (ss-, ds-DNA) and even overstretch ds-DNA on an amphiphile pre-coated graphite surface. DNA-amphiphile complexes form during adsorption of DNA molecules on the amphiphile

pre-coated surface. The complex self-stretches on the HOPG surface. Annealing at 60 °C stretches ds-DNA furthermore up to 1.42 times its original B-form length. ss-DNA can be stretched up to 0.45 nm/base, compared to 0.39 nm/base on poly-L-lysine pre-coated mica [2]. A mechanism for self-stretching is also suggested.

[1] X. Michalet, *Nano Letters* 1 (2001) 341-343 [2] A. T. Woolley, R. T. Kelly, *Nano Letters* 1 (2001) 345-348

CPP 18.7 Tue 11:00 ZEU 114

DNA cholesteric phases: the role of DNA molecular chirality and DNA-DNA electrostatic interactions — ●ANDREY CHERSTVY — IFF, Theorie-II, FZ Jülich, 52425 Jülich, Germany

DNA molecules form dense liquid crystalline twisted phases in vivo and in vitro. How the microscopic DNA chirality is transferred into intermolecular twist in these mesophases and what is the role of chiral DNA-DNA electrostatic interactions is still not completely clear. First, we give an extended overview of experimental observations on DNA cholesteric phases and discuss the factors affecting their stability. Then, we consider the effects of steric and electrostatic interactions of grooved charged helical molecules on the sign of cholesteric twist. We present some theoretical results on the strength of DNA-DNA chiral interactions, on DNA azimuthal correlations in cholesteric phases, on the micron-range pitch of DNA cholesteric phases, and on the regions of existence of DNA chiral phases stabilized by DNA-DNA electrostatic interactions [AC, JPCB, 112 12585 (2008)]. We suggest that 146 bp long DNA fragments with stronger affinities for nucleosome formation can form less chiral phases, with a larger left-handed cholesteric pitch. Also, the value of left-handed pitch formed in assemblies of homologous DNA fragments is predicted to be smaller than that of randomly sequenced DNAs. We expect also the cholesteric assemblies of several-kbp-long DNAs to require higher external osmotic pressures for their stability than the twisted phases of short nucleosomal DNA fragments at the same DNA lattice density.

15 min. break

CPP 18.8 Tue 11:30 ZEU 114

Bundle Formation in Polyelectrolyte Brushes — JENS-UWE GÜNTHER, ●HEIKO AHRENS, and CHRISTIANE A. HELM — Institut für Physik, Uni Greifswald, Felix-Hausdorff-Str. 6, 17487 Greifswald

Bundle formation in the vertically oriented polyelectrolytes within polyelectrolyte brushes is studied with x-ray reflectivity and grazing-incidence diffraction as a function of grafting density and ion concentration. At 0.5 Molar monomer concentration and without added salt, a bundle consists of two chains and is 5 nm long. On the addition of up to 1M CsCl, the aggregation number increases up to 15 whereas the bundle length approaches a limiting value, 2 nm. We suggest that the bundle formation is determined by a balance between long-ranged electrostatic repulsion, whose range and amplitude is decreased on salt addition, and short-ranged attraction.

CPP 18.9 Tue 11:45 ZEU 114

Conformation of poly(styrene sulfonate) layers physisorbed from high salt solution studied by force measurements on two different length scales — ●STEPHAN BLOCK and CHRISTIANE A. HELM — Institut für Physik, Uni Greifswald, Felix-Hausdorff-Str. 6, 17487 Greifswald

The colloidal probe technique (CPT) is used to measure distance-dependent interaction forces between polyelectrolyte layers physisorbed from 1 M NaCl solution in salt solutions between 0.1 mM and 1 M. Both linear polycations (poly(allylamine)hydrochloride, poly-L-lysine) and linear polyanions (poly(styrenesulfonate)) are used. The repulsive interaction energies in the range between 10(-7) and 10(-4) J/m(2) are described by the theory of Alexander and de Gennes for surfaces covered with neutral anchored polymers. However, the brush thickness scales with molecular area and salt concentration with a power of -1/3 as known from a salted brush and reaches approximately 50% of the contour length in diluted solutions. For PSS at low salt conditions, the brush length amounts to 30% of the contour length, a behavior known for polyelectrolyte brushes and attributed to the entropy of the counterions trapped in the brush. A negatively charged AFM tip penetrates the brush-a repulsive electrostatic force between the tip and surface is found, and single chains can be imaged. Thus, with the nanometer-sized AFM tip, the flatly adsorbed fraction of the PSS chains is seen, whereas the micrometer-sized colloidal probe interacts with the fraction of the chains penetrating into solution.

CPP 18.10 Tue 12:00 ZEU 114

Change in Molecular Ordering in Mechanically Stressed Polyelectrolyte Films — JOHANNES FRÜH¹, RUMEN KRASDEV², and RALF KÖHLER^{3,1} — ¹MPI of Colloids and Interfaces, Dept. Interfaces, Potsdam, Germany — ²NMI, WB Bioanalytik, Tübingen, Germany — ³Helmholtz Centre Berlin for Materials and Energy, Dept. SF1, Berlin, Germany

Polyelectrolyte Multilayers (PEM) are organic films which consist in complexed layers of two polyions of opposite charge commonly build-up on solid substrate. The widely used layer-by-layer preparation method allows for a high tunability of the properties of the PEM. Although several studies exist about mechanical behaviour of these films, relatively little is known about the underlying internal structure and the structural changes on molecular level caused by external load/stimulus.

We are interested in the local distribution of micro- and mesoscopic substructures in the PEM-network (e.g., voids or cross-linker points) and their implications on general macroscopic properties, as stability and reversibility (ageing, fatigue) of the films. Especially the effects of external and internal mechanical load shall be examined.

Two strategies are pursued: firstly, the manipulation of internal mechanical stress by incorporation of solvent molecules into the polymer network (swelling experiments); and secondly, the application of external mechanical stress on soft matter-supported PEM samples. Here neutron reflectometry proofs to be a powerful tool due to its ability to test for the thickness of the sample and for its specific material content

at the same time.

CPP 18.11 Tue 12:15 ZEU 114

Immobile Light Water and Proton-Deuterium Exchange in Polyelectrolyte Multilayers — OXANA IVANOVA¹, OLAF SOLTWEDEL¹, ROLAND STEITZ², RALF KÖHLER², and CHRISTIANE A. HELM¹ — ¹Institut für Physik, Uni Greifswald, Felix-Hausdorff-Str. 6, 17487 Greifswald — ²Leibnitz-Zentrum für Material- und Energieforschung Berlin

To describe the swelling of polyelectrolyte multilayers (PEMs) on a molecular scale, the PEM architecture is varied. The polyanion is poly(styrenesulfonate) (PSS) and the polycation poly(allylamine hydrochloride) (PAH). PEM either consists of 10 protonated polyelectrolyte bilayers (p₁₀), 10 deuterated bilayers (d₁₀), or two different blocks, p₅d₅ or d₅p₅. Prior to the exposure to 100 % relative humidity (RH) D₂O or H₂O, the PEM is immersed in liquid D₂O or H₂O, respectively. The obtained scattering length density profiles provide insight into the exchange rates of the constituent molecules: The data indicate that three mobile protons of each PAH monomer are replaced by deuterium ions, yet most of the H₂O molecules found in PEM at 0% RH remain bound at 100% RH D₂O. This is in consistency with the fact that the core of PEM is in a glassy state. At 0% RH, the amount of bound water in the deuterated layers does not depend on the film architecture, whereas in the protonated layers it does.

CPP 19: Focus: Magnetic Soft Matter I

Time: Tuesday 9:30–12:30

Location: ZEU 222

Invited Talk

CPP 19.1 Tue 9:30 ZEU 222

Ferrofluids and their Rheology — STEFAN ODENBACH — Chair of Magnetofluidynamics, TU Dresden, 01062 Dresden

Suspensions of magnetic nanoparticles - commonly called ferrofluids - provide the possibility to control their flow and properties by moderate magnetic fields. After an introduction to ferrofluids, their basic properties and applications (combined with a few small experiments illustrating the magnetic control) the talk will mainly focus on the changes of the rheological properties of ferrofluids in a magnetic field.

Invited Talk

CPP 19.2 Tue 10:00 ZEU 222

Field-dependent structure and rheology of magnetic fluids as seen from theory and simulations — PATRICK ILG — Polymer Physics, ETH Zürich, Department of Materials, CH-8093 Zürich, Switzerland

The interplay between field- and flow-induced structure formation gives raise to very interesting transport properties of magnetic liquids like magnetoviscous and viscoelastic effects [1]. We briefly review some theoretical models of these phenomena, discuss their benefits and limitations and contrast them with simulation approaches [2]. Particular emphasis is laid on the relation between structural and rheological properties as a key issue for improving the current understanding of experimentally observed flow effects. Despite recent progress, there are several experimental findings that still present a challenge for theoretical and/or simulation approaches. Among other things, we mention hexagonal ordering in ferrofluids that might be induced by a delicate balance between steric repulsion and depletion interaction due to excess surfactants [3].

[1] S. Odenbach, J. Phys. Condens. Matter 15 (2003) S1497.

[2] P. Ilg and S. Odenbach, Ferrofluid Structure and Rheology, in "Colloidal Magnetic Fluids", S. Odenbach (Ed.), Springer Lecture Notes in Physics, Vol. 763, 2009.

[3] P. Ilg, Eur. Phys. J. E 26 (2008) 169.

CPP 19.3 Tue 10:30 ZEU 222

Ultra-centrifugation of single-domain magnetite particles and the DeGennes-Pincus approach to ferromagnetic colloids in the dilute regime — ALBERT PHILIPSE — Utrecht University, Van 't Hoff laboratory for physical and colloid chemistry, Padualaan 8, 3584 CH, the Netherlands

A fundamental issue for dipolar colloids is the effect of dipole moments on thermodynamic and transport phenomena. De Gennes and Pincus argued that the thermodynamics of ferromagnetic colloids, at sufficiently low density, can be simply modeled via an effective isotropic

attraction. The present work is motivated by the insight that this very same effective attraction would also determine transport quantities such as sedimentation and diffusion. We have studied sedimentation of stable dispersions of monodisperse magnetic iron-oxide (Fe₃O₄) colloids, with a dipolar coupling constant tuned by the average particle size. We find that the concentration-dependence of sedimentation rates abruptly changes sign, going from pure hard spheres to even weakly dipolar particles. This marked transition does not follow from the De Gennes-Pincus approach for reasons that will be explained. Our results confirm that effective isotropic attractions are not applicable to explain either thermodynamic or transport properties of magnetic fluids.

15 min. break

Invited Talk

CPP 19.4 Tue 11:00 ZEU 222

Mechanical Properties of Uniaxial Magnetic Gels — PHILIPPE MARTINOTY — Institut Charles Sadron, Strasbourg, France

Magnetic gels are composite materials made up of magnetic particles embedded in a polymeric matrix. They are called uniaxial when the magnetic particles are oriented in a permanent way in a given direction.

Two questions are crucial for optimizing uniaxial magnetic gels: how they are formed, and what are their responses to a mechanical field? However, these questions remained unstudied, essentially because the conventional rheometers do not allow performing shear measurements under magnetic field. Here we show some results taken during the formation process of a uniaxial magnetic gel and on the formed material with the piezoelectric rheometer we have recently developed.

This apparatus enables to take measurements of the complex shear modulus in a wide frequency range and for very weak applied strains. The kinetics of formation of the gel was followed by placing the cell in the air-gap of an electromagnet, and the organization of the magnetic particles observed by placing the cell under an optical microscope. Two types of uniaxial magnetic gel were studied; an aqueous gel based on a commercial ferrofluid, and an organic gel containing magnetite particles. This presentation is rounded off by a comparison with the mechanical properties of liquid crystal elastomers.

CPP 19.5 Tue 11:30 ZEU 222

Magnetic Capsules and Pickering Emulsions — ANDREAS KAISER, ROBERT ABRAHAM, and ANNETTE SCHMIDT — Institut für Organische Chemie und Makromolekulare Chemie, Heinrich-Heine-Universität, Universitätsstr. 1, 40225 Düsseldorf, Germany

In our work we present results on magnetic Pickering emulsions, using

superparamagnetic hybrid nanoparticles as susceptible stabilizers. By using the polymer shell of surface grafted iron oxide cores as adaptable solution promoter in a ω -solvent, thermoreversible magnetic fluids are obtained that are mixed with water, leading to stable oil in water (o/w) emulsions. Detailed investigations of the involved phase behaviour will be presented together with investigations on the long-term stability of the magnetic capsules towards temperature and in magnetic fields. Magnetic Pickering emulsions are of interest for advanced drug delivery and release systems.

CPP 19.6 Tue 11:45 ZEU 222

Untersuchung der magnetischen Eigenschaften von Nickel Nanostäben in Hydrogelen — ●PHILIPP BENDER, RAINER BIRNINGER, ANDREAS TSCHÖPE und ANDREAS MICHELS — Universität des Saarlandes, Saarbrücken, Deutschland

Nickel Nanostäbe wurden mit Hilfe einer stromgepulsten Abscheidung von Ni in porösen Aluminiumoxidtemplaten synthetisiert und anschließend mit Natronlauge aus der Oxidmatrix herausgelöst. Durch eine Oberflächenmodifikation der Nanostäbe konnten stabile, wasserbasierte Ferrofluide hergestellt werden, welche anschließend bei 50 °C in verflüssigte Glycergelatine eingerührt wurden. Auf Grund der Thermoreversibilität von Gelatine kommt es bei der Abkühlung des Gelinesols auf Raumtemperatur zur Vernetzung der Gelatinematrix und somit zu einem Einbau der Nickel Nanostäbe in das Gelnetzwerk (isotrope Ferrogele). Zusätzlich ist es möglich durch Anlegen eines äußeren Feldes während der Vernetzung die Nanostäbe auszurichten und dadurch Hydrogele mit einer ausgezeichneten Vorzugsrichtung zu erzeugen (anisotrope Ferrogele).

In der vorliegenden Arbeit wurde mit Hilfe von Magnetisierungsmessungen die Kopplung der magnetischen Eigenschaften der Nanostäbe mit den elastischen Eigenschaften der Gelatinematrix sowohl in isotropen als auch anisotropen Ferrogelen untersucht. Desweiteren wurden temperaturabhängige Hysterese-messungen sowie field- und zero-field-cooling, field-warming (FC/FW, bzw. ZFC/FW) Messungen durchgeführt um die Temperaturabhängigkeit der magneto-elastischen Kopplung innerhalb der Ferrogele zu charakterisieren.

CPP 19.7 Tue 12:00 ZEU 222

Particle co-operated block copolymer self-assembly — ●MOTTAKIN M. ABUL KASHEM¹, JAN PERLICH¹, ALEXANDER DIETHERT¹, WEINAN WANG¹, MINE MEMESA², JOCHEN S. GUTMANN², EVA MAJKOVA³, IGNAĆ CAPEK⁴, STEPHAN V. ROTH⁵, and MÜLLER-BUSCHBAUM PETER¹ — ¹TU München, Physik-Department LS E13, James-Frank-Str.1, Garching, Germany — ²MPI for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany — ³Inst. of Phys.

SAS, Dúbravská 9, SK 84511 Bratislava, Slovakia — ⁴Polymer Inst., SAS, Dúbravská 9, SK 84236 Bratislava, Slovakia — ⁵HASYLAB at DESY, Notkestr. 85, 22603 Hamburg, Germany

We have investigated the role of nanoparticles in particle co-operated self-assembly process and the domain orientation in asymmetric diblock copolymer films in order to create ordered array of magnetic nanoparticles [1-2]. Thin films are prepared from solutions of polystyrene-block-polymethylmethacrylate (PS-b-PMMA) containing varying amount of iron oxide nanoparticles. During annealing, the nanoparticles distribute themselves inside the cylindrical domains of PMMA, which increases the diameters of cylindrical domains and cylinder-to-cylinder distances. Moreover, the nanoparticles contribute to the perpendicular orientation of PMMA domains through balancing the interfacial energy difference between PS and PMMA blocks. The investigations have been carried out by using AFM and SEM, x-ray reflectivity and GISAXS.

1.Abul Kashem, et al. *Macromolecules* 2007, 40, 5075. 2.Abul Kashem, et al. *Macromolecules* 2008, 41, 2186.

CPP 19.8 Tue 12:15 ZEU 222

Surface Instabilities and Magnetic Soft Matter — ●CHRISTIAN GOLLWITZER¹, MARINA KREKHOVA², GÜNTER LATTERMANN², INGO REHBERG¹, and REINHARD RICHTER¹ — ¹Experimentalphysik V, Universität Bayreuth, 95440 Bayreuth, Germany — ²Makromolekulare Chemie I, Universität Bayreuth, 95440 Bayreuth, Germany

Thermoreversible ferrogels are the most recent incarnation of magnetic soft matter [1]. Their mechanical deformation in homogeneous magnetic fields has been studied for the case of a sphere in [2]. We report now on the formation of surface instabilities in a layer of thermoreversible ferrogel when exposed to a vertical magnetic field. Both static and time dependent magnetic fields are employed. Under variations of temperature, the viscoelastic properties of our soft magnetic matter can be tuned. Stress relaxation experiments unveil a critical scaling behaviour of the relaxation time, as predicted in [3]. The resulting magnetic threshold for the formation of Rosensweig-cusps is measured for different temperatures, and compared with theoretical predictions [4]. Details can be found in the preprint [5].

[1] G. Lattermann and M. Krekhova, *Macromol. Rapid Commun.*, 2006, **27**, 1373–1379

[2] C. Gollwitzer, A. Turanov, M. Krekhova, G. Lattermann, I. Rehberg, and R. Richter, *J. Chem. Phys.*, 2008, **128**, 164709.

[3] P. G. de Gennes, *Macromolecules*, 2002, **35**, 3785–3786.

[4] S. Bohlius, H. Brand, H. Pleiner, and M. Gels, *Z. Phys. Chem*, 2006, **220**, 97–104.

[5] <http://arxiv.org/abs/0811.1526>

CPP 20: Focus: Magnetic Soft Matter II

Time: Wednesday 9:30–12:30

Location: ZEU 222

Invited Talk

CPP 20.1 Wed 9:30 ZEU 222

Truncated patterning in the normal field instability — ●ANDREAS BOUDOUVIS — School of Chemical Engineering, National Technical University of Athens, Athens 15780, Greece

The normal field instability sets in a pool of ferrofluid when the strength of a uniform magnetic field, applied in a direction normal to the horizontal free surface of the pool, exceeds a threshold.

Most studied in laterally unbounded pools, the instability gives way to spontaneously formed static patterns of spikes exhibiting striking spatial symmetry, usually hexagonal and rarely square [1, 2].

The finiteness of a pool introduces "imperfections", namely lateral pattern truncation along with side-wall wetting [3]. Of concern here is the normal field instability and the accompanying pattern formation in round containers of moderate diameter. Bifurcation diagrams of truncated patterns of two, three and four spikes are computed by solving the equations of the 3-D capillary magnetohydrostatics with the Galerkin/finite element method. The theoretical predictions, which are in good agreement with experimental measurements, reveal the structure of the solution space, namely the connectivity, the multiplicity and the stability of the truncated patterns, in the studied parameter "window", defined by varying applied field strength and container diameter.

[1] Cowley M D & Rosensweig R E 1967 *J. Fluid Mech.* 30, 671. [2] Gollwitzer C, Matthies G, Richter R, Rehberg I & Tobiska L 2007 *J.*

Fluid Mech. 571, 455. [3] Boudouvis A G, Puchalla J L & Scriven L E 1988 *J. Colloid Interface Sci.* 124, 677.

CPP 20.2 Wed 10:00 ZEU 222

Structure of ferrofluid nanofilms in homogeneous magnetic fields — ●JELENA JORDANOVIC and SABINE H. L. KLAPP — Institut für Theoretische Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin

We report molecular dynamic simulations for a model Stockmayer fluid confined between two plane, parallel walls and subject to an external homogeneous field. The occurring layers, which are characteristic for fluid nanofilms, can be controlled via the field such that for an appropriate film thickness a new layer is created in a perpendicular field while in a parallel field one layer can be destroyed [1]. This field-controlled layering modulation as well as formation of hexagonal or labyrinth in-plane patterns have also been observed in experiments [2,3] and are a promising route for designing novel materials. In our study we examine in detail the dependence of the field-induced structural changes in-plane and normal to the film surfaces on the thermodynamic state [4] for both field directions. Also, we inspect the influence of the attractive contribution of the Lennard-Jones potential on the structural behavior in field. Additionally we investigate a mono- to bilayer transition induced via a perpendicular field to relate our findings to quasi-two-dimensional systems.

[1] J. Jordanovic and S. H. L. Klapp, Phys. Rev. Lett. 101, 038302 (2008).

[2] A. Vorobiev et.al. Phys. Rev. Lett. 93, 267203 (2004).

[3] V. Germain et.al. J. Phys. Chem B 109, 5541 (2004).

[4] J. Jordanovic and S. H. L. Klapp, submitted.

CPP 20.3 Wed 10:15 ZEU 222

Ground state structures in ferrofluid monolayers: Theory and Simulations. — ●SOFIA KANTOROVICH^{1,2}, VICTOR DANILOV¹, TAISIA PROKOPYEVA¹, and CHRISTIAN HOLM² — ¹Ural State University, Ekaterinburg, Russia — ²University of Stuttgart, Stuttgart, Germany

The investigation of the microstructure of ferrofluid monolayers at low temperatures was extended to bidisperse model systems. Previously we have shown that a single ideal ring is the most probable ground state structure for a monodisperse ferrofluid monolayer. Starting with system containing large particles we introduce small particles as defects, and analyze the resulting structures, using a combination of analytical methods and Monte Carlo simulations. The crucial influence of the interaction between particles from different fractions (namely, large and small ones) is demonstrated.

CPP 20.4 Wed 10:30 ZEU 222

Phase transitions and ordering of confined magnetic fluids in applied magnetic fields — ●ISTVAN SZALAI¹ and SIEGFRIED DIETRICH^{2,3} — ¹Institute of Physics, University of Pannonia, H-8201 Veszprem, PO Box 158, Hungary — ²Max-Planck-Institut für Metallforschung, Heisenbergstr. 3, D-70569 Stuttgart, Germany — ³Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Pfaffenwaldring 57, D-70569 Stuttgart, Germany

For the case of the presence of a magnetic field we apply a modified mean-field density functional theory to determine the phase behavior of magnetic fluids in slit-like pores formed by two parallel walls with identical substrate potentials. The magnetic fluid is modeled by the Stockmayer interaction potential. A Carnahan-Starling equation of state based fundamental-measure theory is employed to incorporate the effects of short-ranged hard sphere-like correlations while the long-ranged contributions to the fluid interaction potential are treated perturbatively. The ferromagnetic liquid - ferromagnetic vapor first-order phase transitions and the structural properties of both phases are investigated. The magnetization and susceptibility of the magnetic fluids are also studied. We discuss how the phase diagrams are shifted and distorted upon varying the field strength and the pore width.

CPP 20.5 Wed 10:45 ZEU 222

Gas-liquid critical behavior in fluids of soft-repulsive charged dumbbells — ●HEIKO BRAUN and REINHARD HENTSCHEKE — Fachbereich Mathematik und Naturwissenschaften, Bergische Universität Wuppertal, D-42097 Wuppertal, Germany

The existence of gas-liquid coexistence in dipolar fluids with no other contribution to attractive interaction than dipole-dipole interaction is a basic and open question in the theory of fluids. Recent MC work by Camp and coworkers [1] indicates that a fluid of charged hard dumbbells does exhibit g-l coexistence. This system has the potential to answer the above fundamental question, because the charge-to-charge separation d on the dumbbells may be reduced to, at least in principle, yield the dipolar fluid limit. Here we present MD results for the g-l phase behavior including the critical point of charged soft dumbbells for fixed dipole moment and fixed charges as function of d . We do find a g-l critical point at finite temperature for fixed dipole moment at small d . In this limit, however, we also find that the dumbbells form reversible networks so that the transition possibly is due to the mechanism suggested by Tlustý and Safran [2] for reversible networks.

[1] G. Ganzenmüller, P. J. Camp, J. Chem. Phys. 126, 191104 (2007)

[2] T. Tlustý, S. A. Safran, Science 290, 1328 (2000)

15 min. break

Invited Talk

CPP 20.6 Wed 11:15 ZEU 222

Using triaxial magnetic fields to form optimized particle composites — ●JAMES MARTIN — Sandia National Laboratories, Albuquerque, New Mexico, USA

Complex dynamics can be induced in magnetic particle suspensions by subjecting them to three orthogonal alternating magnetic fields. The range of behavior that can be induced is broad, including particle vortex formation and oscillating sheet-like structures. When such particle suspensions are polymerized in the triaxial field, a variety of surprising structures form - such as particle honeycombs and chain networks - due to the interaction of the viscosity divergence with the heterodyne field frequencies. Such materials are found to have highly optimized magnetic properties and we have completed extensive Brownian Dynamics simulations to understand the emergence of structure in these materials.

CPP 20.7 Wed 11:45 ZEU 222

Shape Discrimination with Hexapole Dipole Interactions in Magic Angle Spinning Colloidal Magnetic Resonance. — PIETRO TIerno¹, STEFFEN SCHREIBER², WALTER ZIMMERMANN², and ●THOMAS FISCHER² — ¹University of Barcelona — ²University of Bayreuth

We study the interactions between magnetically driven anisotropic and isotropic colloidal rotors interacting via induced magnetic dipolar and multipolar forces in a precessing magnetic field. Close to the magic precession angle dipole dipole interactions between the rotors can be tuned such that shape sensitive higher multipole moments allow to assemble originally spherical rotors into clusters of defined shape and size.

CPP 20.8 Wed 12:00 ZEU 222

Brownian ratchet effect in a ferrofluid sample — ●THOMAS JOHN and RALF STANNARIUS — Otto-von-Guericke-Universität Magdeburg, Germany

We investigate experimentally a Brownian ratchet system suggested by Engel et al. [1]. The Brownian ratchet system is based on a magnetic fluid which contains nanometer sized magnetic particles in a thermal bath of carrier fluid. An external static and perpendicular a temporal asymmetric oscillatory magnetic field acts on the particles. Depending on the parameter of this non-rotating field on a spherical ferrofluid sample the induced macroscopic torque is measured. A quantitative comparison of measured torques with predictions from a microscopic [2] and a phenomenological model from M. I. Shliomis [3] are given. Both models describe certain aspects of the measurements only in limited parameter ranges. Several qualitative discrepancies between these models and experiment are found.

[1] A. Engel et al., Phys. Rev. Lett. **91**, 060602 (2003).

[2] A. Engel et al., Phys. Rev. E **70**, 051107 (2004).

[3] M. I. Shliomis, Phys. Rev. Lett. **92**, 188901 (2004).

CPP 20.9 Wed 12:15 ZEU 222

Thermomagnetic convection in magnetic fluids influenced by spatially modulated magnetic fields — ●ADRIAN LANGE and STEFAN ODENBACH — Technische Universität Dresden, Institute of Fluid Mechanics, Chair of Magnetofluidynamics, 01062 Dresden, Germany

The influence of a spatially modulated magnetic field on the convection in a horizontal layer of magnetic fluid bounded by isothermal non-magnetic boundaries is analysed. Such a magnetic field is generated by a spatial modulation of the top and bottom boundary of the fluid layer. Depending on the sign of the relative phases between the modulations, the basic state, the behaviour of the critical Rayleigh number, and the character of the onset of convection is studied. With respect to the latter, it is of particular interest if a Hopf bifurcation can be found as for spatially periodic modulated Rayleigh-Bénard convection [1].

[1] R. Schmitz and W. Zimmermann, Phys. Rev. E **53**, 5993 (1996).

CPP 21: Polymer Physics II

Time: Wednesday 9:30–12:30

Location: ZEU 114

CPP 21.1 Wed 9:30 ZEU 114

Structure analysis with micrometer spatial resolution in polymer fibers — ●NORBERT STRIBECK¹, ULRICH NÖCHEL¹, and ARMANDO ALMENDÁREZ CAMARILLO² — ¹Universität Hamburg, Institut TMC, 20146 Hamburg, Germany — ²Instituto Tecnológico de Celaya, 38010 Celaya Gto., Mexico

The investigation of structure gradients in fibers, cylindrical rods or pipes by the X-ray microbeam scanning technique is put on its theoretical fundament. It is shown that the observed smeared structure information is readily reconstructed by the inverse Abel transform, for which fast and low-noise algorithms are available [1]. As a result, the scattering patterns emanating from the series of volume elements on the fiber radius are obtained (X-ray scattering-fiber computer-tomography, XSF-CT). Perfect reconstruction is achieved when the structure in every voxel shows fiber symmetry (local fiber symmetry, LFS). Violation of LFS results in characteristic reconstruction errors [2]. These can be interpreted in terms of two elementary deviating topologies (tangential grain, radial grain). Application to nanostructure analysis of polymer fibers is demonstrated.

[1] Striebeck *et al.* Macromol. Chem. Phys. (2008) 209(19), 1976-1982[2] Striebeck *et al.* Macromolecules (2008) 41(20), 7637-7647

CPP 21.2 Wed 9:45 ZEU 114

Investigation of changes in crystalline structure during deformation of semi-crystalline polymers by synchrotron radiation — ●KONRAD SCHNEIDER and ANDREAS SCHÖNE — Leibniz Institut für Polymerforschung Dresden e.V., Hohe Strasse 6, 01069 Dresden, Germany

During deformation of semi-crystalline polymers very complex structural changes appear. To distinguish certain processes simultaneous WAXS and SAXS was measured during deformation. The characteristic changes will be presented and discussed in detail. First changes in the crystalline phase appears far before reaching the yielding point. This correlates with the onset of irreversible deformation. In the yielding region radical changes on long- as well as short scale range appear.

CPP 21.3 Wed 10:00 ZEU 114

Molecular weight dependence of the crystalline-amorphous superstructure of semi-crystalline polymers — ●ALBRECHT PETZOLD and THOMAS THURN-ALBRECHT — Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle, Germany

During crystallization polymers form a crystalline-amorphous superstructure consisting of lamellar crystals with a typical thickness of about 10 nm. This non-equilibrium structure is often explained by the kinetics of crystallization during which the crystals which form fastest, are selected. The thickness d_a of the amorphous layers separating adjacent crystals is in most cases not considered. To find out which parameters and physical processes determine d_a , we undertook a systematic study of the corresponding structural parameters by small angle x-ray scattering using a series of polyethyleneoxide (PEO) with different molecular weight as a model system. We show that for this system the thickness of the amorphous layers is a well defined equilibrium quantity which depends only on molecular weight and temperature, and not on the conditions of crystallization, while the thickness of the crystalline layers is strongly influenced by the kinetics of crystallization and lamellar thickening and in general is much less uniform. The fact that d_a increasing with molecular weight indicates that the semi-crystalline morphology is related to structure of the chains in the amorphous melt before crystallization.

CPP 21.4 Wed 10:15 ZEU 114

Studying Radical Polymerization by Single Molecule Spectroscopy — ●DOMINIK WÖLL¹, FRANS DE SCHRYVER², KLAUS MÜLLEN³, and JOHAN HOFKENS² — ¹Zukunftskolleg/Fachbereich Chemie, Universität Konstanz, Universitätsstraße 10, 78457 Konstanz, Germany — ²Laboratory for Photochemistry and Spectroscopy, Celestijnenlaan 200 F, Katholieke Universiteit Leuven, 3001 Heverlee, Belgium — ³Max-Planck-Institut für Polymerforschung, Ackermannweg 10, 55128 Mainz, Germany

The possibility to observe single molecules, first realized about 20 years ago, has opened up a fascinating field of research. Even though poly-

mers are popular systems for single molecule spectroscopy studies, the process of radical polymerization has so far not been studied at the single molecule level.

We investigated how the molecular motion of single fluorescent probes changes during the synthesis of polystyrene, polystyrene networks and polymethylmethacrylate by bulk radical polymerization. As probes, we have chosen perylene diimide derivatives of different sizes and functionalities. The translational motion over the entire conversion range from free diffusion to immobilization of the dyes could be followed by a combination of fluorescence correlation spectroscopy and wide-field microscopy. In contrast to ensemble measurements, the evolution of heterogeneities could be strikingly visualized by SMS. Such heterogeneities not only influence the progress of polymerization but also the properties of the synthesized polymer and are especially pronounced during the formation of networks.

CPP 21.5 Wed 10:30 ZEU 114

Polymer melt dynamics studied by Nuclear Magnetic Resonance — PATRICK HÜBSCH¹, ●FABIAN VACA CHAVEZ¹, WOLFGANG BINDER², RONALD ZIRBS², and KAY SAALWÄCHTER¹ — ¹Institute of Physics - Faculty of Natural Sciences II, Martin-Luther-University Halle-Wittenberg, Betty-Heimann-Str. 7, 06120, Halle, Germany — ²Macromolecular Chemistry Group, Institute of Chemistry, Heinrich Damerow Strasse 4, 06120, Halle, Germany

Proton Multiple-Quantum (MQ) NMR is a powerful technique to investigate polymer dynamics due to its sensitivity to molecular motions on very different timescales [1]. In this work, we apply MQ NMR to linear poly(cis-1,4-isoprene) and poly(isobutylene) of different molecular weight above the glass transition over suitable ranges of temperature, in order to establish the dynamic regimes predicted by the tube model, and, for the first time, to extract actual time scale information. This directly complements many neutron scattering studies, which are restricted to the sub- μ s-timescale. Measurements on PIB-grafted silica particles with different molecular weights and different chain densities on the surface of the particle are also shown. The data is analyzed by establishing scaling laws which can be directly associated with different dynamic regimes predicted by the tube/reptation model [2]. Full analytical analyses based on a correlation function which explicitly includes segmental, Rouse, and reptation dynamics are discussed.

[1] K. Saalwächter, Prog. NMR Spect., **2007**, 51, 1-35. [2] R. Graf, A. Heuer, H.W. Spiess, Phys. Rev. Lett., **1998**, 80, 5738-5741.**15 min. break**

CPP 21.6 Wed 11:00 ZEU 114

Dielectric and electric relaxations at nanometric length scales — ●FRIEDRICH KREMER¹, ANATOLI SERGHEI^{1,2}, MARTIN TRESS¹, JOSHUA RUME SANGORO¹, and CIPRIAN IACOB¹ — ¹Institute for Experimental Physics I, University of Leipzig, Germany — ²Department of Polymer Science and Engineering, University of Massachusetts Amherst, Amherst, MA 01003, USA

Dielectric spectroscopy benefits from the extraordinary advantage that its sensitivity increases with decreasing thickness of a sample capacitor. This enables one for instance to carry out broadband spectroscopic measurements on quasi isolated polymer coils in nano structured capacitor arrangements, having thicknesses as small as 100 nm. It is demonstrated that for polymers like polyvinyl pyridin (P2VP) or polyvinylacetate (PVAC) the dynamic glass transition can be measured for (averaged) sample thickness as small as ~ 2 nm in a wide spectral range (10^{-2} Hz – 10^6 Hz) and at temperatures between 150 K to 350 K. No shift of the mean relaxation rate and no broadening of the relaxation time distribution function are found compared to the bulk liquid.

Electrode polarization is an ubiquitous phenomenon taking place at the interface between a metal and an ionic conductor. A quantitative theory will be presented, which enables one to deduce from its characteristic frequency, temperature and concentration dependencies – by use of a novel formula – the bulk conductivity of the ionic liquid under study. It is shown that the electrical relaxation processes take place within a nanometric layer at the (ionic conductor/metal) interface which can be analysed in detail.

CPP 21.7 Wed 11:15 ZEU 114

Heterogeneous Dynamics of Polymer PMA close to Glass Transition Temperature — ●SUBHASIS ADHIKARI, MARKUS SELMKE, and FRANK CICHOS — Molecular Nano-photonics, Institute of Experimental Physics I, University of Leipzig, 04103 Leipzig, Germany

In the study of glassy polymer systems there has been a long debate about the nature of heterogeneity of the material. There exist mainly two pictures of spatial and dynamic heterogeneities, where on one side the dynamical properties of change with the spatial position in the sample and on the other side with time at the same position of the sample. Recent experiments on single dye molecules in glassy glycerol suggest mainly a spatial heterogeneity, where each molecule shows a different dynamics. In this presentation we present recent results on this issue in long chain polymeric systems. We have analyzed the rotational diffusion dynamics of PDI dye molecule in high molecular weight glassy polymer PMA at both the ensemble and single molecule level close to T_g . Ensemble measurements have been done to compare with the single molecule measurement. From our single molecule measurements we obtain a broad distribution of rotational relaxation times of different individual molecules at a given temperature which indicates that the dynamics in some regions is orders of magnitude faster than the dynamics in other regions only a few nanometres away. Again this distribution becomes broader when temperature decreases to T_g . The rotational correlation function of a single molecule is however well fitted by a stretched exponential decay. This nonexponential behavior gives a clear evidence of existence of dynamical heterogeneity.

CPP 21.8 Wed 11:30 ZEU 114

The glass transition in blends of molecular glasses — ●ROMAN UEBERSCHAER, EVGENY TATAROV, THOMAS FUHRMANN-LIEKER, and JOSEF SALBECK — Universität Kassel, Heinrich-Plett-Straße 40, D-34132 Kassel, Germany

Blends of molecular glasses and their properties are of great interest for applications in optoelectronics. In this contribution we present results of differential-calorimetric measurements on binary blends of spiro-compounds. Spiro-compounds are low-molecular organic glass formers with glass transition temperatures well above 100 °C. The investigation was focused on the composition dependence of the glass transition temperature for two prototype blend systems. One system consists of two components that are miscible over the whole composition range. Applying the Fox law that approximates the inverse glass temperature as the sum of the inverse glass temperatures of the two compatible components weighted by their mass fractions, we found that a modified version of the Fox law where the weighting is related to the mole fraction predicts the glass transition temperature of the blend more accurately. This result might be useful for approximating the phase compositions of partially miscible blends from the corresponding glass transition temperatures. We discuss this issue with respect to the second system that exhibits a broad miscibility gap despite the high entropy of mixing that is expected for low-molecular substances.

CPP 21.9 Wed 11:45 ZEU 114

On the glassy state of multiphase and pure polymer materials — ●STEPHAN ALEXANDER BAEURLE — Institute of Physical and Theoretical Chemistry, Regensburg University, D-93053 Regensburg, Germany

In this presentation we introduce a new glass theory and investigate its suitability for describing the mechanical response of thermoplastic elastomers composed of styrenic-block copolymers. The investigated materials are composed of glassy domains of polystyrene, which physically link soft rubbery chain segments made of either polybutadiene or polyisoprene. We demonstrate that the crossover in the shift factors, observed experimentally to change from Williams-Landel-Ferry to Arrhenius behavior passing through a characteristic crossover temperature T^* from below, coincides with the crossover from power-law to stretched-exponential behavior of the stress relaxation found in re-

cent tensile experiments. Moreover, we show that the characteristic crossover temperature T^* is identical with the underlying true equilibrium second-order phase transition temperature T_2 of the polystyrene crosslinks, predicted by the thermodynamic theory of Gibbs and Di Marzio for pure glassy polystyrene in the infinite-time limit. By combining the recently introduced theory of Di Marzio and Yang with the significant-structure theory of Eyring and Ree, we develop a new glass theory, which is capable of explaining the mechanical response of multiphase as well as pure glassy materials. Moreover, we show a clear evidence for the existence of T_2 postulated in 1950s for pure glasses and hotly debated since then.

CPP 21.10 Wed 12:00 ZEU 114

Build-up and relaxation of stresses in a glass-forming soft-sphere mixture — ●JOCHEN ZAUSCH¹ and JÜRGEN HORBACH² — ¹Inst. f. Physik, Universität Mainz, Staudinger Weg 7, 55099 Mainz — ²Inst. f. Materialphysik im Weltraum, DLR, Linder Höhe, 51147 Köln

Glass-forming liquids under shear often exhibit the effect of shear thinning, i.e. the decrease of viscosity η upon increasing shear rate $\dot{\gamma}$ if $\dot{\gamma} \gtrsim 1/\tau$ (with τ the relaxation time). The viscosity is related to the shear stress $\sigma = \dot{\gamma}\eta$ that is built up due to the external shear field. Employing extensive non-equilibrium Molecular Dynamics computer simulations of a glass-forming binary Yukawa mixture we aim at understanding the transition from a quiescent state to steady shear. To this end, we monitor the stress as a function of the strain $\dot{\gamma}t$ after a suddenly commencing or terminating shear flow.

After switching on the shear field, the stress σ shows an overshoot at a strain $\dot{\gamma}t \approx 0.1$ that marks the transition from elastic to plastic deformation. The stress increase is closely related to the development of structural anisotropies, which we quantify by a projection of the pair correlation function onto a spherical harmonic of degree 2. After switching off the external drive in the elastic regime, stresses decay to zero on the time scale τ , whereas a switch-off in the plastic regime leads to the much faster decay on time scale $1/\dot{\gamma}$. We attribute this behaviour to the different distributions of local shear stresses in these regimes. Our results are corroborated by confocal microscopy experiments of colloidal systems and by a theoretical approach in the framework of mode-coupling theory (J. Phys.: Condens. Matter **20**, 404210 (2008)).

CPP 21.11 Wed 12:15 ZEU 114

Microrheology with Fluorescence Correlation Spectroscopy — ●SILKE RATHGEBER^{1,2}, HANS-JOSEF BEAUVISAGE¹, HUBERT CHEVREAU^{1,3}, NORBERT WILLENBACHER⁴, and CLAUDE OELSCHLAEGER⁴ — ¹Max Planck-Institute for Polymer Research, 55128 Mainz, Germany. — ²Johannes Gutenberg-University Mainz, 55099 Mainz, Germany. — ³Ecole Polytechnique Universitaire de Lille, 59655 Villeeneuve D'Ascq Cedex, France. — ⁴Technical University Karlsruhe, 76131 Karlsruhe, Germany.

We show that fluorescence correlation spectroscopy (FCS) can be applied to passive microrheological (MR) experiments. We performed measurements on a high molecular weight poly(ethylene oxide)-water solution in order to allow direct comparison of the results to the measurements of Weitz and Mason using diffusing wave spectroscopy (DWS) and quasielastic light scattering (QELS). We derived the bulk rheological shear moduli covering more than five decades in frequency ($\omega \leq 10^{-1}$ rad/s to $\omega \geq 10^4$ rad/s). The MR results are compared to those obtained with bulk rheological methods on the same samples using a rotational rheometer as well as a piezo driven squeeze flow apparatus. Good agreement between MR results probing the local rheological response and those obtained from the bulk methods are found. MR with FCS covers a similar ω range as QELS and DWS together with some limitations to higher ω due to the lower spatial resolution of FCS compared to DWS. However, the small sample sizes (10 μ L) and small tracer concentrations (nM) involved in FCS make this method a powerful tool in particular for biological and medical applications.

CPP 22: Fokus: Conjugated Polymers

Time: Wednesday 9:30–12:30

Location: ZEU 160

Topical Talk CPP 22.1 Wed 9:30 ZEU 160
Charge transport in doped poly(p-phenylene vinylene) — Y. ZHANG, B. DE BOER, and P. W. M. BLOM — Zernike Institute for Advanced Materials and Dutch Polymer Institute, University of Groningen, The Netherlands

The hole transport in poly(dialkoxy-p-phenylene vinylene) (PPV) based diodes is known to be space-charge limited (SCL) for Ohmic contacts. At room temperature the SCL current in PPV-derivatives is governed by the dependence of the hole mobility on charge carrier density, whereas at low temperatures the field-dependence prevails [1]. We present controlled p-type doping of MEH-PPV deposited from solution using tetrafluoro-tetracyanoquinodimethane (F4-TCNQ) as a dopant. By using a co-solvent aggregation in solution can be prevented and doped films can be deposited. Upon doping the current-voltage characteristics of MEH-PPV based hole-only devices are increased by several orders of magnitude and a clear Ohmic behavior is observed at low bias. Taking the density dependence of the hole mobility into account the free hole concentration due to doping can be derived. We find that a doping concentration of 1.0 wt.% leads to a free carrier density of $2 \times 10^{22} \text{ m}^{-3}$. Neglectance of the density-dependent mobility would lead to an overestimation of the free hole density by an order of magnitude. The free hole densities are further confirmed by impedance measurements on Schottky diodes based on F4-TCNQ doped MEH-PPV and a silver electrode.

1. C. Tanase, P.W.M. Blom, and D.M. de Leeuw, Phys. Rev. B. 70, 193202 (2004)

Topical Talk CPP 22.2 Wed 10:00 ZEU 160
A realistic description of the charge carrier wavefunction in microcrystalline polymer semiconductors — ALESSANDRO TROISI, DAVID L. CHEUNG, and DAVID P. MCMAHON — Department of Chemistry, University of Warwick, Coventry, UK

The electronic structure of the charge carrier in one of the most commonly used semiconducting polymer (P3HT) is investigated using a combination of classical and quantum chemical methods. It is shown that the carriers are localized in correspondence of long lived traps which are present also in the crystalline phase of the polymer and these traps are characterized with chemical detail. The existence of activated transport also for very ordered polymer phases (regardless of the strength of the polaron formation energy) is explained and the provided chemical description of the trapped states can be used to design materials with improved mobility. It is shown that is possible to use computational chemistry methods to fill the gap between phenomenological descriptions of charge transport in polymers and microscopic description of the individual quantum dynamic process.

Topical Talk CPP 22.3 Wed 10:30 ZEU 160
Influence of microstructure on transport and recombination in conjugated polymer:fullerene blend films — JENNY NELSON¹, AMY BALLANTYNE¹, MARIANO CAMPOY-QUILES¹, TOBY FERENCZI¹, JARVIST FROST¹, PANOS KEIVANIDES¹, JI-SEON KIM¹, JAMES KIRKPATRICK¹, CHRISTIAN MUELLER², DONALD BRADLEY¹, JAMES DURRANT¹, PAUL SMITH², and NATALIE STINGELIN³ — ¹Imperial College London, UK — ²ETH Zuerich, Switzerland — ³Queen Mary University of London, UK

The dynamics of charge carriers in conjugated polymer:small molecule blend solar cells are strongly influenced by the microstructure of the blend films. Efficient photocurrent generation appears to require, at the same time, a high degree of order in local molecular packing (benefitting charge transport and charge separation), a large interface (for charge separation) and significant phase segregation (to minimise charge recombination). In this work, we will show how a combination of spectroscopic techniques, electrical measurements and studies of phase behaviour can be used to build up a picture of the microstructure in a polymer: fullerene blend film, and to relate the microstructure to the dynamics of charge separation, transport and recombination. To interpret the results we use coarse grained models of the evolution of phase morphology and kinetic Monte Carlo models of charge transport and recombination. Finally, we demonstrate that the optimum blend composition for photocurrent generation can be related in a rational way to the phase behaviour of the binary system and in particular to the self-organising tendency of the component materials.

Topical Talk CPP 22.4 Wed 11:00 ZEU 160
Charge transport along isolated conjugated molecular wires — FERDINAND C. GROZEMA and LAURENS D.A. SIEBBELES — DelftChemTech, Delft University of Technology, The Netherlands

In the majority of measurements of charge transport in single molecular wires the molecule is connected to two electrodes. The results obtained from these measurements are often to a large extent determined by the molecule-electrode interface and the transport occurs by direct tunneling with the charge never being fully located on the wire. Therefore is difficult to obtain information on the mobility of charges when they are actually on the molecule. We use a unique combination of techniques that enables us to measure the mobility of charges along conjugated polymers chains that are isolated from each other by bringing them in a dilute solution. Charges are generated by irradiation with pulses of high-energy electrons and the mobility of these charges is determined by contact-less time-resolved microwave conductivity measurements. These experiments have been performed for a wide variety of different types of conjugated polymers and it was found that charge carrier mobility strongly depends on the molecular structure [1-3].

1. P. Prins, F.C. Grozema, J.M. Schins, S. Patil, U. Scherf and L.D.A. Siebbeles, Phys. Rev. Lett., 2006, 96, 146601

2. P. Prins, F.C. Grozema and L.D.A. Siebbeles, J. Phys. Chem. B, 2006, 110, 14659

3. F.C. Grozema, C. Houarner-Rassin, P. Prins, L.D.A. Siebbeles and H.L. Anderson, J. Am. Chem. Soc., 2007, 129, 13370

Topical Talk CPP 22.5 Wed 11:30 ZEU 160
Charge transport: a multiscale model in polymers — JAMES KIRKPATRICK — Department of Physics, Imperial College London, UK

This contribution addresses the relationship between charge transport and polymer chain morphology. It attempts to determine whether our instinctive model of charges rapidly moving along chains and slowly between them is consistent with charge transport parameters computed using state of the art computational methods.

The morphology of polymer films is simulated using molecular dynamics, charge transport parameters are computed using semi classical methods and charge transport is simulated by solution of rate equations. The model system considered is polypyrrole. Global arrangement is manipulated by preparing morphologies with chains aligned along one axis ("fiber"), lying in the plane ("slice") or disordered in all directions ("isotropic"). Local molecular arrangement can also be manipulated by making the chains stiffer, simulating their morphology when oxidized.

Non-adiabatic semi-classical theory will be used to describe hops between different chains. The motion of charges along polymer chains will be approximated as adiabatic hops. The influence of parametrization of charge transport rates on mobility will be studied.

Topical Talk CPP 22.6 Wed 12:00 ZEU 160
From amorphous polymers to discotic liquid crystals - Measuring charge carrier mobility with the time-of-flight technique — FREDERIC LAQUAI¹, DIRK HERTEL², MARCEL KASTLER¹, KLAUS MUELLEN¹, and GERHARD WEGNER¹ — ¹Max-Planck-Institut für Polymerforschung, Mainz, Germany — ²University of Cologne, Germany

The charge carrier mobility is one of the key parameters of conjugated materials that greatly determines the performance of electronic devices. It can be measured by various techniques, for instance, the time-of-flight (TOF) technique, space-charge limited current measurements or pulsed radiolysis time resolved microwave conductivity measurements. Here, the charge-generation-layer TOF technique has been used to study hole mobility of a series of amorphous poly-spirobifluorene copolymers. The copolymers contain different concentrations of triarylamine units in the polymer backbone and have mobilities in the range of $10^{-6} - 10^{-4} \text{ cm}^2/\text{Vs}$. The results of the field and temperature dependent measurements can be well interpreted in the framework of the 3D-Gaussian disorder formalism. The experiments show that high hole mobility does not necessarily lead to high performance in OLEDs. Secondly, the TOF technique has been employed to study hole transport in hexa-peri-hexabenzocoronene molecules that can be organised into face-on or edge-on arrangements between substrates depending on

the nature of the alkyl-chains attached to the molecule. Mobilities of $10^{-3} \text{ cm}^2/\text{Vs}$ have been determined and results could be well analysed

in the framework of a 1D-transport model.

CPP 23: Electronic and Optical Properties

Time: Wednesday 14:00–17:00

Location: ZEU 114

CPP 23.1 Wed 14:00 ZEU 114

Analyzing Anisotropic Light Propagation by Defocused Imaging of Single Emitters — ●REBECCA WAGNER and FRANK CICHOS — Molecular Nanophotonics Group, University of Leipzig, Linnéstraße 5, 04103 Leipzig

Many materials introduce an optical anisotropy to internal emitters due to their internal structure. Layers of oriented polymer molecules have different dielectric constants parallel and perpendicular to the layer, i.e. they are birefringent. Photonic crystals, materials with periodic variation of the dielectric constant, have stop bands for certain directions in which propagation of light is prohibited. These effects have been measured for example by angle resolved fluorescence spectroscopy for ensembles of emitters, thereby averaging over extended areas. However, if the anisotropy is caused by the local environment of the emitters, a spatially-resolved measurement is necessary. We show that optical anisotropy can be measured locally by defocused imaging microscopy of internal emitters. This leads to asymmetric diffraction patterns that contain information about the spatial dependence of the emission. We show how these patterns are influenced by the angle dependence of the refractive index ellipsoid. The technique is demonstrated exemplarily on photonic crystals to measure the fractional local density of states, i.e. the angle dependence of the photonic stop band.

CPP 23.2 Wed 14:15 ZEU 114

2d light point localisation in stretchable planar waveguide — ●ANTON NEULINGER^{1,2}, PETR BARTU¹, ROBERT KOEPE^{1,2}, LISA FALLON³, NIKITA ARNOLD¹, and SIEGFRIED BAUER¹ — ¹Department of Soft Matter Physics (SoMaP), JKU Linz, Altenbergerstr. 69, A-4040 Linz, Austria — ²isiQiri interface technologies GmbH i.G., c/o tech2b, Hafenstr. 47-51, A-4020 Linz, Austria — ³Dublin Institute for Advanced studies (DIAS), 31 Fitzwilliam Place, Dublin 2, Ireland

A fully flexible and stretchable planar waveguide serving as a photoluminescent concentrator, fabricated from a mixture of PDMS with a fluorescence dye, can be used to detect localized light. The incident light is absorbed by the dye, leading to an emission of light with higher wavelength. The emitted light is spreading out in the two dimensional waveguide and detected via embedded Si-photodiodes in the device. Using a simple mathematical model, the position of light spots can then be easily recalculated. These devices can lead to applications, such as human interface devices and artificial skins. This work was partially supported by FWF.

CPP 23.3 Wed 14:30 ZEU 114

Infrared Transition Moment Orientational Analysis (IR - TMOA) — ●PERIKLIS PAPAPOPOULOS, WILHELM KOSSACK, and FRIEDRICH KREMER — Universität Leipzig, Institut für Experimentelle Physik I, Linnéstr. 5, 04103 Leipzig

A novel method is suggested for unraveling the mean orientation and the molecular order parameter in any IR-transparent or translucent material under study. It is based on the analysis of IR transmission spectra as a function of polarization and an intentional inclination of the sample. Taking advantage of the specificity of the IR spectral range, it is based on the analysis of the absorption coefficient $\alpha \sim \left\langle \left(\vec{\mu} \cdot \vec{E} \right)^2 \right\rangle$, where μ is the transition dipole moment and E the electric field of the IR beam, in dependence on the polarization and the angle of inclination. Additionally, for non-scattering samples, the complex refractive index tensor can be determined by using the Fresnel equations. The spatial resolution of the technique is only limited by the wavelength.

Compared to other structural techniques, like X-ray scattering and NMR, this novel method has the advantage that it can give group-specific 3D structural information for samples under varying external conditions. The sample quantity requirements are minimal (down to μg) and time-resolved studies in combination with mechanical or electric measurements may be carried out.

CPP 23.4 Wed 14:45 ZEU 114

Coplanar waveguides - new sample cells for fast and ultrafast investigations — ●MICHAEL GÖRLICH^{1,2,3,4}, KLAUS ATTENKOFER¹, NALAKA KODITUWAKKU¹, MANFRED FICKENSCHER², REINHARD FOJIT³, and IGNAZ EISELE⁴ — ¹Argonne National Laboratory — ²Hochschule München — ³Ketek GmbH — ⁴Universität der Bundeswehr München

Motivated by the idea of using coplanar waveguides (CPW) as a sample cell to trigger and control chemical reactions, the infrastructure for designing, testing, and simulating these transmission lines was developed. Unlike any other method CPWs offer the opportunity to create extreme high field strengths of up to 1V/nm in combination with an excitation length of pico- and sub-picoseconds. A fundamental understanding and characterization of CPWs in different frequency ranges was obtained and theoretical limits to field strength and frequency were derived. A test facility was designed, built, and commissioned to characterize the electric properties of transmission lines built in integrated circuit technology. The important part of the measurements and results will be presented.

CPP 23.5 Wed 15:00 ZEU 114

Oscillator strength of the peptide bond resonances at the C 1s and N 1s X-ray absorption thresholds — ●KURT KUMMER¹, VICTOR SIVKOV², DENIS VYALIKH¹, SERGUEI NEKIPELOV², ANJA BLÜHER³, MICHAEL MERTIG³, and SERGUEI MOLODTSOV¹ — ¹Institute of Solid State Physics, Dresden University of Technology, D-01062 Dresden, Germany — ²Komi Science Center, Russian Academy of Science, Ural Division, Syktyvkar 167982, Russia — ³BioNanotechnology and Structure Formation Group, Max Bergmann Center of Biomaterials and Institute of Materials Science, Technische Universität Dresden, D-01062 Dresden, Germany

X-ray absorption of regularly arrayed two-dimensional bacterial surface layers of *bacillus sphaericus NCTC 9602* was investigated by means of total electron yield measurements. In doing so the spectral dependence of the total absorption cross section in the photon energy range between 280 and 580 eV was obtained, as well as partial absorption cross sections at the C 1s, N 1s and O 1s edges. At each of the three edges a sharp resonance originating in the peptide group showed up. For the very first time, the oscillator strengths of C 1s $\rightarrow \pi^*(\text{CONH})$ and the N 1s $\rightarrow \pi^*(\text{CONH})$ transitions were determined. Furthermore, we demonstrate that the folded structure of the protein leads to an increased oscillator strength of incorporated benzene rings when compared to free benzene molecules.

15 min. break

CPP 23.6 Wed 15:30 ZEU 114

New thiol-gold binding protocol for improving the conductance of double-stranded DNA — ●SHOUPENG LIU¹, BENJAMIN BORNEMANN², ANDREAS MARX², ELKE SCHEER², and ARTUR ERBE¹ — ¹Physics Department, University of Konstanz, D-78457 Konstanz, Germany — ²Chemistry Department, University of Konstanz, D-78457 Konstanz, Germany

Thiol-functionality at 5' ends DNA are normally used to allow its binding to gold electrodes for measuring its conductance. However, poor overlap of the electronic orbitals of the thiols with the Pi-system leads to low conductance of DNA. In this contribution, new oligonucleotides are synthesized that bear short thioalkyl functions at the nucleobases rather than at the phosphor-sugar backbone. We investigated the electronic transport properties of double-stranded DNA ended with these new oligonucleotides by mechanically controllable break junctions (MCBJ). From the measured current-voltage characteristics we deduce a semiconductor-like electronic band-structure. The results suggest a comparatively high conductance with a current of 700 nA in 0.25V, which is higher than in most of the former reports. The improved conductance is suggested to be caused by the thioalkyl group which facilitates charge transfer into the Pi-system of the nucleobases.

CPP 23.7 Wed 15:45 ZEU 114

Advanced Simulation Methods for Charge Transport in OLEDs — ●EVELYNE HUBER, HANSUELI SCHWARZENBACH, ROGER HÄUSERMANN, NILS A. REINKE, and BEAT RUHSTALLER — Zurich University of Applied Science, Institute of Computational Physics, Wildbachstrasse 21, 8401 Winterthur, Switzerland

Until now the system of equations for organic semiconductor device modelling has been predominantly solved in a decoupled way with the Gummel algorithm which can suffer from slow convergence. This limits the use of fitting algorithms for parameter extraction and sweeping. For the design of OLED it is of crucial importance to solve the involved equations efficiently on a PC. OLED simulation requires solving the continuity equations for electrons and holes and the Poisson equation in one dimension. The resulting system of equations is strongly coupled. Introducing disorder and novel mobility models for organic materials leads to highly nonlinear equations. In this study we present OLED simulations where the coupled equations are solved with the Newton algorithm. We combine this method with advanced physical transport models such as Gaussian disorder, density- and field-dependent mobilities and generalized Einstein diffusion. The performance of the presented algorithms is compared.

CPP 23.8 Wed 16:00 ZEU 114

Angular electronic "band structure" of molecules — ●YAROSLAV PAVLYUKH and JAMAL BERAKDAR — Martin-Luther-Universität Halle-Wittenberg

First principles calculations of the electronic structure of spherical molecules reveals that the valence band dispersion and bands filling are almost completely determined by the properties of angular momentum operator. With a very high accuracy we find the single particle states to disperse with the averaged angular momentum ℓ as $E_\ell = E_0 + \ell(\ell + 1)/2R^2$. Angular electronic band bendings at large ℓ and all peculiarities in the band fillings of large fullerenes and their high symmetry derivatives can be explained within a unified picture as bands avoided crossing.

CPP 23.9 Wed 16:15 ZEU 114

Laser-excitation of molecular systems within stochastic time-dependent current-density-functional theory — ●HEIKO APPEL and MASSIMILIANO DI VENTRA — Department of Physics, University of California, San Diego, USA

In this talk we investigate the excited electron dynamics of molecular systems due to laser excitation. The system dynamics is described within the recently proposed stochastic time-dependent current-density-functional theory [1,2]. Work supported in part by Lockheed Martin and DOE.

[1] Massimiliano Di Ventra and Roberto D'Agosta, Phys. Rev. Lett. **98**, 226403 (2007).

[2] Roberto D'Agosta and Massimiliano Di Ventra, Phys. Rev. B **78**, 165105 (2008).

CPP 23.10 Wed 16:30 ZEU 114

Three-Pulse Photon Echo beyond the Impulsive Limit —

●INES MYNTTINEN¹, WICHARD J. D. BEENKEN¹, TÖNU PULLERITS², and ERICH RUNGE¹ — ¹Technische Universität Ilmenau, Germany — ²Lund University, Sweden

We present computational simulations of three-pulse photon echo (3PPE) experiments on Nile-blue as a reference. For the theoretical analysis, we go beyond the impulsive limit in order to simulate the effects of duration and chirp of the incoming laser pulses. In particular, we study the time-integrated intensity of the third order polarization, the frequency-resolved polarization, and the photon-echo peak shift. The latter is defined as the value of the first delay time where the maximum integrated signal intensity occurs for given second delay time. The peak shift is of general importance for the use of 3PPE in condensed-matter studies, since the time evolution of the peak shift was found earlier to reflect the time-correlation function of the system-bath interaction. We found that both, finite pulse duration and chirp, result in a distinct decay of the integrated intensity in dependence on the second delay time. Additionally, the chirp affects the decay of the peak shift. Our results make clear that it is necessary to control the chirp of the pulses in 3PPE experiments. In particular, the frequency-resolved third-order polarization signal allows to distinguish between the fundamental system-bath dynamics and the effects caused by the pulse chirp. Furthermore, careful analysis of the chirp dependence proves to be a tool to extract additional information from 3PPE experiments, which is usually hidden due to the finite pulse duration.

CPP 23.11 Wed 16:45 ZEU 114

Effect of chemical architecture on light-induced deformation in azobenzene polymer films — ●MARINA SAPHIANNIKOVA¹, VLADIMIR TOSHCHEVIKOV^{1,2}, and GERT HEINRICH¹ — ¹Leibniz-Institut für Polymerforschung, Dresden, Germany — ²Institute of Macromolecular Compounds, Saint-Petersburg, Russia

Photoresponsive azobenzene polymers have been extensively explored as highly functional materials which have a fascinating potential for technical applications (data storage media, artificial muscles, etc). We propose a microscopic theory which describes the light-induced deformations in amorphous azobenzene polymers taking the chemical architecture of macromolecules explicitly into account. Our theory provides the values of the light-induced stress comparable and higher than the values of yield stress typical for glassy polymers. Thus, the theory explains the possibility for the inscription of surface relief gratings in glassy azobenzene polymers in the absence of light-induced softening. We show that the photo-elastic behaviour of azobenzene polymers is very sensitive to the chemical architecture. Depending on the chemical architecture, a sample can be either stretched or uniaxially compressed along the electric vector of the linearly polarized light. For some chemical architectures, elongation of a sample displays a non-monotonic behaviour with the light intensity. These predictions are in agreement with experimental observations [1] and MD simulations [2].

This work was supported by the RFBR (08-03-00150).

[1] D.Bublitz et al. Appl. Phys. B 2000, 70, 863

[2] J.Ilnytskyi et al. MCLC 2008, 496, 186

CPP 24: Colloids

Time: Wednesday 14:00–15:15

Location: ZEU 160

CPP 24.1 Wed 14:00 ZEU 160

Forbidden Symmetries in 2D Colloidal Systems — ●JULES MIKHAEL, SEBASTIAN RAUSCH, LAURENT HELDEN, and CLEMENS BECHINGER — 2. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart

Until 1984, it was unanimously established that rotational symmetries like 5-, 7-, 8-fold or higher are forbidden to ordered matter. However some metal alloys, polymers or micelles have defied these crystallographic rules and self-organized into so-called quasicrystals. Only four rotational symmetries mainly the 5-, 8-, 10- and 12-fold were reported although geometrical models predict any n-fold symmetry (where n is an integer number). Why? Are there forbidden symmetries even to quasicrystals?

Here we artificially create one of the symmetries, never observed in nature, by interfering seven coherent laser beams. Due to optical forces, the generated pattern acts as a template for a colloidal

monolayer whose phase behavior is studied in real space. Our results demonstrate that for interference patterns of 7 laser beams the colloids organize in large domains with strict periodic, i.e. crystalline, order. This is in contrast to interference patterns comprised of 5 laser beams where the colloids adopt the quasicrystalline order imposed by the substrate[1]. Based on the substrate potential depth distribution of interference patterns with different rotational symmetries, we provide a possible explanation why 5-, 8-, and 10-fold symmetries can occur in self organized systems while 7-, 9-, 11-fold do not.

[1] Mikhael, Roth, Helden & Bechinger, Nature 454, 501 (2008).

CPP 24.2 Wed 14:15 ZEU 160

Testing geometrical aspects in the particle insertion free energy and depletion interaction between colloids — MARTIN OETTEL, VITALIE BOȚAN, and ●FLORIAN PESTH — University of Mainz, Institute of Physics / KOMET 331, Germany

Morphological measures appear to be a useful tool to calculate the in-

sorption free energies of particles in a solution, which is otherwise a difficult task to calculate in the case of large, irregularly shaped objects. A morphological theorem introduced by Mecke et al. states [1], that if some physical restrictions are imposed on the solute, the insertion free energy depends on only four geometric quantities. The corresponding coefficients can be obtained for the same type of particle but with a more regular shape (spheres, cylinders...) thus simplifying the calculation of the insertion energy. Dumbbell shaped objects are the first non trivial objects for studying the validity of the theorem. The dumbbell insertion free energy is also related to the depletion interaction between two hard spheres or a sphere and a wall immersed in a solvent. For such systems, it has been shown recently that standard techniques such as bulk integral equations and the Derjaguin approximation fail to describe the depletion interaction [2,3]. The morphometric approach is a natural extension of the Derjaguin approximation, is superior to it for intermediate size ratios between solute and solvent particles and compares well to explicit DFT results.

[1] P.-M. König, R. Roth, and K. R. Mecke, PRL 93, 160601 (2004)
 [2] M. Oettel, PRE 69, 041404 (2004) [3] A. R. Herring and J. R. Henderson, PRL 97, 148302 (2006)

CPP 24.3 Wed 14:30 ZEU 160

Effect of Interface Mediated Interaction between Anisotropic Colloids at Fluid Interface — ●EHSAN NORUZIFAR and MARTIN OETTEL — Institut fuer Physik – Johannes Gutenberg-Universitaet, Staudinger Weg 7, 55099 Mainz, Germany

The effective interaction between colloidal particles trapped at the interface between two fluid phases is influenced by the presence of the deformable interface. Interfacial changes in such a system are responsible for new types of interactions that are not present in the bulk. As an instance, thermal fluctuations of the interface induce a Casimir type interaction between nano scale colloids, which was studied extensively for isotropic particles [1]. In the present work, by adding anisotropy to the colloids, we have investigated the effect of these fluctuation induced forces on possible ordering phenomena. On the other hand, for increasing the size of the trapped anisotropic particles, static deformations of the interface lead to more and more dominating capillary interactions between the colloids [2]. In the second part of the work, using this capillary potential, we have studied the dynamic behavior of colloids at the interface by employing Langevin dynamics simulations.

[1] H. Lehle, M.Oettel, and S. Dietrich, Europhys. Lett. 75, 174 (2006), H. Lehle and M. Oettel, Phys. Rev. E 75, 011602 (2007)
 [2] H. Lehle, E. Noruzifar, and M. Oettel, Eur. Phys. J. E 26, 151-160

CPP 25: Diffusion and Dynamics

Time: Wednesday 15:30–17:15

Location: ZEU 160

CPP 25.1 Wed 15:30 ZEU 160

Hot Brownian Motion — ●DANIEL RINGS¹, ROMY RADÜNZ², FRANK CICHOS², and KLAUS KROY¹ — ¹ITP, Uni Leipzig, Germany — ²EXP1, Uni Leipzig, Germany

Brownian motion is abundant throughout the microscopic and mesoscopic world. Since Einstein's seminal work, there is a good understanding of this process under conditions of thermal equilibrium. Brownian motion of particles in media with inhomogeneous temperature distributions poses several new questions. One way – already introduced by Maxwell – to cope with temperature gradients is to modify the boundary conditions at the particle's surface and allow slip in order to account for effects of thermal gradients. This approach is purely phenomenological, however, and does not take into account the temperature-dependence of the solvent viscosity, which is pronounced in water and e. g. hence most relevant for biological systems.

Here, we present a simple theoretical model for a suspension of heated Brownian particles. We determine the Stokes' flow around a spherical particle for radially varying viscosity and thus obtain effective quantities $\tilde{\eta}$, \tilde{T} . With these, we formulate a generalized Stokes-Einstein relation $6\pi\tilde{\eta}RD = k_B\tilde{T}$, which has been justified by a novel experimental technique called Photothermal Correlation Spectroscopy (PhoCS) presented by Romy Radünz also at this conference.

CPP 25.2 Wed 15:45 ZEU 160

Application of photothermal correlation spectroscopy to the

(2008)

CPP 24.4 Wed 14:45 ZEU 160

The effect of mixing and spatial dimension on the glass transition — ●DAVID HAJNAL¹, JOSEPH M. BRADER², and ROLF SCHILLING¹ — ¹Institut für Physik, Johannes Gutenberg-Universität Mainz, Staudinger Weg 7, D-55099 Mainz, Germany — ²Fachbereich Physik, Universität Konstanz, D-78457 Konstanz, Germany

We study the influence of composition changes on the glass transition of binary hard disk and hard sphere mixtures in the framework of mode coupling theory.

We derive a universal formula for the local variation of the critical packing fraction upon composition changes. For low concentration limits of one particle species, we evaluate our formula by using a perturbation ansatz. This new method allows a fast prediction of some properties of the glass transition lines. In addition, we present a glass transition diagram for binary hard disks and compare these two-dimensional results with the corresponding results for hard spheres in three dimensions from previous studies.

CPP 24.5 Wed 15:00 ZEU 160

Influence of the attraction range on the reentrant glass transition in colloid polymer mixtures — ●CARL STILKE and ECKHARD BARTSCH — Institut f. Physikal. Chemie, Universität Freiburg, Albertstr. 21, D-79104 Freiburg

Recently the occurrence of a reentrant glass transition has been observed in a binary mixture of polystyrene microgel colloids in a good, isorefractive solvent to which linear polystyrene with a size ratio $\delta = R_g(\text{polymer})/R(\text{colloid}) = 0.08$ was added [1] to introduce depletion attractions. This phenomenon has been predicted by mode coupling theory (MCT) for such systems [2]. MCT predicts further that for smaller size ratios δ the reentry effect should become even stronger and that for $\delta > 0.0465$ there should emerge a glass-glass transition line ending in a critical point (a A3 singularity in the MCT language).

To check up on these predictions we prepared colloid-polymer mixtures with a size ratio $\delta = 0.03$. The short range order and the dynamics of these colloid-polymer mixtures were then studied with light scattering techniques in order to localize the glass transition lines. As the glass-glass transition line should be most easily detectable by a discontinuous jump in the plateau modulus G_p the rheological behaviour was studied as well. The obtained results are contrasted with the predictions of MCT.

[1] T. Eckert, E. Bartsch, J. Phys.: Condens. Matter 16, S4937,(2004) [2] K. Dawson et al., Phys. Rev. E 63, 011401, (2001)

study of hot Brownian motion — ●ROMY RADÜNZ¹, DANIEL RINGS², KLAUS KROY², and FRANK CICHOS¹ — ¹Molecular Nanophotonics Group, Institute of Experimental Physics I, University Leipzig, Linnéstraße 5, 04103 Leipzig — ²Soft Condensed Matter Theory, Institute of Theoretical Physics, University Leipzig, Vor dem Hospitalore 1, 04103 Leipzig

We introduce a new technique for the measurement of tracer dynamics, which is sensitive to single metal nanoparticles down to a radius of 2.5 nm with a time resolution of a few microseconds. The method is based on a fluctuation analysis of a heterodyne photothermal scattering signal, which is recorded in a simple confocal microscopy setup. It exploits the same principles as fluorescence correlation spectroscopy but targets the use of extremely photostable, non-fluorescent, nanosized tracers as a replacement of fluorescent probes. To validate our approach, we verify that the Stokes-Einstein relation holds for heated diffusing gold nanoparticles, with an effective viscosity and temperature predicted by a semi-quantitative analytical model. We further demonstrate first applications to gold nano-particle diffusion in bio-materials. Due to the photostability and the low size dispersion of gold nanoparticles, the method promises broad applications especially in the field of high throughput biological screening.

CPP 25.3 Wed 16:00 ZEU 160

Dynamic Density-Functional Theory in Flow and Non-uniform Temperature — ●MARKUS HÜTTER¹ and JOSEPH M.

BRADER² — ¹ETH Zürich, Department of Materials, Polymer Physics, CH-8093 Zürich, Switzerland — ²Universität Konstanz, Fachbereich Physik, D-78457 Konstanz, Germany

Dynamic density functional theory has proven to be a useful tool for studying the dynamics of colloidal suspensions. Recent attempts have aimed to incorporate flow, non-uniform temperature gradients and hydrodynamic interactions. In this contribution, we take the first steps towards constructing a unified, thermodynamically consistent theory for the complete colloid plus solvent system. First, in order to examine the effect of strongly non-local effects, we formulate a thermodynamically admissible set of evolution equations for a one-component fluid in terms of the densities of mass, momentum, and internal energy. By using coarse-graining techniques, one can examine how long-range interactions on the particle level affect the macroscopic continuum description. The following conclusions emerge. (i) The body forces in the momentum balance have both energetic and entropic contributions in general, but can not be summarized in terms of a free energy-related term. (ii) The thermal conductivity and the viscosity are non-local in space. Second, we consider the colloid plus solvent system. Specifically, we present the evolution equations for the nonisothermal hydrodynamics of the solvent and for the spatial distribution of the colloids. In this way, it is clarified how the latter evolution equation can be extended to flow and nonisothermal situations.

CPP 25.4 Wed 16:15 ZEU 160

Cluster-resolved scaling theory for particle transport on percolating systems — AXEL KAMMERER, ●FELIX HÖFLING, and THOMAS FRANOSCH — Arnold Sommerfeld Center for Theoretical Physics (ASC) and Center for NanoScience (CeNS), Fakultät für Physik, Ludwig-Maximilians-Universität München, Germany

A Brownian particle moving between randomly distributed obstacles, a variant of the Lorentz model, constitutes a simple model for transport in heterogeneous environments. Three major transport phenomena are observed: normal diffusion, localization, and anomalous transport. All three aspects may be unified into the concept of transport in a medium with a percolation transition. Recent simulations have revealed that the asymptotic subdiffusive behaviour is only slowly approached and the large corrections cannot be ignored [1].

Thus, it is of general interest to develop a systematic description of universal corrections to scaling in percolating systems [2]. We have derived a new universal exponent relation connecting the leading corrections to scaling of the static cluster structure and of the transport dynamics. The derivation relies on a cluster-resolved scaling theory, unifying the scaling of both the cluster size distribution and the dynamics of a random walker. We have corroborated our scaling theory as well as the exponent relation in detail by large-scale simulations for the square lattice.

[1] Höfling, Franosch, and Frey, *Phys. Rev. Lett.* **96**, 165901 (2006).

[2] Kammerer, Höfling, and Franosch, arXiv:0811.1414, to appear in *Europhys. Lett.* (2008).

CPP 25.5 Wed 16:30 ZEU 160

Diffusion of magnetic nickel nanorods in colloidal dispersions — ●ANNEGRET GÜNTHER, ANDREAS MICHELS, ANDREAS TSCHÖPE, and RAINER BIRINGER — Technische Physik, Universität des Saarlandes, Postfach 151150, Geb. D2 2, D-66041 Saarbrücken, Germany

Ni nanorods with varying aspect ratios were synthesized by electrode-

position of Ni into porous alumina templates. The nanorods were extracted from the matrix by dissolution of the alumina and were dispersed in water or water-glycerine mixtures. The dynamics of the rods in colloidal dispersions in terms of the rotational and translational diffusion was investigated. Rotational diffusion of the nanorods was characterized by AC susceptibility measurements from 10 to 10000 Hz and by optical transmission measurements. The translational diffusion was studied by single particle tracking (SPT) of trajectories which were observed by laser scattering in an optical microscope. The rotational and translational diffusion coefficients were analyzed with regard to the aspect ratio of the Ni nanorods.

CPP 25.6 Wed 16:45 ZEU 160

Diffusional and orientational dynamics of various single terylene diimide conjugates in mesoporous materials — ●FLORIAN FEIL, CHRISTOPHE JUNG, JOHANNA KIRSTEIN, JENS MICHAELIS, and CHRISTOPH BRÄUCHLE — Department of Chemistry and Biochemistry, Ludwig-Maximilians-Universität München, Butenandtstrasse 11, 81377 München (Germany)

Mesoporous silica materials are ideally suited as host-guest systems in nanoscience with applications ranging from molecular sieves, catalysts, nanosensors to drug delivery systems. For all these applications a thorough understanding of the interactions between the mesoporous host system and the guest molecules is vital. Here, we use single molecule spectroscopy to study the dynamics of three different terylene diimide dyes acting as molecular probes in hexagonal and lamellar mesoporous silica films. The diffusion behaviour in the hexagonal phase is represented by the trajectories of the single molecules which are highly structured and thus provide information about the underlying host structure, such as domain size or the presence of defects inside the host structure. In the lamellar phase, the differences between the three guests are quite dramatic. Two populations of diffusing molecules could be observed: one with parallel orientation of the molecules to the lamellae and the other with perpendicular orientation. Additionally, switching between the two populations was observed. These data provide new insights into host-guest interactions like the influence of the molecular structure of the guest molecules on their diffusional as well as on their orientational behaviour in structurally confined guest systems.

CPP 25.7 Wed 17:00 ZEU 160

Single molecule studies of mesoporous silica structures for drug-delivery applications — ●TIMO LEBOLD, CHRISTOPHE JUNG, THOMAS BEIN, JENS MICHAELIS, and CHRISTOPH BRÄUCHLE — Center for Nanoscience (CeNS) and Nanosystems Initiative Munich (NIM), Ludwig-Maximilians-Universität München, Department of Chemistry and Biochemistry, Butenandtstraße 11, 81377 München

Novel drug-delivery systems based on nanostructures can provide fundamental progress to many therapies in medicine. We apply mesoporous thin silica films with nanometer-sized pores as drug carriers and incorporate the anti-cancer drug Doxorubicin. The measurements conducted on a single-molecule level provide insights into mechanistic details of the diffusion process. The diffusion dynamics of the drug inside the host channel system is controlled and modified. Further, the release kinetics of the drug is determined and live-cell measurements prove the applicability of the system for drug-delivery. This study demonstrates the high potential of nanoscience for medicine.

CPP 26: Organic Photovoltaics I

Time: Wednesday 14:00–17:00

Location: ZEU 222

CPP 26.1 Wed 14:00 ZEU 222

Efficient Polaron Pair Dissociation in Polymer:Fullerene Blends — ●CARSTEN DEIBEL¹, THOMAS STROBEL¹, and VLADIMIR DYAKONOV^{1,2} — ¹Experimental Physics VI, Institute of Physics, Julius-Maximilians-University of Würzburg, D-97074 Würzburg — ²Bavarian Centre for Applied Energy Research e.V. (ZAE Bayern), D-97074 Würzburg

Organic bulk heterojunction solar cells already achieve energy conversion efficiencies of up to 6%. To a significant part, this is due to the very efficient separation of the bound electron-hole pairs, also called polaron pairs. This event is the intermediate but crucial step between exciton dissociation and charge transport to the electrodes. Using a

simple model of Coulomb attraction of the bound charge carrier pair, the electric field needed to overcome the mutual attraction with a probability of 90% is larger than 10⁸ V/m. In contrast, in good organic solar cells, almost all polaron pairs are separated at fields smaller by a factor of around 50. We attempt an explanation of this significant discrepancy by performing Monte Carlo simulations of hopping transport in a bulk heterojunction blend system. We discuss the influence of phase separation and recombination rate on the efficiency of the polaron pair dissociation.

CPP 26.2 Wed 14:15 ZEU 222

Stability of organic electronics - P3HT as model to study

general mechanistic effects. — ●HOLGER HINTZ¹, HANS-JOACHIM EGELHAAF^{1,2,3}, CHRISTOPH BRABEC³, HEIKO PEISERT¹, and THOMAS CHASSÉ¹ — ¹University of Tübingen, Institute for Theoretical and Physical Chemistry, Auf der Morgenstelle 8, D-72076 Tübingen — ²Christian-Doppler Labor für oberflächenoptische Methoden, Johannes-Kepler University, Altenbergerstraße 69, A-4040 Linz — ³Konarka Austria GmbH, Altenbergerstraße 69, A-4040 Linz

The stability of Polythiophene (P3HT) is still unsatisfactory and the degradation mechanism has not yet been fully understood. Photo-oxidation of thin P3HT layers was performed under ambient conditions and under varying partial pressures of oxygen, water and ozone using Xenon light. The kinetics were monitored by FTIR and UV/VIS spectroscopy and can be described by the laws of photo-oxidation of layer systems, considering the blue-shift of the absorption spectra of formed P3HT fragments. A sublinear dependence of the degradation rate on oxygen partial pressure is monitored, probably due to the formation of singlet oxygen via a long-lived triplet excited state of P3HT. This is supported by strongly reduced degradation rates upon addition of PCBM, due to the quenching of the polymer excited state. Further support comes from the comparison of the temperature dependences of photo degradation and oxygen diffusion. Photo-oxidation at different humidity levels showed enhanced degradation rates in the presence of water. As water in the absence of oxygen does not cause any degradation, this is due to either a solvent effect or a catalytic mechanism.

CPP 26.3 Wed 14:30 ZEU 222

Molecular semiconductor blends: microstructure, charge carrier transport and application in photovoltaic cells — ●ANDREAS OPITZ¹, JULIA WAGNER¹, BERNHARD ECKER¹, WOLFGANG BRÜTTING¹, ALEXANDER HINDERHOFER², and FRANK SCHREIBER² — ¹Institute of Physics, University of Augsburg, Germany — ²Institute of Applied Physics, University of Tübingen, Germany

Blends of organic donor and acceptor materials have the potential of an increase of solar cell efficiency. However, the balance between charge carrier transport in phase-separated structures and exciton dissociation at the donor-acceptor interface has to be optimized. To analyze this relation in more detail the following molecular material combinations were investigated: (i) Copper phthalocyanine (CuPc) combined with fullerene C₆₀ and (ii) CuPc in combination with perfluorinated CuPc (F₁₆CuPc).

Measurements by X-ray diffraction and scanning force microscopy indicate the formation of phase-separated nanocrystals for blends of CuPc/C₆₀ and the formation of mixed crystals in the CuPc/F₁₆CuPc system. The formation of mixed crystals is an interesting feature for organic blends which has not yet been explored in organic solar cells. We will discuss the implications of the different molecular arrangements on the optical and electrical properties as well as for the solar cell performance.

CPP 26.4 Wed 14:45 ZEU 222

Interfacial adhesion in polymer blend P3HT:PCBM solar cells — ●AYSE TURAK¹, JONAS HANISCH², ESTHER BARRENA^{1,3}, ERIK AHLWEDE², and HELMUT DOSCH^{1,3} — ¹Max Planck Institute for Metals Research, Heisenbergstrasse 3, 70569, Stuttgart — ²Zentrum für Sonnenenergie- und Wasserstoff-Forschung (ZSW) Baden-Württemberg, Industriestrasse 6, 70565, Stuttgart — ³Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Pfaffenwaldring 57/VI, 70550 Stuttgart, Germany

The nature of the contact at the electrode/organic interface has a major impact on device performance. Introduction of thin dielectric interlayers such as LiF have been successful in significantly improving device properties. However, examination of the buried interface is generally difficult as deposition of the top electrode may alter the nature of the contact. Using peel-off adhesion analysis with grazing incidence x-ray diffraction, atomic force microscopy and optical imaging, we have assessed the quality of the buried interfacial layer in P3HT:PCBM solar cells in the presence of interlayers. We see increased adhesion of the Al cathode without the interlayer, suggesting broader interfacial mixing of the Al with the polymer without LiF as a blocking interlayer. The confinement of the charge extraction to a well defined interface may be used to explain improved device performance with LiF interlayers.

CPP 26.5 Wed 15:00 ZEU 222

Block copolymer templating: a bicontinuous double gyroid hybrid solar cell — ●EDWARD CROSSLAND¹, SABINE LUDWIGS¹, MARC HILLMYER², ULRICH WIESNER³, HENRY SNAITH⁴, and ULLRICH STEINER⁵ — ¹Freiburg Institute for Advanced Studies, Germany —

²University of Minnesota — ³Cornell University — ⁴University of Oxford — ⁵University of Cambridge

The conversion of light to electrical energy in hybrid solar cells based on organic-ceramic composites demands engineering of highly distributed, yet interconnected heterojunctions on the 10nm length scale. Microphase separation of block copolymers offers an extremely versatile bottom-up approach to high aspect ratio patterning of functional materials on these macromolecular scales in thin films. We fabricated highly ordered arrays of semiconductor nanostructures using selectively degradable block copolymers as porous electrochemical templates. Cylinder-forming poly(4-fluorostyrene)-b-(D,L-lactide) films were aligned using electric fields to template freestanding vertical nanowire arrays over 1 μ m long and 10nm in diameter while the network phase of a bicontinuous double gyroid morphology could be replicated without external alignment. Charge transport and recombination rates as well as photovoltaic power conversion efficiencies were probed in each morphology incorporated into dye sensitized solid-state and liquid-electrolyte solar cells. These results mark the first successful application of the gyroid morphology in a functioning electronic device. This templating technique is fully extendable to a enormous range of potentially high performance heterojunction systems.

CPP 26.6 Wed 15:15 ZEU 222

Preparation of hybrid solar cells from CdSe nanocrystals and poly(3-hexylthiophene) — ●FOLKER ZUTZ, MARC-DANIEL HEINEMANN, IRINA LOKTEVA, JOANNA KOLNY-OLESIK, INGO RIEDEL, HOLGER BORCHERT, and JÜRGEN PARISI — University of Oldenburg, Department of Physics, Energy and Semiconductor Research Laboratory, Carl-von-Ossietzky Str. 9-11, 26129 Oldenburg, Germany

Colloidally prepared semiconductor nanocrystals with particle sizes of a few nanometers possess particular physical and chemical properties. One example is the size-dependent band gap which enables tuning of optical properties by controlling the particle size. One potential application is the use of nanocrystals as a component in hybrid solar cells. Similar to organic composites of polymer and fullerenes, a nanocrystal-polymer composite is a donor/acceptor system where photo-generated charge carriers can be efficiently separated because of the affinity of the nanocrystals and polymers to accept electrons and holes, respectively. In contrast to fullerenes, semiconductor nanocrystals can additionally act as absorber themselves. This offers possibilities to optimize the exploitation of the solar spectrum. In the present work, we prepared high-quality CdSe nanocrystals. Composites of the nanocrystals and polymere (P3HT) were successfully used to prepare laboratory solar cells which were characterized by I-V curves and measurements of the external quantum efficiency. Further experiments with different ratios of Cadmium to Selenium in the nanocrystals and different ratios of CdSe nanocrystals to polymere in the semiconductor blend were made. The results were compared with purely organic composites.

CPP 26.7 Wed 15:30 ZEU 222

Hybrid Organic-Inorganic Bulk Heterojunctions with Silicon Nanocrystals for Solar Cells — ●SABRINA NIESAR¹, ROLAND DIETMÜLLER¹, ANDRÉ EBBERS², MARTIN TROCHA², HARTMUT WIGGERS³, and MARTIN STUTZMANN¹ — ¹Walter Schottky Institut, Technische Universität München, Am Coulombwall 3, 85748 Garching, Germany — ²Evonik Degussa GmbH, Paul-Baumann-Str.1, 45772 Marl, Germany — ³Institut für Verbrennung und Gasdynamik, Universität Duisburg-Essen, Lotharstr. 1, 47048 Duisburg, Germany

Hybrid organic-inorganic solar cells, which incorporate both, organic and inorganic semiconductors, have received a lot of attention during the last years. Such solar cells typically consist of a bulk heterostructure made of organic semiconducting polymers and semiconducting nanocrystals. These hybrid organic-inorganic solar cells can benefit from the solution processing and from the broad spectral absorption range of semiconductor nanocrystals. We have studied hybrid bulk heterojunctions between Silicon nanocrystals (Si-nc), which have been synthesized by decomposition of silane in a microwave plasma reactor, and the organic hole conductor poly(3-hexylthiophene-2,5-diyl) (P3HT). Hybrid bulk heterojunction solar cells with P3HT and Si-nc have been produced and characterized by current-voltage measurements. For these devices, we have demonstrated by spectrally resolved photocurrent measurements that both components of the solar cell, the Si-nc and the P3HT, contribute to the photocurrent. Current-voltage measurements under white light illumination with 100 mW/cm² show a high open circuit voltage of up to 0.7 V.

CPP 26.8 Wed 15:45 ZEU 222

Inverted Bulk Heterojunction Solar Cells — ●SOFIE KHALIL and KLAUS MEERHOLZ — University of Cologne, Institute for Physical Chemistry, Luxemburger Str. 116, 50969 Cologne, Germany

Solution processed polymer photovoltaics are nowadays a very promising low-cost fabrication technology for renewable energy sources. Nevertheless research made onto bulk heterojunction (BHJ) with structure: ITO/ PEDOT:PSS/ blends of regioregular poly-3-hexylthiophene (RR-P3HT) and the fullerene derivative [6,6]-phenyl C61 butyric acid methyl ester (PCBM) / Ca:Ag showed inherent lifetime limitations due to the use of PEDOT:PSS and low work-function metal electrode. In this talk we will show an alternative device with a new stacking order of layers: the inverted solar cells. In these devices to avoid the air sensitive and lifetime limiting materials we use a stable transparent anode electrode with lower energy level than the stable high-work function metal top electrode. The direction of the carrier flow is therefore inverted due to the inversion of the direction of the internal field. Inverted bulk-heterojunction solar cell made RR-P3HT and PCBM as the active layer in the structure: ITO / TiO_x / RR-P3HT-PCBM / metal electrode were studied. The transparent TiO_x acts as electron-collecting electrode and the metal electrode as hole-collecting electrode. Different parameters have been investigated: thickness and treatment of the TiO_x layer, solvent, thickness of the active layer, molecular weight of the polymer, post-annealing process, work-function of the metal electrode. And then a comparison of lifetime between a regular solar cell and an inverted one will be presented.

CPP 26.9 Wed 16:00 ZEU 222

Transparent Metal Electrodes for Organic Solar Cells — ●JAN MEISS, MORITZ K. RIEDE, and KARL LEO — Institut fuer Angewandte Photophysik, Technische Universitaet Dresden, 01062 Dresden - <http://www.iapp.de>

Organic solar cells (OSC) are emerging as possible inexpensive alternative to inorganic photovoltaics. Current issues of OSC are the high price of indium tin oxide (ITO), the most commonly used transparent contacting material, and the fact that glass is used as substrate in almost all cases. We are exploring alternatives to the scarce and expensive ITO and investigate alternative OSC configurations, i.e. top-illuminated and inverted solar cells.

In this contribution, top-illuminated small-molecule organic solar cells with transparent metal cathodes consisting of different combinations of Al, Ag and Au are presented. The whole device stack has been prepared by thermal evaporation under vacuum. It is shown that multi-layer metal cathodes employing surface modifying interlayers achieve by far superior performance compared to single-layer cathodes. Scanning electron and atomic force microscopy show that this can be attributed to significantly improved morphology in multi-layer devices; these conclusions are supported by the electrical properties in the current-voltage curves. By additionally enhancing light incoupling with a capping layer and utilizing microcavity effects, promising efficiencies of over 2.2% are obtained for zinc phthalocyanine / C60 bulk heterojunction solar cells containing standard materials.

CPP 26.10 Wed 16:15 ZEU 222

Effects of geminate and bimolecular recombination on the performance of polymeric-small molecular solar cells — ●MARCEL SCHUBERT¹, CHUNHONG YIN¹, MAURO CASTELLANI¹, ALAN SELLINGER², and DIETER NEHER¹ — ¹University of Potsdam, Institute of Physics and Astronomy, 14476 Potsdam-Golm, Germany — ²IMRE and A*Star, 3 Research Link, 117602 Republic of Singapore

Many physical properties of organic photovoltaics are related to the nature of the geminate pair, an intermediate state that forms after dissociation of photogenerated excitons and prior to free charge carrier generation. Whereas it was found that photocurrent generation is dominated by the strong field dependent process of geminate pair dis-

sociation, the recombination of uncorrelated free charge carriers and the formation of space charge seem to play a minor role in the prominent P3HT/PCBM combination. The situation may change, when using different D/A combinations or other soluble acceptor molecules.

We present organic solar cells comprising a novel small molecule based on 2-vinyl-4,5-dicyanoimidazole (Vinazene) as acceptor and M3EH-PPV as donor. While bilayer devices show promising results with a fill factor up to 57 %, the IU-characteristics of bulk heterojunction devices are dominated by bimolecular recombination and space charge effects even at moderate illumination intensities. Photo-CELIV measurements were performed to study the bimolecular recombination in detail. By combining photo-CELIV results with PL and IU measurements we are able to analyze the interrelation of recombination losses, free charge carrier generation and exciplex formation.

CPP 26.11 Wed 16:30 ZEU 222

Highly doped layers as efficient electron-hole conversion contact for tandem organic solar cells — ●RONNY TIMMRECK, SELINA OLTTHOF, MORITZ RIEDE, and KARL LEO — Institut für angewandte Photophysik, TU Dresden, Dresden, Germany

To achieve high power conversion efficiencies with stacked organic solar cells, several requirements concerning their layer structure have to be fulfilled. A key feature is an efficient conversion contact at the interface between the single solar cells of a stacked cell: Here, an electron current has to be converted into a hole current without loss of energy. We investigate such contacts for small-molecule organic solar cells and present an approach adopted from inorganic tandem solar cells by using highly doped organic layers. We also compare metal-cluster based conversion contacts reported in literature to our new approach. For this purpose, comparable structures are characterised by UPS, by I-V-characteristics of organic p/n-heterojunctions, and by I-V-characteristics of corresponding solar cells. The experiments show that our approach is superior to the metal cluster based approach, e.g. it allows a full addition of the open circuit voltage Voc of the subcells independent from the used organic materials. It is thus possible to avoid the metal clusters which allows for a wider choice of materials and has advantages for future mass production. Using these results, a possible working mechanism of these contacts is discussed: high recombination rates at the conversion contact result in low sheet resistances and a removal of quasi-Fermi level splitting such that no reverse voltage occurs which would reduce Voc of the stacked solar cell.

CPP 26.12 Wed 16:45 ZEU 222

Light- and touch-point localization using flexible large area organic photodiodes — ●PETR BARTU¹, ROBERT KOEPPE^{1,2,3}, SIEGFRIED BAUER¹, and NIYAZI SERDAR SARICIFTCI² — ¹Department of Soft Matter Physics (SoMaP), JKU Linz, Altenbergerstr. 69, A-4040 Linz, Austria — ²Linz Institute for Organic Solar Cells (LIOS), JKU Linz, Altenbergerstr. 69, A-4040 Linz, Austria — ³isiQiri interface technologies GmbH i.G., c/o tech2b, Hafenstr. 47-51, A-4020 Linz, Austria

A large area photodiode using a heterojunction of zinc-phthalocyanine and fullerene C60 as active layer sandwiched between resistive electrodes of Poly(ethylenedioxythiophenes) Polystyrenesulfonate (PEDOT:PSS) and semitransparent aluminum can be used as a two dimensional position sensitive device for detecting light spots. The current generated in the photodiode drops over resistive electrodes to the edges of the device and depends on the distance between the excitation and the point where the resistive electrode is connected with the outer circuit. For precise tuning of the device, a variation of the electrode sheet resistance as well as a change in modulation of the frequency can be used. Additionally, localized out-coupling of light from a waveguide of silicone rubber by pressure allows the construction of a pressure sensitive optical touchpad.

CPP 27: Symposium Self-Organizing Surfaces and Interfaces

Time: Wednesday 14:00–17:15

Location: BAR SCHÖ

see SYSO for the program of the session

CPP 28: POSTERS Interfaces and Thin Films

Time: Wednesday 17:00–19:00

Location: P3

CPP 28.1 Wed 17:00 P3

High Frequency QCM Flow cell with Enhanced Accuracy for Liquid and Biochemical Sensing — ●BRIGITTE PAULA SAGMEISTER¹, SIEGFRIED BAUER¹, REINHARD SCHWÖDIAUER¹, and HERMANN GRUBER² — ¹Soft Matter Physics, Johannes Kepler University, Altenberger Str. 69, A-4040 Linz, Austria — ²Institute for Biophysics, Johannes Kepler University, Altenberger Str. 69, A-4040 Linz, Austria

The quartz crystal microbalance (QCM) has been proven to be a highly sensitive mass detector which found its way into biomedical sciences. The measuring technique is ideally suited for online detection of biological and chemical analytes and gets along without labelling them. Most biosensing systems based on thickness shear mode resonators work with resonance frequencies between 5 and 20 MHz and use commercially available flow cells. The utilisation of high frequency fundamental (HFF) quartz resonators, with resonance frequencies up to 200 MHz, could further improve the sensitivity of such systems. We present a fully biocompatible flow cell, designed for HFF quartz resonators. For the development of a biosensor we solved important questions like the functionalization of the small and fragile sensor surface, the sensitive and repeatable detection of dissolved analytes and the regeneration of the sensor. The system performance is further evaluated by a number of experiments including the step-wise growth of a protein multilayer system by an alternating immobilisation of streptavidin and biotinylated immunoglobulin G, as well as the detection of specific antibody-antigen reactions.

CPP 28.2 Wed 17:00 P3

Supported Lipid Bilayers on Spacious and pH Responsive Polymer Cushions with Varied Hydrophilicity — ●LARS RENNERT¹, TILO POMPE¹, REGIS LEMAITRE², DAVID DRECHSEL², and CARSTEN WERNER¹ — ¹Leibniz Institute of Polymer Research Dresden, Max Bergmann Center of Biomaterials Dresden, Germany — ²Max-Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany

We report on the successful formation of supported multicomponent lipid bilayer membranes (sLBMs) from natural occurring lipids as well as synthetic lipids on a set of polymer cushions consisting of alternating maleic acid copolymers. Maleic acid copolymers provide a versatile platform to adjust the physico-chemical behaviour by the choice of the comonomer unit. The formation of sLBMs was triggered by a transient reduction of the electrostatic repulsion between the polymer cushions and the lipid vesicles by lowering the solutions pH to 4. Upon formation the stability of sLBMs was not affected by subsequent variations of the environmental pH to 7.2. The degree of hydrophilicity and swelling of the anionic polymer cushions was found to determine both the kinetics of the membrane formation and the mobility of the sLBM. An increase in cushion hydrophilicity correlated with a strong increase in the diffusion coefficient of the lipids. The observations strongly support the important role of the support's polarity for the fluidity of the sLBM. The investigated polymer cushions are considered to open new options for the in situ modulation of sLBM characteristics for the successful integration of functional transmembrane proteins.

CPP 28.3 Wed 17:00 P3

Controlled Wrinkling as a novel method for the fabrication of patterned surfaces — ●ALEXANDRA SCHWEIKART¹, CONGHUA LU², and ANDREAS FERY¹ — ¹University of Bayreuth, Physical Chemistry Department II, Bayreuth, Germany — ²MPI for Colloids and Interfaces, Department of Interfaces, Golm, Germany

Surfaces that are patterned on the sub-micron- or nanoscale are of great interest as building blocks for devices in areas as diverse as photonics (diffraction gratings), sensorics (pressure sensors), biotechnology (direction of cell growth), catalysis and stamps for microcontact printing. We present a new, lithography-free approach for creating such surfaces that is based on controlled wrinkling. Wrinkles develop if a soft substrate covered by a hard film is exposed to strain. Given the case that strain is controlled well and homogenous, wrinkle patterns are highly regular. They can be of sub-micron periodicity while the lateral dimensions of the substrate can be macroscopic. We use this approach to direct colloidal crystal assembly by using a template assisted self-assembly process. In the first part, we discuss recent experiments

on the mechanics of surface wrinkling on the micron/submicron scale. In the second part, we focus on applications of wrinkled surfaces for structuring and templating. Here, we show that the interaction between colloidal particles and wrinkled substrates as well as capillary forces direct colloids and nanoparticles into wrinkles with high regularity.

CPP 28.4 Wed 17:00 P3

High resolution, non-destructive, and quantitative material characterization on the nanoscale by HarmoniX-microscopy — ●HARTMUT STADLER — Veeco Instruments GmbH, Dynamostr. 19, D-68165 Mannheim (Germany)

The miniaturization of devices and functions down to the nanoscale regime require techniques for localized investigation of material properties. Particularly interesting are quantitative data on elastic, viscous or adhesive properties of thin layers or films (e.g. for their tribological or rheological behavior). Some of the already known and commercially available SPM modes (force-distance based or similar) reveal these properties to some extent, but they are limited in lateral/vertical resolution, sample compatibility, or speed of data acquisition.

Recently, HarmoniX-microscopy has been introduced as a new scanning probe mode, based on the well known and widely used standard tapping mode. HarmoniX allows nanoscale mapping of material properties such as elasticity, adhesion, and dissipation by analyzing the full spectrum of motion of special probes designed for high bandwidth measurement of tip forces. From the spectra, the force distance curves during the tapping cycles and the respective material properties of the sample can be extracted, and displayed as lateral maps in realtime. HarmoniX microscopy is hundreds of times faster than other quantitative material mapping techniques such as force volume, but retains the high resolution, non-destructive qualities of tapping mode imaging.

The fundamentals, instrumental aspects, and first applications of the new technique will be reviewed in this contribution.

CPP 28.5 Wed 17:00 P3

Growth of gold thin films on PVK-coated nanostructured titanium dioxide — STEPHAN V. ROTH², ●GERD HERZOG^{1,2}, RALF RÖHLSBERGER², SEBASTIEN COUET², KAI SCHLAGE², ANDRE ROTHKIRCH², ANDREAS TIMMANN², RALPH DÖHRMANN², NADJA REIMERS², HEINZ GRAAFSMA², MICHAEL LOHMANN², D. BISCHOFF², GUNAR KAUNE³, MATTHIAS RUDERER³, WEINAN WANG³, MOTTAKIN M. ABUL KASHEM³, EZZELDIN METWALLI³, WILFRIED WURTH¹, PETER MÜLLER-BUSCHBAUM³, and RAINER GEHRKE² — ¹Institut für Experimentalphysik der Universität Hamburg, Luruper Chaussee 149, D-22761 — ²HASYLAB at DESY, Notkestr. 85, D-22603 Hamburg, Germany — ³Physik-Department E13, TU München, James-Frank-Str. 1, D-85748 Garching, Germany

PVK-coated nanostructured TiO₂ films are candidates for photo-voltaic devices. To create an electrode, gold is sputter deposited onto the TiO₂/PVK film. Grazing incidence small angle x-ray scattering (GISAXS) is used for in situ investigation of gold cluster growth. Out of plane scans show two clearly separated peaks which leads to the conclusion that a bimodal distribution of particles is present, which we call large and small clusters. The temporal development of out of plane scans illustrates the kinetics of the radius of small clusters, while detector scans and off detector scans at the small clusters' Yoneda peak are used to discover the vertical growth of large and small clusters, respectively. Since the radius of the large clusters is found to be constant, they are thought to be voids in the polymer film caused by roughness in the TiO₂ layer which are filled with gold atoms.

CPP 28.6 Wed 17:00 P3

Glass transition in ultra thin polymeric films measured by differential AC chip calorimetry — ●HEIKO HUTH¹, DONGSHAN ZHOU², and CHRISTOPH SCHICK¹ — ¹University of Rostock, Institute of Physics Universitätsplatz 3, 18051 Rostock, Germany — ²Dept. of Polymer Science and Eng., Nanjing University, Nanjing, 210093, China

The film thickness dependency of glass transition in polymer films is still controversially discussed. For different experimental probes different dependencies are observed and a generally accepted link to molecular mobility is not yet established. Calorimetry has proven to provide

useful information about glass transition, because it establishes a direct link to energetic characterization. In several cases a direct comparison with results from other dynamic methods like dielectric spectroscopy is possible giving further insights. For thin films in the micro...nm range standard calorimetric methods are mostly not applicable. In the recent years there are new developments in the field of calorimetry which overcome these limitations. We set up a differential AC-chip calorimeter capable to measure the glass transition in nanometer thin films with pJ/K sensitivity. Changes in heat capacity can be measured for sample masses below one nanogram as needed for the study of the glass transition in nanometer thin polymeric films. No thickness dependency of the glass transition temperature was observed within the error limits - neither at constant frequency nor for the traces in the activation diagrams.

CPP 28.7 Wed 17:00 P3

Designing the interfacial properties of Langmuir monolayers from amphiphilic diblock copolymers — KATJA TRENKENSCHUH¹, FELIX SCHACHER², AXEL H. E. MÜLLER², and ●LARISA TSARKOVA¹ — ¹Physikalische Chemie II, Universität Bayreuth, D 95440 Bayreuth, Deutschland — ²Macromolekulare Chemie II, Universität Bayreuth, D 95440 Bayreuth, Deutschland

We followed changes in the molecular arrangement of amphiphilic diblock copolymers at air-water interface which were associated with the variation of the molecular composition. We demonstrate that the main characteristics of the surface pressure – area per molecule ($\pi - A$) isotherms strongly depend on the mechanical properties of the hydrophobic block (polystyrene (PS) or polybutadiene (PB)), and on the volume fraction of the hydrophilic block poly(N, N-dimethylaminoethyl-methacrylate) (PDMAEMA). In the case of a majority PB block, the interfacial assembling shows clear dependence on the chain relaxation, while a PS majority block leads to a significantly larger mechanical stability of the monolayers. The contribution of the PDMAEMA block is noticeable at low compressions and at low pH values due to the protonation of the chains. The nanostructure of Langmuir-Blodgett films was investigated with scanning force microscopy (SFM). We captured the details of the phase transition from a network of PS-core worm-like micelles to densely packed PS-core spherical domains through increasing the monolayer compression. Our results further establish the generality of the molecular-structure guided assembling phenomena.

CPP 28.8 Wed 17:00 P3

Voltage-dependent uptake of L-glutamate by polypyrrole films analysed in situ with EQCM — ●KATHRIN FUCHS, ELIZABETH VON HAUFF, and JÜRGEN PARISI — Energy- and Semiconductor Research Laboratory, Department of Physics, University of Oldenburg, Carl-von-Ossietzky-Strasse 9-11, D-26111 Oldenburg

L-glutamate is an important neurotransmitter in the human central nervous system. Molecular selective surfaces which can control the concentration of biomolecules such as glutamate could find a broad range of application in the fields of biology and medicine.

For this purpose, electropolymerized polypyrrole (PPy) films doped with glutamate were characterized as glutamate-selective surfaces for the uptake and release of L-glutamate via a variable potential. The films were deposited potentiostatically on gold electrodes and 5 MHz Au-coated AT-cut quartz crystals, respectively, in an aqueous solution containing 0.4 M pyrrole and 0.5 M sodium L-glutamate. After deposition PPy films were overoxidized potentiodynamically in aqueous 0,1 M NaOH in order to create a complementary cavity for the recognition of L-glutamate molecules [1]. Subsequently, the efficiency of the PPy film for the uptake and release of L-, D-Glutamate and chlorine depending on the applied voltage was analysed in situ with an electrochemical quartz crystal microbalance (EQCM). Furthermore the morphology of the films were investigated with a scanning electron microscope.

[1] B. Deore, Z. Chen, and T. Nagaoka, *Anal. Sci.*, 15, 827, 1999

CPP 28.9 Wed 17:00 P3

Inkjet Printing of Polymer Microspheres — ENRICO SOWADE¹, JENS HAMMERSCHMIDT¹, DAVID POLSTER², REBECCA WAGNER³, THOMAS BAUMGÄRTEL⁴, ●THOMAS BLAUDECK¹, HARALD GRAAF², FRANK CICHOS³, CHRISTIAN VON BORCZYKOWSKI², and REINHARD R. BAUMANN¹ — ¹Print and Media Technology, 09107 Chemnitz, Germany. — ²Optical Spectroscopy and Molecular Physics, Chemnitz University of Technology, 09107 Chemnitz, Germany. — ³Molecular Nanophotonics, University of Leipzig, 04103 Leipzig. — ⁴Graduate

School of Engineering Science, Osaka University, Osaka 560-8531, Japan.

During this decade, drop-on-demand piezo inkjet printing has gained considerable interest as it allows for a personalized and patterned deposition of thin functional films at ambient conditions. We report about libraries of inkjetted polymer microspheres with varying drop-to-drop space, head-to-substrate distance, solvent composition and substrate properties. The layers are characterized by AFM and optical microscopy aiming to understand the self-assembly phenomena of the spheres on the substrate.

CPP 28.10 Wed 17:00 P3

Solvent content in thin spin-coated polymer nanocomposite films — ●JAN PERLICH¹, EZZELDIN METWALLI¹, MINE MEMESA², ROBERT GEORGH³, JOCHEN S. GUTMANN^{2,4}, and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik-Department LS E13, James-Franck-Str. 1, 85748 Garching (Germany) — ²Max-Planck Institute for Polymer Research, Ackermannweg 10, D-55128 Mainz (Germany) — ³FRM-II, TU München, Lichtenbergstr. 1, 85747 Garching (Germany) — ⁴Inst. Phys. Chem., Johannes Gutenberg Universität, Jakob-Welder-Weg 10, 55099 Mainz (Germany)

The amphiphilic diblock copolymer P(S-b-EO) is used as template to synthesize nanocomposite films composed of ordered titania nanoparticles. In this approach a so-called "good-poor solvent pair" induced phase separation process is coupled with sol-gel chemistry. As result of the complex force balance, different nanocomposite morphologies can be obtained by adjusting the relative weight fractions between the sol-gel components, i.e. 1,4-dioxane, HCl and titania precursor. Directly after spin-coating the thin polymer nanocomposite films are investigated with neutron reflectivity (NR). The use of deuterated solvents generates contrast for the NR experiment. In NR a narrow range around the critical edge of total external reflection is probed with high resolution. Due to the high sensitivity of the position of the critical edge on the ratio of protonated P(S-b-EO) and deuterated solvent (1,4-dioxane), the exact position of the critical edge enables to determine the content of remaining solvent. The focus is on the systematic variation of the sol-gel components addressing different morphologies.

CPP 28.11 Wed 17:00 P3

Mechanical stability and permeability of porous polyaniline films fabricated by using polymer matrixes as templates — ALEXANDER SOKOLYUK^{1,2}, VLADIMIR G. SERGEYEV¹, and ●LARISA TSARKOVA² — ¹Polymer Division, Department of Chemistry, Moscow State University, 119992, Moscow Russia — ²Physikalische Chemie II, Makromolekulare Chemie II,

Nanostructured polyaniline (PANI) composites have high potential in chemo- and biosensor technology due to their high sensitivity and fast response. We report the preparation of porous 3D interconnected structure of PANI by using as templates polymer films with varied mechanical and physico-chemical properties. Micro-structured layers of PANI have been characterized with SEM, SFM techniques and by contact angle measurements. The permeability of the nano-composites has been investigated by exposing the films to the vapor of organic solvent or water, and by monitoring the response using in-situ spectroscopic ellipsometry. We demonstrate that incorporation of PANI particles into the polystyrene (PS) films dramatically affects the mechanical stability of the resulting composite, independent on the thickness of the underlying PS template. Both the mechanical stability and permeability of PANI-based composite films are improved by using templates from elastomeric block copolymers or from amphiphilic block copolymers.

CPP 28.12 Wed 17:00 P3

Orientation and spatial distribution of dyes binding to SiO₂ surfaces — ●SCHUBERT SEBASTIAN, TÄUBER DANIELA, KOWERKO DANNY, SCHUSTER JÖRG, and VON BORCZYKOWSKI CHRISTIAN — nanoMA TU-Chemnitz, Institut für Physik, 09107 Chemnitz.

Silica surfaces are widely used e.g. in the fabrication of organic electronic devices. Yet many details of the interactions between silica surfaces and organic molecules which are crucial for their electrical properties and thus for device performance are not fully understood.

Here we use ensemble fluorescence and single molecule methods to explore the spatial distribution, molecular orientation and spectral dynamics of differently functionalized dyes on silica surfaces [1]. This allows us to draw conclusions on preferential geometrical orientations and physio-chemical binding affinities depending on the chemical structure of participating molecules and silica surfaces.

[1] D. Kowanko, J. Schuster, Ch. von Borczyskowski: Molecular Physics submitted

CPP 28.13 Wed 17:00 P3

Application of in-situ ellipsometry for the investigation of stimuli-responsive polymer brushes and adsorption processes thereon — ●EVA BITTRICH¹, DENNIS AULICH², KLAUS - JOCHEN EICHHORN¹, KARSTEN HINRICHS², PETRA UHLMANN¹, and MANFRED STAMM¹ — ¹Leibniz Institute of Polymer Research Dresden, Hohe Str. 6, 01069 Dresden, Germany — ²ISAS - Institute for Analytical Sciences, Department Berlin, Albert-Einstein-Str. 9, 12489 Berlin, Germany

Thin polymer brushes, with the polymer chains grafted chemically by one end to the surface, have thoroughly proven their ability to modify physico-chemical interface properties as well as the adsorption behaviour of proteins at artificial surfaces. With the help of in-situ spectroscopic ellipsometry these thin polymer films can be investigated according to their swelling behaviour and adsorption processes at the polymer-solution interface.

We report on swelling measurements of homopolymer and mixed polymer brushes consisting of pH- and temperature sensitive polymer chains. Furthermore we investigated the adsorption of human serum albumin, a protein of the blood plasma, onto charged polymer brushes. Here we monitored the influence of changes in the environmental conditions and the composition of the polymer brush on the adsorbed amount as well as the optical properties of the protein layer.

CPP 28.14 Wed 17:00 P3

Collective behavior during dewetting — ●CRISTINA-MARIA POP¹, ANA MARIA FLORESCU², YVES BRÉCHET³, and ZOLTÁN NÉDA⁴ — ¹Arnold Sommerfeld Center and CeNS, Ludwig-Maximilians-Universität München, Germany — ²LSP, Université Joseph Fourier, St Martin d'Hères Cedex, France — ³SiMAP-ENSEEG, Institut National Polytechnique de Grenoble, St Martin d'Hères Cedex, France — ⁴Babeş-Bolyai University, Cluj-Napoca, Romania

When a liquid film on a substrate is unstable, dry spots appear and the liquid breaks into droplets: this phenomenon is called dewetting. It can be observed every day on a windshield or in a cooking pan, and the stability of liquid films on solid substrates is crucial for numerous technological applications. In biology, dewetting governs the dynamics of adhesion on wet substrates in the case of mushroom spores or living cells. Dewetting can take place through amplification of capillary waves in thin films, or by spontaneous nucleation and growth in thicker films.

We studied the mechanism of dewetting by introducing a two-dimensional model in which the dynamics of the dewetting hole is given by capillarity (the line tension which tends to shrink the hole, and the difference between the surface energy of the substrate when dry and wet). Dissipation makes the motion overdamped. With the aid of this model we performed numerical simulations which enabled us to find the critical parameters for the growth of a dewetting hole, and to study the collective dynamics of many holes in a dewetting process with spontaneous nucleation. Thus we obtained a size distribution of the liquid droplets on the substrate after dewetting has taken place.

CPP 28.15 Wed 17:00 P3

Effect of geometrical confinement and surface charge on the structuring in colloidal silica suspensions — ●YAN ZENG¹, SABINE KLAPP², and REGINE V. KLITZING¹ — ¹Stranski-Laboratorium für Physikalische & Theoretische Chemie, Institut für Chemie, TU Berlin — ²Institut für Theoretische Physik, Freie Universität Berlin

This work focuses on the effect of geometric confinement on the structuring of colloidal suspensions in thin film geometry. Colloidal silica suspensions with different particle concentration and ionic strength allow a deeper insight into the ion distribution around the particles. Results from colloidal probe atomic force microscopy (CP-AFM) force-distance measurements in films are compared with results from small-angle X-ray scattering (SAXS) in bulk. It is found that the characteristic lengths obtained from force oscillation measured by AFM, correlate well with the intermediate particle distance from the structure peak measured by SAXS, scale with particle concentration with an exponent of -1/3. In order to study the effect of the surface elasticity the bare silicon surfaces are modified by polymer coatings. The effect on the structuring of particles is measured by AFM and compared with our preliminary results from Thin Film Pressure Balance (TFPB).

CPP 28.16 Wed 17:00 P3

Optical microscopy of colloidal polymeric thin films - ordering on large length scales — ●JANNIS LEHMANN^{1,2}, GERD HERZOG^{1,3}, ADELIN BUFFET¹, PETER MÜLLER-BUSCHBAUM⁴, RAINER GEHRKE¹, and STEPHAN V. ROTH¹ — ¹DESY, Notkestr. 85, D-22607 Hamburg, Germany — ²Univ. Hamburg, Dep. f. Physik, Jungiusstr. 9, D-20355 Hamburg, Germany — ³ExpPh, Univ. Hamburg, Luruper Chaussee 149, D-22761 Hamburg, Germany — ⁴Physik-Department E13, TU München, D-85748 Garching, Germany

Colloidal films are widely applied in many areas of research and technology, e.g. magnetic data storage or due to their optical properties [1,2,3]. We focused on the long-range order of spin-coated (on top of basic cleaned Si-wafers) colloidal polystyrene spheres (diameter 100nm) by using optical microscopy. We investigated the influence of colloidal concentration, spin-coating parameters and annealing on the structure of the colloidal film. Especially, annealing is performed far below as well as near the glass transition temperature of polystyrene of about 100°C to investigate the influence of mobility on the structure of the film during. We clearly see a regular periodic constitution of colloid-islands, which are homogeneously ordered on the surface. This long-range order extends from some ten micrometers to over several millimeters.

[1] Abul Kashem et al., *Macromolecules* 40, 5075-5083 (2007)

[2] Siffalovic et al., *Phys. Rev. B* 76, 195432 (2007)

[3] Roth et al., *Appl. Phys. Lett.* 91, 091915 (2007)

CPP 28.17 Wed 17:00 P3

AFM based approach to measure adhesion energies of micron sized particles predicated on JKR apparatus — ●JOHANN ERATH and ANDREAS FERY — University Bayreuth, Universitätsstr. 30, 95440 Bayreuth, Germany

Determination of adhesion energies is of interest for both fundamental science and applications. The aim of this contribution is to introduce a novel, AFM based approach for the case of soft surfaces.

Our approach builds up on the so called JKR (Johnson, Kendall and Roberts) apparatus. This device is used for macroscopic measurements and is based on the fact that the contact area of elastomeric lenses is only dependent on adhesion energy as well as elastic properties and load force. Thus, adhesion energy can be determined from measurement of contact area as a function of load.

In our case, the same principle is used for micron sized particles made from PDMS. We attach the particles to an AFM setup (soft colloidal probe AFM), whereby one can control the load and simultaneously measure the particle-surface contact area using microinterferometry.

We discuss the potential and advantages of this microscopic approach compared to classic JKR apparatus.

CPP 28.18 Wed 17:00 P3

Surface energy patterns generated by single pulse laser interference lithography — ●TOBIAS GELDHAUSER¹, STEFAN WALHEIM², THOMAS SCHIMMEL^{2,3}, PAUL LEIDERER¹, and JOHANNES BONEBERG¹ — ¹Universität Konstanz, 78457 Konstanz, Deutschland — ²Institute of Nanotechnology (INT), Forschungszentrum Karlsruhe, 76021 Karlsruhe, Deutschland — ³Institute of Applied Physics, Center for Functional Nanostructures (CFN), Universität Karlsruhe, 76128 Karlsruhe, Deutschland

Single pulse laser interference lithography is used to structure self-assembled monolayers of thiol on gold by thermal desorption in a rapid and large area (mm²) process. The desired structure can be varied by different angles of incidence and numbers of interfering laser beams. The structuring process is investigated by attenuated total reflection and AFM measurements. For comparison with the experiment 1D and 2D simulations of temporal heat distributions are presented. As a verification of this patterning process and example structures down to 200nm in width generated by demixing of polymers, sol-gel and guided assembly of colloids are shown.

CPP 28.19 Wed 17:00 P3

The bending rigidity of the liquid/vapour interface of water — ●FELIX SEDLMEIER, DOMINIK HORINEK, and ROLAND R. NETZ — Physik Department, Technische Universität München, 85748 Garching, Deutschland

Whenever two liquid phases are in contact, thermally excited fluctuations of the interface position, i.e. capillary waves, occur. At large length scales, they are well described by a constant interfacial tension in the framework of capillary wave theory. On smaller scales, however, deviations from capillary wave theory arise, which lead to an effective

surface tension that is a function of the wave vector of the excitation modes. The coefficient of the quadratic order term of the effective surface tension can be identified with Helfrich's bending rigidity, the sign and magnitude of which has been a long standing issue in theoretical as well as experimental research. Also, simulation studies of simple liquids have not given a conclusive answer yet. One of the main problems in the analysis of capillary waves at liquid interfaces is that at small scales interfacial fluctuations are entangled with bulk-like density fluctuations. For an unambiguous determination of the bending rigidity, these contributions have to be separated. We present results from large scale molecular dynamics simulations that elucidate the effect of this entanglement and give quantitative results for the bending rigidity of the liquid/vapour interface of water.

CPP 28.20 Wed 17:00 P3

Internal structure of PNIPAM microgel particles — ●MARTIN MEDEBACH¹, ANNA BURMISTROVA¹, MATTHIAS KARG¹, YVONNE HERTLE², WEINAN WANG³, PETER MÜLLER-BUSCHBAUM³, and REGINE V. KLITZING¹ — ¹Technische Universität Berlin — ²Universität Bayreuth — ³Technische Universität München

Thermosensitive microgel particles are of great interest in basic research and also for technical applications. For instance Poly-(N-Isopropylacrylamide), PNIPAM, undergoes a temperature induced phase transition at approx. 32 °C. This transition leads to shrinking by a factor of 10, while the shrinking effect at the solid/liquid interface is only about factor 2 perpendicular to the surface. These findings raise the question how the interactions with the solid surface affect the internal structure of the microgel particles. We report about experiments (GISANS, SANS, AFM and ellipsometry) with charged PNIPAM microgel particles (diameter in bulk between 100 to 1000 nm, depending on the degree of swelling) adsorbed on oppositely charged Silicon wafers. The PNIPAM particles are copolymerized with 5% acrylic acid and they are adsorbed on top of a Silicon wafer that is coated with Polyethyleneimine (PEI). The particles are close packed. From ellipsometry and AFM measurement the swelling is observed normally and laterally (AFM) to the surface. SANS experiments show the correlation length in the bulk system while GISANS measure the correlation length of the absorbed particles in lateral direction. Taken all experiments together we can describe the change of the internal structure during the swelling.

CPP 28.21 Wed 17:00 P3

AFM Studies of photoswitchable nanocomposite films — ●M. MÜLLER¹, Y. GONZALEZ-GARCIA¹, C. PAKULA², V. ZAPOROJTCHEK², F. FAUPEL², and O. MAGNUSSEN¹ — ¹Institut für Experimentelle und Angewandte Physik, Leibnizstrasse 19, Universität Kiel — ²Lehrstuhl für Materialverbunde, Kaiserstrasse 2, Universität Kiel

Photoswitchable conductive nanocomposites of metal nanoparticles and polymers containing photoisomerizable groups may have interesting applications as sensors and photoswitchable filters. We have investigated composite films of Au clusters and PMMA with embedded azobenzene, which can be optical switched between the trans and the cis isomer, resulting in photo-induced changes in the film conductivity. The film morphology and local conductivity have been characterized by a conductive sensing AFM (CS-AFM) with integrated UV/visible optics that allows in situ studies of illumination effects. According to these studies the change in configuration is accompanied by changes in the nanoscale film morphology, such as changes in free volume and a decrease of the surface roughness.

CPP 28.22 Wed 17:00 P3

Block Copolymer Templating using Periodic Chemical Nano-Patterns Induced with the Tip of an Atomic Force Microscope — ●TOBIAS HEILER¹, REGINA WEINGAERTNER², VASSILIOS KAPAKLIS³, ROLAND GROEGER², STEFAN WALHEIM¹ and THOMAS SCHIMMEL^{1,2} — ¹Institute of Nanotechnology (INT), Forschungszentrum Karlsruhe, Germany — ²Institute of Applied Physics and DFG-Center for Functional Nanostructures (CFN), Universität Karlsruhe, Germany — ³present address: Engineering Science Department, University of Patras, 26504 Patras, Greece

The nanoscale phase morphology of an amphiphilic block copolymer film was controlled by a chemical periodic surface energy pattern made by molecular exchange with the tip of an Atomic Force Microscope (AFM). The two polymer components of the copolymer, as well as the two surface molecules of the chemically patterned substrate possess a high contrast in polarity, so that a defect-

tolerant pattern replication with a line width of 40 nm in the polymer film is observed after a short (vapor-)annealing process. We used polyethylenoxide-polyisoprene-polyethylenoxide block copolymers and methyl- vs. carboxyl-terminated alkane thiols as self-assembled monolayers.

CPP 28.23 Wed 17:00 P3

Transient waviness of polymer films during spin-coating — ●JOERG PFEIFER¹, STEFAN WALHEIM², and THOMAS SCHIMMEL^{1,2} — ¹Institute of Applied Physics and DFG-Center for Functional Nanostructures (CFN), Universität Karlsruhe, Germany — ²Institute of Nanotechnology (INT), Forschungszentrum Karlsruhe, Germany

The development of roughness (waviness) during spin-coating of polymer films is a well known phenomenon of high technological relevance. We have investigated the transient formation of such waves in film thickness using time-resolved light reflectance measurements during the spin-coating process. Our model system (Polystyrene (PS) in Cyclohexane) develops this instability during the last 200 milliseconds of the drying process. By controlling the process atmosphere containing a defined load of solvent vapour, the formation and recovery of film waviness (wavelength: 20-50 micron) was observed. In this way, we were able to pre-adjust the amplitude of the developing waves from zero to 100 nm in films with an average thickness of 200 nm. The results of our quantitative investigations give rise to a model of solvent-polymer phase separation during spin-coating as the driving mechanism for this widely observed instability.

CPP 28.24 Wed 17:00 P3

Polymer phase separation on surface energy patterns generated by single pulse laser interference — ●ALEXANDER FOERSTER¹, TOBIAS GELDHAUSER², JOHANNES BONEBERG², PAUL LEIDERER², STEFAN WALHEIM¹, and THOMAS SCHIMMEL^{1,3} — ¹Institute of Nanotechnology (INT), Forschungszentrum Karlsruhe, Germany — ²Department of Physics, Universität Konstanz, Germany — ³Institute of Applied Physics and DFG-Center for Functional Nanostructures (CFN), Universität Karlsruhe, Germany

Single pulse laser interference lithography is used to structure self-assembled monolayers of thiols on gold. The molecular desorption process is investigated by attenuated total reflection measurements. The resulting surface energy patterns are investigated by AFM and are used to control the phase morphology of a polymer blend - subsequently spin-cast on these structured surfaces. The laser lithography was realized with different wavelengths (266, 532, and 1064 nm) which shows that the structuring is a thermal process. As a first demonstration of this process, structures down to 800 nm period and 300 nm width are fabricated. Ref.: Langmuir 24 (22), 13155-13160 (2008)

CPP 28.25 Wed 17:00 P3

A transient triple layer leads to a purely lateral morphology in a spin-cast polymer blend film — ●CHENG HUANG¹, AARON WEIS², FENGZHEN ZHANG³, OTHMAR MARTI³, STEFAN WALHEIM¹, and THOMAS SCHIMMEL^{1,2} — ¹Institute of Nanotechnology (INT), Forschungszentrum Karlsruhe, Germany — ²Institute of Applied Physics and DFG-Center for Functional Nanostructures (CFN), Universität Karlsruhe, Germany — ³Institute for Experimental Physics, Universität Ulm, Germany

We study the phase separation process of PS/PMMA during spin-coating from a Methyl-Ethyl-Ketone (MEK) solution. Using this solvent this polymer blend forms a purely lateral structure on a hydrophilic substrate with PS cylinders in PMMA matrix. Our results of time-resolved reflectometry point in the direction of a transient triple layer formation during the spin-coating process which then transforms via an instability into the final lateral morphology. The process parameters can be tuned so that a purely horizontally layered situation can be observed in the dried state. Humidity, spin rate and the concentration of the polymer blend solution are the most important parameters which define the final structure. The PS or PMMA phase was later selectively dissolved and the film was subsequently used as a lithographic mask.

CPP 28.26 Wed 17:00 P3

Thickness dependence of diffusion in thin liquid crystalline films — ●BENJAMIN SCHULZ, JÖRG SCHUSTER, and CHRISTIAN VON BORCZYKOWSKI — TU Chemnitz, Institut für Physik, 09107 Chemnitz

Liquid crystals are of high technical interest especially for the use in

liquid crystal displays. As all applications are based on the orientational behaviour of the molecules, especially on surfaces, it is important to examine the molecular alignment and mobility in proximity to solid interfaces.

We are using single molecule microscopy to track the trajectories of dyes dissolved in the liquid crystal. This allows us to directly access to the molecular movement in the specimen. We are using specially tailored perylene dye molecules that align in the liquid crystal matrix and which are thus a good representation of the real behaviour of the liquid crystal molecules. The comparison with the diffusive behaviour of randomly aligning dye molecules gives us the chance to investigate the local structure on the surface. We find a drastic slowdown of diffusion as the film thickness decreases for both types of tracers, however, with a different thickness dependence. Film thickness is hereby varied from extremely thin quasi 2D films consisting of a single smectic double layer, up to quasi bulk material, where a crossover to 3D structured films (FCDs) is observed.

With our method we try to establish a model of the structure of extremely thin smectic liquid crystals, a question which is not yet re-

solved in literature, by relating the diffusive behaviour of the liquid crystals to the three dimensional patterning.

CPP 28.27 Wed 17:00 P3

Thermotropic liquid crystal foams — •TORSTEN TRITTEL, THOMAS JOHN, and RALF STANNARIUS — Otto-von-Guericke-Universität Magdeburg

Foams made from surfactant solutions are well investigated and understood, but there is no information about properties of foams made from pure thermotropic materials. This new type of foams has advantages compared with ordinary soap foams. For example, higher stability and slower drainage. In our experiments, we investigate two-dimensional foams, made from liquid crystals in the smectic A phase, with the aid of digital image analysis. We focus on the temporal evolution (ageing) of these foams, especially in the long time regime, where scaling behaviour occurs. The evolution of the mean bubble radius (R) and distribution functions, e.g. bubble size distribution, are determined and compared with soap foams.

CPP 29: Symposium Organic Photovoltaics

Time: Thursday 9:30–12:30

Location: BAR SCHÖ

see SYOP for the program of the session

CPP 30: Symposium Self-Organizing Surfaces and Interfaces

Time: Thursday 9:30–12:30

Location: GÖR 226

see SYSO for the program of the session

CPP 31: Symposium Self-Organizing Surfaces and Interfaces

Time: Thursday 14:00–17:00

Location: GÖR 226

see SYSO for the program of the session

CPP 32: Polymer Physics III

Time: Thursday 9:30–12:00

Location: ZEU 222

CPP 32.1 Thu 9:30 ZEU 222

Bulk Behaviour of Random Block Copolymers — •BIRGER STEINMÜLLER and MARCUS MÜLLER — Institut für Theoretische Physik, Georg-August-Universität Göttingen

The microphase separation of random block copolymers is a promising route for fabricating fuel cell membranes. In order to describe this process on time and length scales, which are not accessible by atomistic simulations, we resort to coarse-grained models. We use a coarse-grained bead-spring model in conjunction with MD simulations and study a soft-particle model by Single-Chain-in-Mean-Field (SCMF) simulations. The advantages of the MD model are its operation with a model of higher resolution than SCMF, therefore it can be better mapped to results of atomistic simulations, and that it permits a more immediate access to dynamical quantities of polymer melts and solutions. The SCMF model on the other hand is a simpler one, which employs softer interactions and is thus computationally far more efficient. We want to propose a strategy for mapping the SCMF to the MD model. Thus, we will be able to benefit from the advantages of both models.

We discuss our results with a focus on the methodology used to parametrize the SCMF model with the aim of reproducing the mesoscale behaviour of the MD model. The approach is validated by comparing structural properties of the models on said scale.

CPP 32.2 Thu 9:45 ZEU 222

Modelling of hysteresis behaviour of multigraft copolymers — •RALF SCHLEGEL¹, DANIEL WILKIN¹, ULRIKE STAUDINGER^{1,5}, ROLAND WEIDISCH¹, JIMMY W. MAYS², DAVID UHRIG³, and NIKOS HADJICHRISTIDIS⁴ — ¹Institute of Materials Science and Technology (IMT), Friedrich-Schiller-University Jena, Löbdergraben 32, D-07743

Jena, Germany — ²Department of Chemistry, University of Tennessee, Knoxville, USA — ³Center for Nanophase Materials Science at ORNL, PO BOX 2008 MS6494, Knoxville, TN USA — ⁴Department of Chemistry, University of Athens, Athens 15771 Greece — ⁵current address: Institute of Materials Science, Technische Universität Dresden, 01062 Dresden, Germany

Multigraft copolymers are thermoplastic elastomers with a special molecular architecture. Polystyrene(PS) arms are grafted regularly spaced and with different functionalities onto a rubbery polyisoprene(PI) backbone chain. Graft functionality and the number of grafting points can be controlled at synthesis level. The hysteresis properties of multigraft copolymers have been critically investigated. TEM investigations revealed that the materials are showing micro phase separation. The non-affine tube model of Kaliske and Heinrich was applied and adapted to the stress release curve of the materials. In addition to the model parameters a parameter describing the stress softening is attained. Multigraft copolymers with tetra and hexafunctional molecular architecture were characterized. Significant low stress softening characteristics were observed for the tetrafunctional materials with spherical PS micro domains.

CPP 32.3 Thu 10:00 ZEU 222

Traveling spatially periodic forcing of phase separation — •VANESSA WEITH, ALEXEI KREKHOV, and WALTER ZIMMERMANN — Theoretische Physik I, Universität Bayreuth, 95440 Bayreuth, Germany

Within the framework of a suitably generalized Cahn-Hilliard model [1,2] we present a theoretical analysis of phase separation of binary polymer mixtures in the presence of spatially periodic forcing of wavenumber q traveling with a velocity v .

We found that for a stationary forcing ($v = 0$) phase separation is locked beyond a critical forcing amplitude $a_0(q)$ to periodic patterns of wavenumber $Q = q$. This critical amplitude is increased at increasing the pulling velocity v . The bifurcation diagram, the existence range of the periodic solutions, as well as the dynamics of phase separation influenced by the forcing have been studied.

We have also investigated the existence and stability of subharmonic periodic patterns of wavenumber $Q = q/m$ ($m \geq 2$) and their spatio-temporal behaviour for the cases $v = 0$ and $v \neq 0$. We obtained that the critical forcing amplitudes for the stabilization of subharmonic periodic patterns are larger than for the harmonic solution with $Q = q$.

- [1] A. P. Krekhov and L. Kramer, Phys. Rev. E **70**, 061801 (2004)
 [2] V. Weith, A. Krekhov and W. Zimmermann, Eur. Phys. J. B, in press (2008)

CPP 32.4 Thu 10:15 ZEU 222

Modelling agglomeration effects in CNT/polymer composites — ●MARINA SAPHIANNIKOVA, SVEN RICHTER, and GERT HEINRICH — Leibniz-Institute für Polymerforschung, Hohe str. 6, 01069 Dresden

Theoretical description of viscoelastic properties of the polymer melts, filled with attractively interacting anisometric particles, represents a great challenge. Such filler particles tend to build a network-like superstructure [1] which is very fragile and can be easily broken in external flow fields. In the quiescent state the particles agglomerate again, slowly restoring the network superstructure. In this study, to describe the agglomeration/deagglomeration process of anisometric particles, we use a superposition approach, in which the total stress is represented by a sum of three stresses: 1) the viscoelastic stress arising in the polymer matrix, 2) the hydrodynamic reinforcement due to the presence of anisometric particles, 3) the viscoelastic stress arising in the filler network. The latter is represented by a nonlinear variant of the Maxwell model combined with a usual kinetic equation for the scalar structural parameter that describes the instantaneous state of filler network at particular flow conditions. This approach is verified in a number of linear and nonlinear shear experiments carried out on polycarbonate composites filled with carbon nanotubes [2].

This work was supported by the BMBF grant CarboNet No.03X0504E.

- [1] F.R.Costa et al. Adv. Polym. Sci. 210, 101 (2008) [2] S.Richter et al. Submitted to Macromol. Symp., Macromolecules

CPP 32.5 Thu 10:30 ZEU 222

Anisotropy of the dynamic mechanical properties of strongly stretched polymer networks — ●VLADIMIR TOSHCHEVNIKOV^{1,2}, GERT HEINRICH¹, and YULI GOTLIB² — ¹Leibniz Institut für Polymerforschung, Dresden, Germany — ²Institute of Macromolecular Compounds, Saint-Petersburg, Russia

Superposition of large static and small oscillating strains has been proposed recently as a method for studying the structure of polymer networks [1,2]. The main goal of the present work is to study the anisotropy of the dynamic mechanical properties of strongly stretched polymer networks with respect to the direction of a static strain. This is of importance to understand the crack propagation in rubbers, which is determined by the dynamics of highly stretched network portions near crack tips under pulsed loading conditions (<http://www.ipfdd.de/FOR597>). We show that a stretched polymer network is characterized by the anisotropy of viscoelastic properties: frequency dependent shear modulus is different for different geometries of applying the shear (parallel or perpendicular to the axis of deformation). For all geometries of the shear, fine structure of the relaxation spectrum leads to the broadening of the frequency dependences of loss moduli which can display several maxima at strong deformations. Theoretically calculated frequency dependences of the loss and storage moduli are in a good agreement with experimental data [2].

This work was supported by the RFBR (08-03-00150).

- [1] V.L.Bodneva et al. Polymer Science 2005, 47, 409
 [2] E.Munch et al. Polymer 2006, 47, 3477

15 min. break

CPP 32.6 Thu 11:00 ZEU 222

Combination of μ GISAXS and imaging ellipsometry - a new versatile instrument for the surface sensitive investigation of polymer films — ●VOLKER KÖRSTGENS¹, ROBERT MEIER¹, JOHANNES WIEDERSICH¹, STEPHAN V. ROTH² und PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik-Department LS E13, James-Frank-Str. 1, D-85747 Garching — ²HASYLAB at DESY, Notkestr.

85, D-22607 Hamburg

For the structural investigation of polymer thin films the method μ GISAXS (grazing incidence small angle x-ray scattering with a μ m-sized beam) is well established and very powerful. It gives access to lateral structures at the surface as well as buried structures of inhomogeneous samples such as gradient films. Whereas in the common set-up available at a few beamlines at synchrotron radiation sources the samples are investigated with μ GISAXS and simultaneously with optical microscopy, we introduce an advanced method with in-situ imaging ellipsometry replacing the optical microscopy. Therewith a comprehensive sample characterization is possible including local film thickness and optical properties combined with structural information with a spatial resolution depending on the size of the x-ray beam. The scope of the instrument is illustrated with investigations on different polymer samples. Full capability of the method will be reached with implementation in the newly developed μ SAXS/WAXS beamline at the novel high-brilliance synchrotron radiation source PETRA3 at DESY, Hamburg beginning its operation in fall 2009.

This project is financially supported by BMBF grant 05KS7WO1.

CPP 32.7 Thu 11:15 ZEU 222

Investigating industrial processes at the future microSAXS/WAXS beamline at PETRA III — ●STEPHAN V. ROTH, ADELIN BUFFET, RALPH DÖHRMANN, HERMANN FRANZ, RAINER GEHRKE, HEINZ GRAAFSMA, PATRICK GRÖGOR, ULRICH ULRICH HAHN, MICHAEL LOHMANN, RALF RÖHLSBERGER, HORST SCHULTE-SCHREPPING, and EDGAR WECKERT — HASYLAB at DESY, Notkestr. 85, D-22607 Hamburg, Germany

Micro- and nanofocused x-ray beams combined with small- and wide-angle x-ray scattering (SAXS/WAXS) are powerful tools to investigate nanocomposite and hierarchical materials on multiple length scales. In 2009, the microfocusSAXS/WAXS beamline P03 will become operational at PETRA III. This beamline combines high resolution in both real and reciprocal space with beam sizes ranging from 40 μ m to 100nm. The low divergence offered by the high- β -undulator allows for installing ultraSAXS geometries in combination with such small beams. We present the detailed layout of the μ SAXS/WAXS beamline. Strong emphasis is put on the future improvements of the various experimental IN-SITU scanning techniques, such as nano- and microbeam GISAXS [1,2] and micro/nanoSAXS tomography [3] as well as its possible combinations with high-throughput and industrial processing methods for thin film technology and fluidics.

- [1] S.V. Roth et al., Appl. Phys. Lett 91, 091915 (2007)
 [2] E. Metwalli et al., Langmuir 24, 4265 (2008)
 [3] C. Schroer et al., Appl. Phys. Lett. 88, 164102 (2006)

CPP 32.8 Thu 11:30 ZEU 222

Recent Experiments at the SAXS Beamline BW4 — ●ANDREAS TIMMANN, RALPH DÖHRMANN, TOM SCHUBERT, STEPHAN V. ROTH, and RAINER GEHRKE — HASYLAB at DESY, Notkestr. 85, D-22603 Hamburg, Germany

The BW4 beamline at HASYLAB is a versatile small-angle x-ray scattering (SAXS) beamline. It offers transmission and grazing incidence SAXS using sample-detector distances (D_{SD}) between one meter and 13 meters. For $D_{SD} < 2$ m it also offers a moderate micro-focus of 22 \times 40 μ m² at sample position. All SAXS techniques can be combined with wide-angle x-ray scattering.[1]

Recently we conducted in-situ GISAXS experiments such as rheology and sputter-deposition.[2,3]

We also examined a beryllium compound refractive lens (Be-CRL) as focusing optic for USAXS geometries. Its usage results in an undistorted beam and the background is considerable lower than that caused by focusing mirrors[4]

References:

- [1] Roth et al., Rev. Sci. Instrum., 2006, 77, 085106
 [2] Timmann et al., App. Phys. Let., 2007, 91, 213102
 [3] E. Metwalli et al., Langmuir, 2008, 24, 4265
 [4] Timmann et al., Rev. Sci. Instrum., submitted

CPP 32.9 Thu 11:45 ZEU 222

High Intensity - High Resolution Small-Angle Neutron Diffractometers of JCNS at FRM II — ●AUREL RADULESCU — Jülich Centre for Neutron Science (JCNS), Forschungszentrum Jülich GmbH, 85747 Garching, Deutschland

The KWS-1 and KWS-2 small-angle neutron diffractometers of Jülich Centre for Neutron Science are currently reconstructed at the Research

Neutron Source Heinz Maier-Leibnitz (FRM II) in Garching-München. With a high flux supplied by the cold neutron source of FRM II and the newly designed optimized neutron guide and with a new collimation system allowing a larger experimental flexibility the instruments will be dedicated facilities for structural studies in the field of soft-matter and magnetic systems. The standard of 5x5 cm² neutron guides leads to high intensities with standard resolution and provides a maximum flux close to world leading SANS instruments, as for example D22, ILL-Grenoble. Further support is obtained by neutron lenses that allow for larger sample apertures of 5x5 cm² without losing any res-

olution. High counting rates (up to 600kHz) will be detectable with a dead-time of about 0.6 microsec for either homogeneous or strong inhomogeneous scattering patterns distributed on the scintillation detector. The high resolution mode is supported by a chopper, which will allow a variation of the wavelength spread between 10% (as delivered by the velocity selector) and 1%. Additionally, the neutron lenses in combination with small collimation apertures lead to smallest Q-vectors of around 0.0001 1/Å. The high intensity and high resolution options of the KWS-1 and KWS-2 SANS instruments will be presented in details.

CPP 33: Organic Photovoltaics II

Time: Thursday 14:00–16:00

Location: ZEU 222

CPP 33.1 Thu 14:00 ZEU 222

Interplay between morphology and energy levels in conjugated polymers: A theoretical view — ●GEORG HEIMEL¹, INGO SALZMANN¹, STEFFEN DUHM², JÜRGEN P. RABE¹, and NORBERT KOCH¹ — ¹Institut für Physik, Humboldt-Universität zu Berlin, Newtonstr. 15, D-12489, Berlin, Germany — ²Graduate School of Advanced Integration Science, Chiba University, Japan

Conjugated polymers are important constituents of organic electronic devices and it is both the bulk properties and the interfaces, which decisively determine device performance. For example, the preparation conditions are known to crucially impact the thin-film morphology of the prototypical π -conjugated polymer region-regular poly(3-hexylthiophene) and, consequently, also the device characteristics of, e.g., organic solar cells based on this material (rr-P3HT). We present first-principles calculations on highly ordered monolayers of rr-P3HT and a fluorinated derivative with the backbone orientations varying continuously from face-on to edge-on. Supported by electrostatic modeling, we find that the backbone orientation importantly influences the energy-level positions in these films due to intra-molecular surface dipoles; we find variations of up to 1.5 eV. As a consequence, also the energy-level alignment at ubiquitous inorganic/organic and organic/organic interfaces can be expected to depend critically on thin-film morphology. Our results provide further insight into the structure-property relationship in an important class of materials and imply novel strategies for molecular, polymer, and device design.

CPP 33.2 Thu 14:15 ZEU 222

Investigation of the preparation process of dye sensitized photovoltaic cells by AFM, Kelvin Probe Force Microscopy and X-ray diffraction — ●HARALD GRAAF¹, CARSTEN MÄDLER¹, MIRKO KEHR¹, and TORSTEN OEKERMANN² — ¹Institute of Physics, University of Technology Chemnitz, 09107 Chemnitz, Germany — ²Institute of Physical Chemistry and Electrochemistry, Leibniz University Hannover, 30167 Hannover, Germany

Dye-sensitized photovoltaic cells with zinc oxide (ZnO) as the inorganic semiconductor and organic dye molecules as the sensitizer are well known devices with high efficiency. Such cells are prepared by electrochemical deposition of an aqueous zinc salt solution including dye molecules. After deposition the dye is desorbed to obtain a porous ZnO network followed by re-adsorption of the dye as a sensitizer. Up to now studies concerning the influence of different processing steps on the structure of the ZnO are sparse. We discuss the growth mechanism during film deposition and the crystal structure changes of the ZnO accompanying the desorption process, which is performed in an alkaline aqueous solution. X-ray investigation shows the influence of the dye on the structure of the formed ZnO/dye hybrid film. AFM topography and Kelvin Probe Force Microscopy investigations suggest the following deposition process: at first dye molecules are adsorbed on the electrode followed by ZnO formation within the pores of the organic network. This ZnO, which shows high crystallinity, seems to be oriented with the zinc face up.

CPP 33.3 Thu 14:30 ZEU 222

Nanoscale Near-field Spectroscopic Investigation of the Interplay between Local Film Morphology and the P3HT/PCBM Organic Solar Cell Efficiency — ●DAI ZHANG¹, XIAO WANG¹, KAI BRAUN¹, HANS-JOACHIM EGELHAAF², and ALFRED J. MEIXNER¹ — ¹Institute of Physical and Theoretical Chemistry, University of Tuebingen, Germany — ²Christian-Doppler-Lab for Surface Optical Meth-

ods, Johannes-Kepler-University and Konarka GmbH, Linz, Austria

The interplay between the local film morphology and the organic solar cell efficiency is systematically investigated by apertureless near-field scanning optical microscopy (SNOM). A home-built parabolic mirror assisted SNOM is used to collect both the topography and optical (Raman and photoluminescence (PL)) information from the Poly(3-hexylthiophene) (P3HT) and [6,6]-phenyl C₆₁ butyric acid methyl ester (PCBM) blend film. Molecular domains composed of either PCBM or P3HT at nanometer scale are successfully determined by their corresponding Raman fingerprint information and PL information. The regioregularity of P3HT polymer influenced by the clustering of PCBM during thermal annealing is compared considering the FWHM broadening of the C=C vibration Raman peak. The influences of the local film morphology and the local distribution of P3HT/PCBM on the solar cell efficiency are discussed based on the different PL quenching levels induced by the exciton dissociation and electron transfer at P3HT/PCBM interfaces.

CPP 33.4 Thu 14:45 ZEU 222

Ultrahigh time resolution nonlinear spectroscopy of polymer/fullerene blends — ●SARAH MARIA FALKE¹, DANIELE BRIDA², GIULIO CERULLO², and CHRISTOPH LIENAU¹ — ¹Institut für Physik, Carl von Ossietzky Universität Oldenburg, 26129 Oldenburg, Germany — ²Dipartimento di Fisica, Politecnico di Milano, 20133 Milano, Italy

Blends of polymers and fullerene derivatives are important prototype structures for efficient photoinduced charge generation and transport in organic photovoltaic devices. It is well established that photoexcitation of polymer/fullerene blends can result in an efficient ultrafast charge transfer from the excited polymer to the electron accepting fullerene moiety. It is generally believed that this charge transfer occurs within 50-100 fs [1]. Here we study ultrafast nonlinear spectra of pristine polymers (poly(3-hexylthiophene-2,5-diyl), P3HT) and polymer/fullerene ([6,6]-phenyl-C₆₁ butyric acid methyl ester, PCBM) blends with a high time resolution of only 5 fs using a novel two-color pump-probe setup with broadband detection range. By comparing transient spectra of polymers and the polymer blend we observe an extremely rapid buildup of a band between 450 nm and 525 nm in the blend, occurring on a sub-10-fs time scale. Since the band is generally assigned to the stimulated emission from the indirectly excited fullerene moiety, our results indicate excitation transfer from the photoexcited polymer to the fullerene moiety on a sub-10-fs time scale, much faster than previously thought. The implications of these results for the microscopic charge generation processes in polymer/fullerene blends are discussed. [1] C.J. Brabec, Chem. Phys. Lett. **340**, 232 (2001).

CPP 33.5 Thu 15:00 ZEU 222

A synthetic way towards rational design of discotic liquid crystals with high charge carrier mobilities — ●DENIS ANDRIENKO¹, XINLIANG FENG¹, VALENTINA MARCON¹, WOJCIECH PISULA¹, JAMES KIRKPATRICK², FERDINAND GROZEMA³, KURT KREMER¹, and KLAUS MUELLEN¹ — ¹Max Planck Institute for Polymer Research, Mainz, Germany — ²Imperial College London, UK — ³Delft University of Technology, The Netherlands

Conjugated materials offer the revolutionary prospect of producing semiconductor devices at low cost. The best to date discotics are built around the coronene unit and possess six fold symmetry. In the discotic phase six fold symmetric molecules stack with an average azimuthal twist of 30 deg, whereas the angle which would lead to the

greatest electronic coupling and hence highest charge mobility is 60 deg. Here, a molecule with three fold symmetry and alternating hydrophilic/hydrophobic side chains is synthesized and X-ray scattering is used to prove the formation of the desired helical microstructure. Pulse radiolysis time resolved microwave conductivity measurements show that the material has indeed a very high mobility in the plastic crystalline phase, in the range of $0.1 - 0.2 \text{ cm}^2/\text{Vs}$. The physical structure of the assemblies of molecules are simulated using molecular dynamics. This, together with quantum chemical techniques, allows the computation of charge mobilities without fitting parameters. The calculations prove that mobility is still limited by structural defects and that a defect free assembly would lead to mobilities in excess of $10 \text{ cm}^2/\text{Vs}$.

CPP 33.6 Thu 15:15 ZEU 222

Absorption enhancement in excitonic solar cells by a photonic crystal top layer — ●STEFAN GULDIN¹, NICOLAS TETREAULT^{1,3}, MATHIAS KOLLE¹, SVEN HÜTTNER¹, MARK WELLAND², PETER MÜLLER-BUSCHBAUM⁴, RICHARD FRIEND¹, and ULLRICH STEINER¹ — ¹Cavendish Laboratory, University of Cambridge, UK — ²Nanoscience Center, University of Cambridge, UK — ³LPI, Ecole Polytechnique Federale de Lausanne, CH — ⁴Physik-Department, E13, TU München

Photonic crystal structures have been identified by theorists as a candidate to enhance the still relatively low response of excitonic photovoltaic cells in the near infrared. We present a new material route that enables the fabrication of a double layer dye-sensitised solar cell, including a mesoporous TiO₂ underlayer with high surface area and an optically active TiO₂ photonic crystal layer. A diblock copolymer acts as a structural directing agent for the mesoporous TiO₂, arranging the sol-gel-derived material into a highly ordered nanostructure. The hybrid underlayer is not porous in its unannealed state and thus allows the self-assembly and infiltration of a photonic crystal template. This approach represents, to our knowledge, the first successful method that couples a photonic crystal top layer into a functioning dye-sensitised solar cell with front illumination, opening up a vast parameter space for effective light management. In this first attempt an increase in normalised photon to electron conversion of 20.4% was observed in the range from 520 nm to 725 nm (at the tail of the dye absorption spectrum).

CPP 33.7 Thu 15:30 ZEU 222

Investigation of ageing processes in bulk-heterojunction

P3HT:PCBM organic solar cells by means of impedance spectroscopy — ●ULI WÜRFEL^{1,3}, BAS V. D. WIEL², BIRGER ZIMMERMANN^{1,3}, and MICHAEL NIGGEMANN³ — ¹Freiburg Materials Research Centre, Freiburg, Germany — ²Universiteit Utrecht, Netherlands — ³Fraunhofer Institute for Solar Energy Systems, Freiburg, Germany

The improvement of the long term stability is one important task in the development of organic photovoltaic (OPV) devices. Although promising device stabilities in the order of years can be expected the degradation mechanisms are not understood completely. They have to be identified to define conditions for accelerated degradation experiments to predict the lifetime of a device. Oxygen and water are well known as most harmful chemical species for OPV devices. We will present results of accelerated ageing experiments done on bulk-heterojunction P3HT:PCBM solar cells. The cells were placed in a gas tight flow cell and exposed either to ambient air, pure dry oxygen or nitrogen saturated with water vapour. They were repeatedly measured by recording dark and illuminated current-voltage characteristics and a series of impedance spectra for different applied bias voltages. By means of the impedance spectra it is possible to distinguish between different degradation phenomena - like e.g. doping and interface degradation - and gain a deeper understanding of the underlying processes. Finally, simulations were carried out to model the change in the physical properties of the organic semiconductor and its impact on the device performance.

CPP 33.8 Thu 15:45 ZEU 222

Influence of polymer solar cell geometry on device parameters — BURHAN MUHSIN¹, JOACHIM RENZ¹, KARL-HEINZ DRÜE², GERHARD GOBSCH¹, and ●HARALD HOPPE¹ — ¹Institute of Physics, Ilmenau Technical University, Weimarer Str. 32, 98693 Ilmenau, Germany — ²Electronic Technology, Ilmenau Technical University, Gustav-Kirchhoff-Str. 7, 98693 Ilmenau, Germany

In order to study the influence of the device shape on the solar cell device parameters, we systematically varied its geometry. By determining all sheet and contact resistances in the device, we were able to correlate the series resistance with the geometry of the device using a simple model for its calculation. As a result, rules for optimal design of solar modules were derived. However, further refinement of the calculation is required in order to minimize the deviation between calculus and experiment.

CPP 34: Microfluidics I: Applications and Devices

Time: Thursday 9:30–12:30

Location: ZEU 160

CPP 34.1 Thu 9:30 ZEU 160

Ship-in-a-Bottle Assembly of Linked Geometrically Coupled Microdevices — ●TOBIAS SAWETZKI¹, SABRI RAHMOUNI¹, DAVID W.M. MARR², and CLEMENS BECHINGER^{1,3} — ¹2. Physikalisches Institut, Universität Stuttgart — ²Chemical Engineering Department, Colorado School of Mines, Golden — ³Max-Planck-Institut für Metallforschung, Stuttgart

To realize complex microfluidic systems the ability to drive and control the single components in an integrated and cooperative fashion is required. In current microfluidic chips the actuation and manipulation of individual units is often done on a single-device level by applying macroscopic methods such as external pressure. The need for connections to the macroscopic world for every single device on the chip hinders both, the portability and the development of highly complex architectures on Lab-on-a-Chip systems. We present a new method [1] to build, actuate and control microfluidic systems with only one external source of power. Magnetic fields are not only used to *in-situ* assemble paramagnetic colloidal particles in confining geometries, but also to power the components non-invasively and massively parallel. By combining local geometry of channel architecture with this single global field, the functionality of a constituent device is only defined by the shape of colloidal cluster and surrounding. Applying this method, we present a full set of basic microfluidic components like pumps, valves and mixers, and demonstrate that more complex operations can be performed by linking individual units together.

[1] Sawetzki *et al.* PNAS, Dec. 08

CPP 34.2 Thu 9:45 ZEU 160

Separation of magnetic beads by a combination of magnetic and hydrodynamic forces — ●FRANK WITTBRACHT, ALEXANDER WEDDEMANN, ALEXANDER AUGE, and ANDREAS HÜTTEN — Universität Bielefeld, Universitätsstraße 25, D-33615 Bielefeld

Lab-on-a-chip technologies have gained importance in recent years. The integration of all functions and components needed for the analysis of a sample on microfluidic chips has to be achieved. Magnetic materials are widely used in these systems for various applications such as magnetohydrodynamic pumps and valves. Especially in terms of separation and detection of biological samples magnetic materials are suitable.

In this work a microfluidic separation system for magnetic beads is experimentally realized according to theoretical simulations. The separation of magnetic beads is achieved by magnetic gradient fields resulting from conducting lines near the microfluidic channel. Experimental results are compared to calculated results.

CPP 34.3 Thu 10:00 ZEU 160

Manipulation of nanoparticles by turbulent electrohydrodynamic flows — ●MICHAEL BOETTCHER, MAGNUS JAEGER, and CLAUDUS DUSCHL — Fraunhofer Institute for Biomedical Engineering (IBMT), Am Muehlenberg 13, 14476 Potsdam, Germany

Several methods for the manipulation of micro- and nanoparticles have attracted interest in medicine and biotechnology. Especially, lab-on-chip systems (LOC) found their applications due to their fine fluid channels being of the same length scale as the objects under test. An attribute of these micrometre-sized channels is a continuous fluid

flow. In conventional LOCs these flows are often generated by external pressure-driven pumps. A alternative path to establish a fluid transport is a high-frequency, electrical travelling wave. This mechanism can be integrated directly into the chip and works without any moving parts. To this end, an array of parallel electrode elements provides the driving, electrical field. Under special circumstances, the induced fluid flow is accompanied by vortices above the electrodes. The establishment of these turbulent flows in our microfluidic device - which is defined by small Reynolds numbers and, therefore, a laminar flow - indicated a potential of the system for a new application. Our goal is to optimise these vortices to manipulate especially nanometre-sized particles e. g. viruses. For that it is essential to get a better understanding of the vortices. We use the travelling wave mechanism to accumulate artificial, fluorescent beads. The advantage of our system is the defined accumulation of nanometre-sized particles in the absence of any filtering material.

CPP 34.4 Thu 10:15 ZEU 160

Static and dynamic surface-coatings in quartz crystal- and Poly(dimethylsiloxane)-microfluidic channels — ●MARTINA EVERWAND, JAN REGTMEIER, and DARIO ANSELMETTI — Bielefeld University, Experimental Biophysics & Applied Nanoscience, Universitätsstr. 25, 33615 Bielefeld, Germany

For bioanalytical applications, the surface properties of the Lab-on-a-Chip device are of great relevance, e.g. for limiting the band broadening in electroosmotic flow applications.

Therefore we have investigated three different coatings Poly(L-lysine)-poly(ethylene glycol) (PLL-PEG), F108 and n-Dodecyl-D-Maltoside Methyl Cellulose (DDM-MC)) in quartz-crystal and Poly(dimethylsiloxane) (PDMS) microfluidic systems with respect of their electroosmotic flow, protein adhesion and contact angle properties. We used either static or dynamical coating, where the polymers were incubated and rinsed prior usage or where the polymers were directly added to the separation solution.

In summary, all three coatings were able to reduce the electroosmotic flow and protein adsorption in quartz as well as in Poly(dimethylsiloxane) microchips. The highest reductions were obtained for the dynamically coated n-Dodecyl-Maltoside Cellulose polymer.

CPP 34.5 Thu 10:30 ZEU 160

Internal flow and surfactants' dynamics in confined emulsions — ●AUDREY STEINBERGER¹, RALF SEEMANN^{1,2}, and STEPHAN HERMINGHAUS¹ — ¹MPI for Dynamics and Selforganization, D-37073 Goettingen — ²Experimental Physics, Saarland University, D-66041 Saarbruecken

We study the flow of emulsions confined in microchannels whose lateral dimensions are on the same scale as the size of the drops. This system is not only a promising tool for handling liquids in microfluidic processes but also a convenient model system to study the dissipation mechanisms associated to the flow of confined emulsions. Interfacial friction induces a recirculation flow -controlling the mixing- within the droplets. Our aim is to investigate the interaction between those internal flows and the dynamics of the surfactants used to stabilize the emulsion: what is the effect of the viscous stress on the surfactants' layer that surrounds the drops and stabilizes the emulsion? Reciprocally, what is the impact of the surfactants' frictional properties significantly on the internal flow? And what happens in very concentrated emulsions, where the thickness of the continuous phase lamellas separating the drops becomes very small, and possibly reduces to a surfactant bilayer?

To answer those questions, we have developed a micro-PIV setup that allows us to measure simultaneously the velocity field within the drops and the local concentration of fluorescent surfactants on two separate color channels. Here we describe this setup and report on the first results we obtained with it.

15 min. break

CPP 34.6 Thu 11:00 ZEU 160

Phase Transition Behaviour of Nanopore Confined Liquids explored by Capillary Rise Experiments — ●SIMON GRUENER and PATRICK HUBER — Saarland University

We present measurements on the capillary rise (spontaneous imbibition) of liquids into silica monoliths (porous Vycor) permeated by tortuous pores with radii of about 5 nm. The flow properties are studied as

a function of the complexity of the building blocks of the liquids (water, n-alkanes and liquid crystals). In this talk I will present measurements that permit detailed insights into the phase transition behaviour of selected liquids during the imbibition process. First and foremost I will focus on the well-known surface freezing effect in tetracosane. Because of the striking impact of this phenomenon on the surface tension of the liquid the capillarity driven imbibition process is perfectly suitable for such examinations. This work has been supported within the DFG priority program 1164, Nano- & Microfluidics (Grant No. Hu 850/2).

CPP 34.7 Thu 11:15 ZEU 160

Focusing X-ray beam by dynamic compound refractive lenses in a microfluidic device — ●YASUTAKA IWASHITA¹, CHRISTIAN BAHR¹, RALF SEEMANN^{1,2}, and STEPHAN HERMINGHAUS¹ — ¹MPI for Dynamics and Self-Organization, D-37073 Goettingen — ²Experimental Physics, Saarland University, D-66041 Saarbruecken

Compound refractive lenses (CRL), composed of a large number of individual lenses of small radii in a row embedded in a solid medium, have been developed as X-ray lenses [1]. To broaden the possibilities and functions of CRL's, we designed a 'dynamic CRL' composed of gas bubbles in a liquid, where the bubbles are generated *in situ* and flowing consecutively in a microfluidic device. Here, the lamellae between the bubbles act as lenses. Due to the continuous renewal of the materials, this system leads to a high stability against high X-ray intensities. Furthermore, the variation of bubble shape controlled via flow parameters allows *in situ* optimization of the optical properties.

We generate dynamic CRL structures with gas - octadecane foams stabilized by surface freezing and gas - dodecylcyanobiphenyl (liquid crystal) foam stabilized by surface ordering. The advantages of these systems are high X-ray transmittance and stabilization without surfactants. As an example, the theoretically estimated lens properties of a generated dynamic foam, i.e., the focal length, gain and transmittance along the optical axis, were 97.7 μm , 1800 and 50.3 %, respectively, for X-ray energy of 8 keV.

[1] A. Snigirev, V. Kohn, I. Snigireva and B. Lengeler, *Nature* 384(6604), 49(1996).

CPP 34.8 Thu 11:30 ZEU 160

Stability and transitions of droplet arrangements confined in microchannels — ●ENKHTUUL SURENJAV¹, JULIA BURKHARDT¹, MARTIN BRINKMANN¹, STEPHAN HERMINGHAUS¹, and RALF SEEMANN^{1,2} — ¹MPIDS, Göttingen, Germany — ²Experimental Physics, Saarland University, Saarbrücken, Germany

We focus on organization and manipulation of monodisperse gel emulsions in microchannels both in dynamic and static droplet arrangements. Transitions between certain foam-like topologies in an emulsion flowing through a channel can be induced e.g. by varying the geometry of the channel. Due to the finite energy required to change a certain droplet arrangement ("T1"-Transition) topology transitions are inherently hysteretic and depend not only on the droplet size but also on the volume fraction of the dispersed phase. By incorporating corners into the microfluidic channel network we performed precise manipulation of the individual droplet positions with respect to the neighboring droplets. The number of phase shifts as a function of drop size, volume fraction and corner angles were studied and show reasonable agreement with the theoretical consideration based on the path length differences. In stopped flow conditions, quasi two-dimensional structural transitions of static emulsion topologies have been studied as a function of lateral force. By applying a lateral force to the static droplet arrangement, we could vary the equilibrium conditions of different arrangements due to the variation of dispersed phase volume fraction during the droplet compression. We compared the experimental results with the numerical calculation and found qualitative agreement.

CPP 34.9 Thu 11:45 ZEU 160

Microfluidic Physics of Self-synchronizing Picolitre Droplet Generation — ●VENKATACHALAM CHOKKALINGAM¹, STEPHAN HERMINGHAUS¹, and RALF SEEMANN^{1,2} — ¹Max Planck Institute for Dynamics and Self-Organization, Goettingen, Germany. — ²Experimental Physics, Sarland University, Germany.

The in-situ generation of pairs of droplets with excellent monodispersity is essential for quantitative (bio-) chemical reactions in a droplet based microfluidic chip. In the presented work we demonstrate the simultaneous, self-synchronized production of droplets with high dispersed phase volume fraction (up to about 96 %) and excellent monodispersity (variance of the droplet diameter < 1.2 %) with

two different contents by step emulsification. The synchronization is achieved by a pressure cross talk of two connected production units while retaining all relevant properties of a single step-emulsification unit. Pairs and triplets of droplets can be achieved. While the drop volumes of the two droplet types may be different up to a factor of two, the excellent monodispersity of each type is retained.

CPP 34.10 Thu 12:00 ZEU 160

Promoting selective gold immobilization onto polymer nanotemplates using solution flow-stream technique — ●EZZELDIN METWALLI¹, JEAN-FRANCOIS MOULIN², JAN PERLICH¹, WEINAN WANG¹, ALEXANDER DIETER¹, STEPHAN V. ROTH³, and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik Department LS E13, James-Franck-Str.1, 85747 Garching, Germany — ²FRM II, TU München, 85747 Garching, Germany — ³HASYLAB at DESY, Notke Str. 85, 22603 Hamburg, Germany

Guiding gold nanoparticles aggregation into an ordered nano-patterned structure has attracted an immense attention due to applications in nanoelectronics, bioelectronics, and gas sensors. In the current investigation, gold nanoparticles were cast onto nanostructured polymer templates using solutions subjected to hydrodynamic flow by utilizing a simple flow device. Phase-separated polystyrene-block-polyethylene P(S-b-E) diblock copolymer film with parallel cylinder morphology is selected as a nanostructured polymer template. Using in situ grazing incidence small angle X-ray scattering (GISAXS), the progressive gold deposition from solution at various flow rates onto the polymer template attached to the X-ray transparent flow-channel is investigated. The continuously flowing stream of gold solution causes a systematic increase of the X-ray contrast between both phase-separated blocks of the block copolymer template indicating a flow-induced selective gold

immobilization. With further gold nanoparticles upload by the continuous flow, the selectivity characteristic of the flow deposition method diminishes with the formation of an almost uniform gold layer.

CPP 34.11 Thu 12:15 ZEU 160

Lattice Boltzmann studies of finite size driven droplet evaporation and droplet dynamics — ●FATHOLLAH VARNIK — Interdisciplinary Center for Advanced Materials Simulation, Ruhr University Bochum, Germany

The lattice Boltzmann (LB) method has received growing interest both in the scientific and the engineering community. Significant extensions and ramifications of the LB method have been proposed allowing the study of a rich variety of fluid dynamics problems such as the flow through porous media, two phase flows [1] as well as roughness effects on transitional flows [2], to name just a few.

The lattice Boltzmann method proves itself as a particularly powerful tool when it comes to a study of intricate boundary conditions such as chemical and topographical heterogeneity [3].

Here, the method is applied for a study of interesting issues such as instability (evaporation) of droplets in a system with a finite size as well as to the dynamics of droplets.

[1] X. Shan and H. Chen, Phys. Rev. E 47, 1815 (1993); and Phys. Rev. E 49, 2941 (1994); M. R. Swift, W. R. Osborn, and J. M. Yeomans, Phys. Rev. Lett. 75, 830 (1995); and A. J. Briant, A. J. Wagner, and J. M. Yeomans, Phys. Rev. E 69, 031602 (2004).

[2] F. Varnik, D. Dorner, and D. Raabe, J. Fluid Mech. 573, 191 (2007); F. Varnik and D. Raabe, Modell. Simul. Mater. Sci. Eng. 14, 857 (2006).

[3] F. Varnik, P. Truman, Bin Wu, P. Uhlmann, M. Stamm, D. Raabe, Phys. Fluid. 20, 072104 (2008).

CPP 35: Microfluidics II: Boundary conditions

Time: Thursday 14:00–15:30

Location: ZEU 160

CPP 35.1 Thu 14:00 ZEU 160

Simulations of lubrication force experiments — ●JENS HARTING¹, CHRISTIAN KUNERT¹, and OLGA I. VINOGRADOVA² — ¹Institut für Computerphysik, Pfaffenwaldring 27, 70569 Stuttgart, Germany — ²A.N. Frumkin Institute of Physical Chemistry and Electrochemistry, Russian Academy of Sciences, 31 Leninsky Prospect, 119991 Moscow, Russia

When an object that is submerged in a liquid is approached towards a surface, the lubrication force raises. The measurement of the lubrication force gives an insight in the flow profile near objects and thus one can deduce the flow boundary condition. In particular, such a measurement can be used to study the effect of boundary slippage. Therefore many groups perform experiments, where a colloidal sphere is attached to the cantilever of an atomic force microscope (AFM) to measure the lubrication force. For the ideal situation of a perfect sphere being approached with a small, constant velocity towards a perfectly smooth wall a theoretical description is well known and a correction for boundary slip can be applied. In the case of rough boundaries and non-constant approaching velocity a theoretical description is missing. In this contribution we present lattice Boltzmann simulations of such non ideal cases and show that the known theory holds even for very rough surfaces if one applies an effective boundary.

CPP 35.2 Thu 14:30 ZEU 160

The microscopic origin of surface slip: Looking at the boundary layer of sheared liquids on solid surfaces — ●PHILIPP GUTFREUND^{1,2}, MAXIMILIAN WOLFF^{1,2}, STEFAN GERTH³, ANDREAS MAGERL³, and HARTMUT ZABEL² — ¹Institut Laue-Langevin — ²Ruhr-Universität Bochum — ³Universität Erlangen-Nürnberg

According to text-book physics the contacting layer of a flowing liquid is sticking to the solid boundary and from this a smooth velocity profile develops into the bulk of the liquid, which is in agreement with many macroscopic experimental observations. However, recently, both experiments and theory have shown that on a microscopic scale simple liquids may undergo significant slip at a solid wall. Different mechanisms can be evoked to address slip like the formation of a thin depletion layer or a molecular ordering in the liquid near the interface. For most liquids, the short length scales important for slip effects are difficult to probe directly and non destructively. Grazing incident neu-

tron scattering techniques have proved to be a very sensitive tool for the detection of depletion effects and structural arrangements close to solid-liquid walls. We will present recent results obtained by Neutron Reflectivity (NR) and Grazing Incidence Neutron Diffraction (GIND) studies on the depth profile and structure of the boundary layer of sheared hexadecane, that is known to show surface slip, on differently coated solid surfaces. The NR results for deuterated hexadecane show a depletion layer of about 2 nm and the GIND patterns show that the liquid structure factor seems to be influenced by shear.

CPP 35.3 Thu 14:45 ZEU 160

Altering the boundary conditions to influence flow dynamics of a liquid film — ●MATTHIAS LESSEL, OLIVER BÄUMCHEN, and KARIN JACOBS — Saarland University, Experimental Physics, D-66041 Saarbrücken

In the course of the miniaturization of fluidic devices, the typical diameter of flow channels becomes smaller and smaller. Typically, the velocity of the liquid at the boundary to a channel wall is zero, a parabolic velocity profile is measured and high pressure is needed to move the liquid.

We study the impact of surface modifications on the slip length on a model system: polymer films on tailored Si wafers. To induce flow we use the dewetting process, which is driven by an internal force governed by the effective interface potential. In our case, hydrophobic substrates (Si wafers covered by octadecyltrichlorosilane (OTS), dodecyltrichlorosilane (DTS), or Teflon (AF1600)) are only partial wetted by the polystyrene melt. They are ideal smooth substrates. So, roughness effects could be neglected.

Using optical microscopy we found at constant temperature an increase of the dewetting velocity on substrates which show slippage. The slip lengths could be calculated by observing the growth of dewetting holes in the film. The slip lengths lay in the range from several nanometers for AF 1600 to several micrometers for DTS. These results could be approved by analyzing the rim shapes around the holes using AFM. The shapes were found to be influenced by slippage too.

CPP 35.4 Thu 15:00 ZEU 160

In-situ investigation of the solid/liquid interface 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 — ²Inst. f. Phys. Chem., Uni HH, Grindelallee 117, D-20145 Hamburg, Germany

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

The experiments were performed the beamline BW4 at HASYLAB, Hamburg [1] using the microfocuss set-up. We present the results of the investigation of a 13 wt.% solution of a poly-(isoprene-block-ethylene oxide) in water. The block degrees of polymerization of the isoprene and the polyethylene oxide were 55 and 170, respectively. The shear stress was applied by a stress-controlled Bohlin CVO rheometer in a plate-plate-geometry with a diameter of 20 mm and a gap of 1 mm. We investigated the interface layer of the solution with the rotor of the shear geometry at different temperatures. Under shear a desorption of the micelles from the rotor plate was observed, which is independent of the actual shear rate. [2]

References:

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

[2] Timmann et al., App. Phys. Lett., 2007, 91, 213102

CPP 35.5 Thu 15:15 ZEU 160

Shear induced relaxation of polymer micelles at the solid-liquid interface — ●MAX WOLFF^{1,2,3}, ROLAND STEITZ⁴, PHILIPP GUTFREUND^{1,2}, NICOLE VOSS⁵, STEFAN GERTH⁵, MARCO WALZ⁵, ANDREAS MAGERL⁵, and HARTMUT ZABEL¹ — ¹Institute for Solid State Physics/EP IV, Ruhr-University Bochum, Germany. — ²Institute Laue-Langevin, Grenoble, France. — ³Materials Physics, Uppsala University, Sweden. — ⁴Helmholtz Centre Berlin for Materials and Energy, Berlin, Germany. — ⁵Crystallography and Structural Physics, University of Erlangen-Nürnberg, Erlangen, Germany.

Mixtures of amphiphilic block copolymers with a selective solvent are known to form various structures. Applying external fields such as shear can dramatically change the overall structure of the sample. In most cases, crystallites become aligned.

A 20 % aqueous solution of F127 was investigated by combining rheology in a cone/plate-geometry and surface-sensitive grazing incident neutron scattering. The crystalline structure formed by the polymer micelles becomes less pronounced for low shear rates, but correlations increase for higher shear rates. After stopping shear a slow relaxation of the micelles is found in the vicinity of a hydrophilic silicon wall, while a fast relaxation is observed in the boundary layer against the hydrophobic silicon wall (weak micelle-wall interaction). The results show that in the vicinity of the interface wall-particle interactions compete heavily with the shear force acting on the liquid [1].

[1] M. Wolff et al., Langmuir (Letter) 24, 11331 (2008).

CPP 36: Microfluidics III: Soft Objects in Flow

Time: Thursday 15:45–17:00

Location: ZEU 160

Topical Talk CPP 36.1 Thu 15:45 ZEU 160
Modifying Single Particle Diffusion by Chemical Surface Patterning — MARTIN PUMPA and ●FRANK CICHOS — Molecular Nanophotonics Group, University Leipzig

Molecular dynamics at solid/liquid interfaces is among other effects defined by the strength of the interaction of the liquid with the solid surface. The hydrodynamic boundary conditions define the hydrodynamic friction a particle or molecule experiences close to this interface. Thus control of the surface properties of a solid substrate provides a route to control the interfacial molecular dynamics in liquid films. Within this contribution, we present first experimental results on a controlled manipulation of single molecule diffusion by chemically patterning glass surfaces. Using micro-contact printing, we prepare a hydrophilic/hydrophobic pattern on the surface. Typical dimensions of the structure of this pattern are on the order of a few micrometers. These surfaces are mounted in a surface forces apparatus, where the liquid covering the pattern is confined down to a film thickness of a few 100 nanometers. To study molecular dynamics, we employ single molecule tracking of labeled colloids dispersed in the liquid. A new correlation analysis of particle mobility and particle position reveals a clear spatial correlation between chemical surface preparation and particle diffusion.

CPP 36.2 Thu 16:15 ZEU 160

Dynamics of suspended particles diffusing through small walls — ●LAURA ALMENAR^{1,2} and MARKUS RAUSCHER^{1,2} — ¹Max-Planck-Institut für Metallforschung, Stuttgart, Germany — ²ITAP, Universität Stuttgart, Stuttgart, Germany

We study the dynamics of suspended particles in small channels in the presence of flow (in particular Poiseuille flow). We describe the transport taking into account the interactions among the particles as well as with the walls. We extend our study to include the effect of hydrodynamic interactions between particles and walls. With hydrodynamic chromatography as an application in mind we aim for a better understanding of these transport processes.

We focus first on steady state situations and we calculate the size-dependent throughput of the particles using a finite element method. It will be compared with the case of non-interacting particles. The throughput is enhanced or decreased as compared to the non-interacting case depending on the size ratio of the particles and the interaction radius.

CPP 36.3 Thu 16:30 ZEU 160

Self Assembled Supramolecular Structures using Microfluidic Gel Emulsions: Applications in Molecular Electronic Cir-

cuits — ●SHASHI THUTUPALLI¹, SHUANG HOU¹, RALF SEEMANN^{1,2}, MARCEL MAYOR³, and STEPHAN HERMINGHAUS¹ — ¹Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — ²Experimental Physics, Saarland University, Saarbrücken, Germany — ³Department of Chemistry, University of Basel, Switzerland

Hierarchical supramolecular structures in nature are seamlessly linked over several length scales. Synthetic systems with similar integration have been built using two approaches - top down and bottom up. We employ a combination of both, using droplet microfluidics and molecular design, to demonstrate the possibility of self assembled molecular circuits. Using microfluidic gel emulsions, we generate 100's of lipid bilayers that can hold self inserting (amphiphilic) conducting molecules that span the bilayer. Aqueous compartments on either side of the bilayers are then used as electrical contacts establishing self assembled nanogaps for molecular electronics. Further, the droplets in the microfluidic channel assemble into precise arrangements, forming well controlled circuits of conducting molecular rods. Special integrated microelectrodes are used as electrical probes. In such a setup, we show insertion of an electrochromic dye, Di-4-ANEPPS into bilayers of monoolein and record its fluorescence intensity variation with an applied voltage. As a first step to building functional circuits, we also present preliminary results with synthetic conducting molecules.

CPP 36.4 Thu 16:45 ZEU 160

Development and validation of a simplified particulate model for the simulation of blood flow in arbitrary geometries — ●FLORIAN JANOSCHEK and JENS HARTING — Institute for Computational Physics, Pfaffenwaldring 27, D-70569 Stuttgart, Germany

Simulation of human blood flow is a demanding task both in terms of the complexity of applicable models as well as the computational effort. One reason is the particulate nature of blood which in first approximation may be treated as a suspension of red blood cells (RBC) in blood plasma. A second reason is that in realistic geometries typical length scales vary over several orders of magnitude.

By coupling a simple molecular dynamics algorithm for modeling the RBC to the lattice Boltzmann method we obtain an efficient and versatile parallel code that keeps the particulate nature of the RBC and takes full hydrodynamic interactions into account. Different from other lattice Boltzmann-based approaches we do not model the deformability of the RBC itself but instead cover it by soft anisotropic potentials between each two particles as well as between each particle and the confining geometry.

Due to this simplifications our model is computationally efficient enough to simulate the high numbers of RBC that occur in vessels of intermediate size. To validate our model we compare our numerical

results to experimental data obtained from the literature.

CPP 37: Biopolymers (joint session CPP/BP)

Time: Thursday 14:30–17:30

Location: ZEU 114

CPP 37.1 Thu 14:30 ZEU 114

Secondary structure of polyalanine peptides [Ac-Ala_nLysH⁺ (n=5, 10, 15, 19)] in vacuo – part I (experiment) — ●PETER KUPSER, FRAUKE BIERAU, GERT VON HELDEN, MARIANA ROSSI, VOLKER BLUM, MATTHIAS SCHEFFLER, and GERARD MEIJER — Fritz-Haber-Institut, D-14195 Berlin, Germany

While vibrational spectroscopy is one of the key techniques to determine the three-dimensional folding arrangements of biological molecules in solution, infrared experiments of gas-phase peptides and proteins can provide information on intrinsic molecular structural properties without interactions with the surrounding solvent molecules [1]. This is also of great interest for theoreticians to test and enhance their models for determining the structure of biomolecules.

Ac-Ala_n-LysH⁺ (n=5, 10, 15, 19) peptides in the gas phase can serve as model systems for a helical secondary structure [2]. Infrared multiphoton dissociation experiments in the regions of the amide I (C=O stretching vibration around 1700 cm⁻¹) and amide II (N-H bending vibration around 1500 cm⁻¹) band on these polyalanine peptides at room temperature were performed using the free electron laser FELIX. The position of the amide I band shifts to lower energies with increasing number of alanines in the chain. Experimental results will be presented and discussed. [1] G. von Helden *et al.*, PCCP 7, 1345 (2005). [2] R. R. Hudgins *et al.*, JACS 120, 12974 (1998).

CPP 37.2 Thu 14:45 ZEU 114

Secondary structure of polyalanine peptides [Ac-Ala_nLysH⁺ (n=5, 10, 15)] in vacuo – part II (density functional theory) — ●MARIANA ROSSI, VOLKER BLUM, PETER KUPSER, GERT VON HELDEN, FRAUKE BIERAU, GERARD MEIJER, and MATTHIAS SCHEFFLER — Fritz-Haber-Institut, D-14195 Berlin, Germany

Predicting the conformation(s) of biomolecules from first principles is an important challenge, requiring *both* an accurate energetic description of single conformers *and* an efficient strategy to explore the combinatorial explosion of potential candidate structures. We here study the secondary structure of Ac-Ala_nLysH⁺ (n=5, 10, 15) polyalanine peptides *in vacuo*, based on density-functional theory in the generalized gradient approximation with van der Waals corrections (GGA+vdW), using the FHI-aims code [1]. We verify our results by comparing calculated vibrational spectra with experimental room-temperature multiphoton IR spectra obtained using the FELIX free-electron laser. We use a force field (OPLS) to screen roughly the conformational energetics of as many structure candidates as possible (>10⁴ in practice), following up with GGA+vdW for a wide range of low-energy conformers. Consistent with earlier indications [2], we find that Ac-Ala₅LysH⁺ is helical, with a close energetic competition between α - and 3_{10} -like conformers. We show how the LysH⁺ termination acts to induce helices also for longer peptides, and that the inclusion of vdW contributions is critical to decide the detailed energy hierarchy. [1] V. Blum, *et al.*, Comput. Phys. Comm., accepted (2008). [2] R. Hudgins *et al.*, JACS 120, 12974 (1998).

CPP 37.3 Thu 15:00 ZEU 114

Role of van der Waals interactions for the intrinsic stability of polyalanine helices — ●ALEXANDRE TKATCHENKO¹, VOLKER BLUM¹, JOEL IRETA², and MATTHIAS SCHEFFLER¹ — ¹Fritz-Haber-Institut der MPG, Berlin, Germany — ²Dep. Quimica, UAM-Iztapalapa, Mexico

The helical motif is an ubiquitous conformation adopted by amino acid residues in a protein structure and helix formation is the simplest example of the protein folding process. How stable is the folded peptide helix in comparison to a random coil structure? What are the interactions responsible for stabilizing the helical conformation? Answering these questions has thus a direct implication for understanding protein folding. In this work we use density functional theory (DFT) augmented with a non-empirical correction for van der Waals (vdW) forces to study the stability of alanine polypeptide helices *in vacuo*. We find a large stabilization of the native helical forms when vdW correction is used. It amounts to 121%, 157% and 83% on top of

the Perdew-Burke-Ernzerhof (PBE) functional in the case of infinite α , π and 3_{10} helices, respectively. Thus, the experimentally observed α helix is significantly stabilized by vdW forces both over the fully extended and the 3_{10} conformations. Our findings also suggest an explanation to the remarkable stability of gas-phase alanine helices up to high temperatures [M. Kohtani *et al.* JACS 126, 7420 (2004)].

CPP 37.4 Thu 15:15 ZEU 114

Investigation of pulp fiber surfaces and cross-sections using atomic force microscopy — ●FRANZ SCHMIED^{1,4}, CHRISTIAN TEICHERT^{1,4}, LISBETH KAPPEL^{2,4}, ULRICH HIRN^{2,4}, and ROBERT SCHENNACH^{3,4} — ¹Institute of Physics, Montanuniversität Leoben, Franz Josef Straße 18, 8700 Leoben, Austria — ²Institute of Solid State Physics, Graz University of Technology, Petersgasse 16/2, 8010 Graz — ³Institute for Paper, Pulp and Fiber Technology, Graz University of Technology, Kopernikusgasse 24/II, 8010 Graz — ⁴CD-Laboratory for Surface Chemical and Physical Fundamentals of Paper Strength, Graz University of Technology, Petersgasse 16/2, 8010 Graz

Paper is made up of wood fibers. The nano- and microstructure of the fibers, as well as the influence of this structure on the inter-fiber bond strength are not yet completely understood. For improvement of paper strength, a deeper insight into this correlation is desirable because the structure is - besides the chemical composition - the most important influence on the mechanical paper properties. For our investigations we applied atomic-force microscopy (AFM) with phase imaging to study the surface of unbleached chemical pulp fibers and visualized the single fibrils. Further we report investigations of treated pulp fiber surfaces with different amounts of lignin. We quantify the geometry of precipitated lignin and characterize cross-sections of embedded paper sheets. The study showed that AFM is an appropriate tool to characterize the surface morphology of chemical pulp fibers on the nanometer scale.

Supported by **Mondi** and the **Christian Doppler Research Society**, Vienna, Austria.

CPP 37.5 Thu 15:30 ZEU 114

Silkworm silk under tensile stress as a function of humidity investigated by neutron spectroscopy — ●WIEBKE KNOLL¹, TILO SEYDEL², MALTE OGURRECK¹, IMKE DIDDENS³, CEDRIC DICKO³, and MARTIN MÜLLER⁴ — ¹IEAP, Universität Kiel — ²ILL, Grenoble — ³Department of Zoology, Oxford — ⁴GKSS, Geesthacht

Natural silk fibres exhibit extraordinary mechanical properties, combining high tensile strength with a high elongation at failure. The mesoscopic structure with crystalline regions embedded in a softer disordered matrix is the key to these properties. We measured the molecular vibrational response of Bombyx mori silkworm silk fibres *in situ* upon externally applied tensile stress using cold neutron time-of-flight spectroscopy. Adding to a previous study on dry silk fibers we recently investigated humid silk fibers. The aligned silk fibers are therefore exposed to a tensile force along the fiber axis generated by a stretching machine in a humidity chamber. The applied force was sufficient to reach the yield point of plastic deformation. It is already known from X-ray studies that most of the deformation upon extension of the fibres is due to the amorphous regions of the silk. The neutron results on dry fibers indicate that the externally applied force is not reflected by any noticeable effect on the molecular vibrational or diffusional/reorientational properties of the amorphous silk protein. However, on humid fibers we observed a quasielastic broadening of the scattering function, which is due to polymer chain mobility enhanced by the adsorbed water. This effect increases with stretching the humid silk fibers.

CPP 37.6 Thu 15:45 ZEU 114

Anisotropic elastic properties of cellulose measured using inelastic X-ray scattering — IMKE DIDDENS¹, BRIDGET MURPHY¹, MICHAEL KRISCH², and ●MARTIN MÜLLER³ — ¹IEAP, Universität Kiel, 24098 Kiel — ²ESRF, BP 220, 38043 Grenoble, France — ³GKSS Forschungszentrum Geesthacht, Max-Planck-Str. 1, 21502 Geesthacht

Plant fibers such as linen are remarkably stiff materials in the lon-

gitudinal direction of the fiber. As plant cell walls are composites made of cellulose nanocrystals, the so-called microfibrils, embedded in a disordered matrix, those nanocrystals should exhibit an even higher elastic modulus G . We have determined the elastic properties of cellulose microfibrils via the sound velocities measured by inelastic X-ray scattering (IXS). The IXS technique is particularly sensitive to crystal properties by discriminating the contribution of disordered material. A strong anisotropy is observed [1], with a much lower elastic modulus perpendicular to the fiber direction ($G_1 = 15$ GPa) than parallel to it ($G_2 = 220$ GPa). The latter modulus is considerably higher than all values previously determined and will have a significant impact on models for the elastic properties of cellulose microfibrils and of composites based on them.

[1] I. Diddens, B. Murphy, M. Krisch, M. Müller, *Macromolecules*, ASAP online, in press.

15 min. break

CPP 37.7 Thu 16:15 ZEU 114

Proteins on Surfaces investigated by Microbeam Grazing Incidence Small Angle X-ray Scattering — ●RONALD GEBHARDT¹, CHRISTIAN RIEKEL¹, CHARLOTTE VENDRELY², MANFRED BURGHAMMER¹, and PETER MÜLLER-BUSCHBAUM³ — ¹European Synchrotron Radiation Facility, B.P. 220, F-38043 Grenoble Cedex, France — ²Université de Cergy-Pontoise, ERRMECE, F-95000, Cergy-Pontoise, France — ³TU München, Physik Department E13, München, Germany

Grazing incidence small angle scattering with a 1 micron x-ray beam (μ GISAXS) is applied to study structural ordering of casein micelles and fibroin in solution cast films. μ GISAXS scans provide the possibility to locate highly ordered areas and to investigate variation in the molecular packing.

In the case of the casein micelles, ordered film structures have been generated by decreasing their natural size dispersion. While dynamic light scattering was used to characterize the different size fractions in solution, μ GISAXS and roughness are measured on the resulting casein films. GISAXS-Patterns are analyzed by simulations providing the dimension and nearest neighbor distances of casein micelles.

In the case of fibroin, ordering of nano-fibers formed during the drying process is investigated. The experimental data are analyzed by simulations and compared to SEM, AFM and Raman scattering experiments.

CPP 37.8 Thu 16:30 ZEU 114

Adsorption kinetics of proteins on tailored surfaces: An ellipsometry study — ●SAMUEL GRANDTHYLL, HENDRIK HÄHL, HUBERT MANTZ, and KARIN JACOBS — Saarland University, Experimental Physics, D-66041 Saarbruecken, Germany

The adsorption of proteins onto solid surfaces is an everyday phenomenon. For a better understanding of the driving forces inducing the formation of the initial protein layer, we have studied the adsorption kinetics of three different proteins: Bovine serum albumin (BSA), α -amylase and lysozyme.

Our focus had been on the influence of the substrate, where lock-and-key mechanism between protein and surface were absent. It is already textbook knowledge that protein adsorption is influenced by short-range forces arising from the surface chemistry and Coulomb interaction due to unscreened charges. We could show that also long-range van der Waals forces present between the protein and the sample substrate are important. These interactions depend on the thickness of the oxide layer of a silicon wafer and thus are easily alterable [1].

Ellipsometry measurements show that the kinetics of BSA and α -amylase on native thin oxide layers does not follow a standard adsorption model, because the kinetics curve is separated by two kinks. By including conformational changes of the proteins into Monte Carlo simulations, the experimental results could be qualitatively reproduced [2].

[1] A. Quinn et al., *EPL*, **81**, 56003, (2008)

[2] M. Bellion et al., *J. Phys.: Condens. Mat.* **20**, 404226, (2008)

CPP 37.9 Thu 16:45 ZEU 114

Translocation of biopolymers through narrow and wide nanopores: a multiscale computational approach — ●MARIA FYTA^{1,5}, SIMONE MELCHIONNA^{1,2}, MASSIMO BERNASCHI³, SAURO SUCCI^{3,4}, and EFTHIMIOS KAXIRAS^{1,4} — ¹Department of Physics and

School of Engineering and Applied Sciences, Harvard University, Cambridge, MA, USA — ²INFM-SOFT, Department of Physics, Università di Roma La Sapienza, P.le A. Moro 2, 00185 Rome, Italy — ³Istituto Applicazioni Calcolo, CNR, Viale del Policlinico 137, 00161, Roma, Italy — ⁴Initiative in Innovative Computing, Harvard University, Cambridge, MA, USA — ⁵Present address: Physics Department, Technical University of Munich, Germany

Our recently developed novel multiscale approach which concurrently couples a mesoscopic fluid solvent with molecular motion has been efficiently applied to the problem of biopolymer translocation through nanopores. We present results from thousands of numerical simulations of long biopolymers up to 8000 monomers passing through pores of various sizes. The statistical scaling behavior of the translocation process is reproduced with remarkable accuracy. Our results provide valuable insight into the cooperative aspects of biopolymer and hydrodynamic motion. The statistical and dynamical features of the translocation process are incorporated into a phenomenological model for the power law dependence of the translocation time on the biopolymer length. In the case of wide pores, there is clear evidence of folding quantization, leading to a deviation from the single-exponent power-law characterizing the single-file translocation through narrow pores.

CPP 37.10 Thu 17:00 ZEU 114

Hydration behavior of casein micelles in thin film geometry: A GISANS study — ●EZZELDIN METWALLI¹, JEAN-FRANCOIS MOULIN², RONALD GEBHARDT³, ROBERT CUBITT⁴, ALEXANDER TOLKACH⁵, ULRICH KULOZIK⁵, and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik Department LS E13, James-Frank-Str.1, 85747 Garching, Germany — ²FRM II, TU München, 85747 Garching, Germany — ³ESRF, b.p. 220, 38043 Grenoble, France — ⁴ILL, 6 rue Jules Horowitz, b.p. 156, 38042 Grenoble, France — ⁵TU München, Chair for Food Process Engineering and Dairy Technology, 85354 Freising-Weihnstefan, Germany

The water content of the casein micelle films in water vapor atmosphere is investigated using time-resolved grazing incidence small-angle neutron scattering (GISANS). Initial dry casein films are prepared with spin coating method. At 30 °C the formation of a water equilibrated casein protein film is reached after 11 min with a total content of 0.36 g water/ g protein. With increasing water vapor temperature up to 70 °C an increase in the water content is found. With GISANS, lateral structures in the nano-meter scale are resolved during the swelling experiment at different temperatures and modeled using two spheres named micelles and mini-micelles. Upon water uptake, molecular assemblies in the size range of 15 nm (mini-micelle) is attributed to the formation of high contrast D2O outer shell on the small objects that already exist in the protein film [1]. These results are discussed and compared with various proposed models on the casein micelle structures. [1] E. Metwalli et al., *Langmuir* accepted 2008.

CPP 37.11 Thu 17:15 ZEU 114

Photo-CIDNP study of transient radicals of Met-Gly and Gly-Met peptides — OLGA MOROZOVA¹, SERGEY KORCHAR², HANS-MARTIN VIETH², and ●ALEXANDRA YURKOVSKAYA^{1,2} — ¹International Tomography Center, Institutskaya 3a, Novosibirsk, Russia — ²FB Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin

Photo-reactions of methionine containing dipeptides, glycylmethionine (Gly-Met) and methionylglycine (Met-Gly) were studied by time-resolved Chemically Induced Dynamic Nuclear Polarization (CIDNP) a method particularly sensitive to short-lived radical species. In aqueous solution we established several competing reaction pathways following triplet quenching of the photosensitizer 4-carboxybenzophenone depending on the pH: for Gly-Met electron transfer from the sulfur atom takes place, also from the terminal amino group. Two channels of triplet quenching are distinguishable also for Met-Gly: electron transfer from the amino group and from the sulfur atom, here with the formation of a cation radical with a three electron two center S-N bond. At pH < pKa of the terminal amino group Met-Gly forms a linear S-centered radical succeeded by a five-membered cyclic radical. At pH > pKa both peptides form aminium radicals by electron transfer from their N-terminal amino group with deprotonation to the aminyl radical. The radicals were characterized using the dependence of CIDNP on the magnetic field. The potential of the CIDNP techniques in studying other complex biological radical reactions will be discussed. Financial support by the RFBR projects # 08-03-00539, EU FP6 projects "Bio-DNP" and MIF2-CT-2006-022008 is acknowledged.

CPP 38: POSTERS Micro- and Nanofluidics

Time: Thursday 17:00–19:30

Location: P3

CPP 38.1 Thu 17:00 P3

Colloids dragged through a polymer solution: Experiment, theory, and simulation — ●CHRISTOF GUTSCHE¹, FRIEDRICH KREMER¹, MATTHIAS KRÜGER², MARKUS RAUSCHER², RUDOLF WEEBER³, and JENS HARTING³ — ¹Institut für Experimentalphysik I, Universität Leipzig, 04103 Leipzig, Germany — ²Max-Planck-Institut für Metallforschung, Heisenbergstr. 3, 70569 Stuttgart, Germany and Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany — ³Institut für Computerphysik, Universität Stuttgart, Pfaffenwaldring 27, 70569 Stuttgart, Germany

Complex fluids in general and colloid-polymer mixtures in particular are an ideal model system for studying the structure and phase behavior of multicomponent systems. We present optical tweezer based microrheological measurements of the drag force on colloids pulled through a solution of lambda-DNA used here as a monodisperse model polymer. The experiments show a drag force that is larger than expected from the Stokes formula and the independently measured viscosity of the DNA solution. We attribute this to the accumulation of DNA in front of the colloid and the reduced DNA density behind the colloid.

C.Gutsche, F. Kremer, M. Krüger, M. Rauscher, R. Weeber, J. Harting. J. Chem. Phys. 129, 084902 (2008)

CPP 38.2 Thu 17:00 P3

Reversible single bacterial cell localization in microfluidic PDMS devices — ●LUKAS GALLA, DOMINIK GREIF, JAN REGTMEIER, and DARIO ANSELMETTI — Bielefeld University, Experimental Biophysics & Applied Nanoscience, Universitätsstr. 25, 33615 Bielefeld, Germany

For successful optical investigations of bacteria cells it is beneficial to use a method that allows a reversible and defined positioning of single cells at physiological conditions.

Here, we present two approaches for single cell and particle localization in a microfluidic poly(dimethylsiloxane) (PDMS) device. Firstly, in structured microchannels with obstacles at defined positions we used electrokinetic driving forces and electrodeless dielectrophoresis for particle trapping. Secondly, branched channel systems with 1 μ m-intersection points in combination with hydrostatic flux control also allow an exact positioning of particles. In order to prevent unspecific particle adsorption, the channel surface of both types of PDMS chips was coated with a triblock-copolymer (F108).

The functionality of these two approaches was confirmed in experiments with 1,9 μ m fluorescent beads followed by successful localizations of bacterial cells (*S. meliloti* 1021, 0,5 μ m x 3 μ m) suspended in culture medium. No reduction of the cell viability was observed. Both approaches demonstrate the efficiency of the single bacterial cell trapping methods and open the way for new designs of single cell experiments.

CPP 38.3 Thu 17:00 P3

Motion of an elastic capsule in time dependent shear flow — ●STEFFEN KESSLER, REIMAR FINKEN, and UDO SEIFERT — II. Institute of Theoretical Physics, University of Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart

The motion of an elastic 3d capsule in a linear shear flow with time-dependent shear rate is studied both numerically and analytically using an extended Keller-Skalak model. Since the ellipsoidal shape of the capsule is fixed here, only two degrees of freedom remain: the orientation of the capsule with respect to the shear flow, and the internal motion of the membrane with respect to the fixed shape.

For a given shape, the capsule dynamics in time-constant shear flow depends on the applied shear rate and the viscosity contrast between inner and outer fluid. In the corresponding phase diagram tumbling and tank-treading regimes are separated by an "intermittent" regime where the capsule is simultaneously tank-treading and tumbling.

In the case of a time-oscillating shear rate, numerical examples show that tumbling motions can be induced from the tank-treading regime if the shear rate enters the tank-treading regime during its oscillation. Furthermore, numerical results for the mean tumbling rate show an interesting resonance dependence on the applied oscillation frequency, superimposed onto a smooth background vanishing at a cut-off frequency. These findings can be understood analytically for quasispher-

ical capsules and parameters close to the critical point of the phase diagram. A mapping of the system onto a discrete model for low frequencies explains the resonance pattern of the tumbling-rate.

CPP 38.4 Thu 17:00 P3

Hydrodynamically induced attraction and repulsion of rotated dumbbells — ●STEFFEN SCHREIBER and WALTER ZIMMERMANN — Theoretische Physik I, Universität Bayreuth, 95440 Bayreuth, Germany

Two asymmetric and hydrodynamically interacting dumbbells are rotated in a solvent. We show that different shapes of the two dumbbells break the symmetry with respect to a time translation by half a rotational period which causes either a hydrodynamically induced attraction or repulsion between them, depending on the specific shapes. We present phase diagrams of this novel dynamical effect and a reduced model for a qualitative explanation.

CPP 38.5 Thu 17:00 P3

Experimentierkiste "Den Geheimnissen der Flüssigkeiten auf der Spur" — ●FRANK MÜLLER, ATANASKA KASABOVA, MATTHIAS LIENARD, CHRISTIAN ZEITZ, PETER LOSKILL, SAMUEL GRANDTHYLL and KARIN JACOBS — Institut für Experimentalphysik, Universität des Saarlandes, 66041 Saarbrücken

Obwohl Technologie von Jugendlichen akzeptiert wird, sei es in Form von Laptops oder Mobiltelefonen, beschränkt sich das Interesse meist auf die passive Nutzung. Dabei steht eher die Tatsache im Vordergrund, dass "das neue Handy" diese oder jene zusätzliche Spielart aufweist, die Frage nach dem "Warum" oder "Wie" ist aber eher von untergeordneter Bedeutung. Eine Möglichkeit, das Interesse und Technik und Wissenschaft zu fördern, besteht darin, die Vermittlung von wissenschaftlichen Inhalten über die Wandtafel hinaus zu präsentieren und Schülern die Möglichkeit zu geben, selbst aktiv tätig zu sein. Die hier präsentierte "Experimentierkiste" ist für den Einsatz an Schulen im Rahmen des Schwerpunktprogramms SPP 1164 "Nano & Microfluidics" konzipiert worden und beinhaltet 12 Experimente, die von einer Schulklasse im Rahmen einer 1-2 stündigen Veranstaltung bearbeitet werden können. Bei den in Auszügen gezeigten Experimenten wurde besonders Wert auf die einfache Gestaltung gelegt, deren "Zutaten" in jedem Supermarktregal zu finden sind. So steht jedem, dessen Interesse an der einen oder anderen Fragestellung im Rahmen der schulischen Präsentation einmal geweckt worden ist, die Möglichkeit offen, seine "Forschung" zu Hause zu vertiefen.

www.softmatter.de -> Lab-in-a-box

CPP 38.6 Thu 17:00 P3

Roughness affects slippage and slippage affects hydrodynamic instabilities — ●LUDOVIC MARQUANT, MATTHIAS LESSEL, OLIVER BÄUMCHEN, JULIA MAINKA, FRANK MÜLLER, and KARIN JACOBS — Saarland University, Experimental Physics, D-66041 Saarbrücken

Dewetting experiments have proven to be ideally suited to probe the flow dynamics of liquids on solids. Here we focus on the boundary condition at the solid/liquid interface. Under certain conditions, the details of which we will present, the liquid can slip over the solid, leading to higher flow velocities and less drag. In our study we prepare polystyrene films below the entanglement length on top of hydrophobized substrates. The surface functionalization is done by preparing self-assembled monolayers of dodecyl- (DTS) or octadecyl-trichlorosilane (OTS) or by spin casting a thin AF1600 film.

We show that i) roughness affects slippage and that ii) hydrodynamic instabilities similar to the Rayleigh-Plateau instability, are influenced by slippage.

CPP 38.7 Thu 17:00 P3

Near-Surface Structure and Dynamics Explored by Grazing Incidence Neutron Scattering — ●MARCO WALZ¹, MAX WOLFF^{2,3}, NICOLE VOSS¹, PHILIPP GUTFREUND^{2,3}, HARTMUT ZABEL¹, and ANDREAS MAGERL¹ — ¹Crystallography and Structural Physics, Univ. Erlangen-Nürnberg — ²Solid State Physics, Ruhr-Univ. Bochum, Germany — ³Institut Laue-Langevin, Grenoble, France

Even in simple fluids the conventional non-slip boundary condition becomes microscopically void. Surface slip characterized by the slip length may become macroscopic, and a large slip length implies a pro-

nounced anomaly in the shear flow adjacent to a solid surface, where the anomaly itself is only present in a thin layer next to the solid interface within the order of nanometers. For an understanding of boundary slip, the anomalies in the structural and dynamical properties in the interface layer need to be understood. To highlight the properties of the boundary layer we carried out Grazing Incidence Small Angle Neutron Scattering (GISANS) and, for the first time, a Neutron Spin-Echo experiment under condition of Grazing Incidence (GINSE). Our investigation of a concentrated tri-block copolymer solution shows that the local structure depends on the distance to the interface and the chemical termination of the solid boundary. However, the key for the understanding of slip may also be related to a change in the local dynamics of a liquid at an interface and under flow. We have verified that the investigation of the dynamics of the sample with the GINSE technique is feasible, and we present data taken near the critical angle of total reflection.

CPP 38.8 Thu 17:00 P3

Dewetting of thin liquid films on viscoelastic substrates — ●KONSTANTINA KOSTOUROU¹, DIRK PESCHKA³, ANDREAS MÜNCH², BARBARA WAGNER³, STEPHAN HERMINGHAUS¹, and RALF SEEMANN^{1,4} — ¹Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — ²School of Mathematical Sciences, University of Nottingham, UK — ³Weierstrass Institute for Applied Analysis and Stochastics, Berlin, Germany — ⁴Experimental Physics, Saarland University, Germany

We study the dewetting of thin polymer films on viscoelastic (PDMS and molten PMMA) substrates. Experimentally we observe that the dewetting rates increase as we increase the substrate elasticity, whereas they show a two-phase behavior as we tune the substrate viscosity. Furthermore, we find that characteristic rim shapes and substrate deformations depend on the viscoelasticity of the underlying substrate. In our theoretical approach we couple the Navier-Stokes equations to a Kelvin-Voigt model to describe the liquid and solid phase respectively. We derive a set of one-dimensional thin-film equations for the liquid film and the solid substrate, where the depth averaged velocity of the liquid and the deformation of the solid substrate is largely tangential to the liquid-solid interface. Finally, we compare the experimental results with the predictions of our model. Whereas we observe a deviation in the case of the PDMS substrates, we find them to be in good agreement in the case of the PMMA substrates. Specifically, our model is able to define both the dewetting dynamics of our system and the deformation of the substrate close to the three phase contact line.

CPP 38.9 Thu 17:00 P3

Polystyrene nanodroplets on rubber elastic substrates — ●KONSTANTINA KOSTOUROU¹, STEPHAN HERMINGHAUS¹, and RALF SEEMANN^{1,2} — ¹Max Planck Institute for Dynamics and Self-Organization, D-37073 Göttingen, Germany — ²Experimental Physics, Saarland University, D-66041 Saarbrücken, Germany

We study the shape of polystyrene (PS) nanodroplets on substrates of cross-linked Polydimethylsiloxane (PDMS). These drops deform the rubber elastic substrate onto which they are seated. The three phase contact line is lifted upwards by the interfacial energies, whereas the interface between the drop and the substrate is pushed downwards due to the Laplace pressure of the droplet. The upward deformation of the PDMS is measured by imaging the sessile droplets by atomic force microscopy (AFM) and its exact position is determined by overlapping the topography and the phase signal ("top side"). To measure the downward deformation of the PDMS we lift off the PS droplet from the substrate and image the deformation that is frozen into the "bottom side" of the droplet. By analyzing the profiles of the bottom side of the droplet and assuming that our system can be defined by the Hertzian model for a rigid sphere in contact with a soft elastic plane, we can calculate quantitatively the Elastic Modulus of the substrate, that is in very good agreement with values extracted by other independent techniques (rheology, nanoindentation). Furthermore, the lift-off technique allows us to image the upward displacement of the three phase contact line and to compare it to the results of the deformation in the vicinity of the three phase contact line from the "top side".

CPP 38.10 Thu 17:00 P3

Static and Dynamics of Wet Granular Materials — ●SOMNATH KARMAKAR^{1,2}, MICHAEL SIPAHI¹, MARIO SCHEEL¹, MARC SCHABER², MARTIN BRINKMANN¹, MARCO DI MICHEL³, STEPHAN HERMINGHAUS¹, and RALF SEEMANN^{1,2} — ¹Max Planck Institute for Dynamics and

Self-Organization, Göttingen, Germany — ²Universität des Saarlandes, Saarbrücken, Germany — ³ESRF, Grenoble, France

When a small amount of liquid is added to dry granular matter, a network of capillary bridges is formed exerting an attractive force between granules and the granular pile turns into a moldable material. The resulting network of liquid morphologies changes dramatically with liquid content and wettability of the granules. We study the mechanical properties, i.e. tensile strength, yield stress and critical fluidization acceleration of wet granular materials with different wettability and grain shape like sand, glass, and basalt beads for various liquid contents. Our experimental observations show, that in case of a liquid with small contact angle, the mechanical properties of a granular pile are largely independent of the amount of added-liquid over a wide range. In case of a large contact angle, however, the mechanical properties are strongly dependent on the liquid content. We resolve this experimental finding by imaging the liquid distribution inside the granular piles, using X-ray microtomography.

CPP 38.11 Thu 17:00 P3

Contact angle determination in multicomponent lattice Boltzmann models — ●SEBASTIAN SCHMIESCHEK and JENS HARTING — Institut für Computerphysik, Pfaffenwaldring 27, 70569 Stuttgart

Droplets on hydrophobic surfaces are common in microfluidic applications and there exists a number of commonly used multicomponent and multiphase lattice Boltzmann schemes to study such systems. In this contribution we focus on a popular implementation of a multicomponent model as introduced by Shan and Chen. Here, interactions between different components are implemented as repulsive forces whose strength is determined by phenomenological parameters. In this contribution we present simulations of a droplet on a hydrophobic surface. We investigate the dependence of the contact angle on the simulation parameters and quantitatively compare different approaches to measure it.

CPP 38.12 Thu 17:00 P3

Wetting of hydrophilic periodic nanotemplates on Si surfaces — STEFAN HEINDL¹, ●ALFRED PLETTL¹, SABINE HILD², and PAUL ZIEMANN¹ — ¹Institut für Festkörperphysik, Universität Ulm, D-89069 Ulm, Germany — ²Institut für Polymerwissenschaften, Universität Linz, A-4040 Linz, Austria

To influence the wetting behavior of a Si surface, periodically ordered nanomasks were prepared by either a micellar [1] or a miniemulsion technique [2] and used to fabricate extended arrays of nanopillars on a Si wafer by RIE etching [3]. These methods allow a systematic variation of the height and density of such structures. The degree of hydrophobicity of the samples was additionally modified by coating with hexamethyldisilane (HMDS) or octadecyltrilsilane (OTS). Wetting of water was studied by measuring contact angles as well as spreading-receding hysteresis behavior. The specific effect of the nanostructures is to increase the contact angles and enhance hysteresis.

By combining the above nanopatterning techniques with conventional electron beam lithography and a cryogenic Si deep etching, two different roughness scales can be superimposed. The resulting effect on wetting may contribute to an understanding of the well-known Lotus effect.

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

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

[3] F. Weigl et al., Diamond and rel. Mat.15, 1689 (2006).

CPP 38.13 Thu 17:00 P3

Stability of droplets: A free energy based lattice Boltzmann study — ●MARKUS GROSS^{1,2}, FATHOLLAH VARNIK^{1,2}, and DIERK RAABE¹ — ¹Max-Planck Institut für Eisenforschung, Düsseldorf, Germany — ²Interdisciplinary Center for Advanced Materials Simulation, Ruhr-Universität Bochum, Germany

Liquid droplets are very important in many scientific research branches and their study has attracted much interest for a long time. In this work we investigate the behavior of droplets via a mesoscale computer simulation approach, the Lattice Boltzmann method.

In the first part, we consider the stability of a droplet and its saturated vapor inside a finite volume, an issue of considerable importance in nanotechnology. Results obtained within our simulations show the same system size dependence as obtained via analytic approximations to the underlying free energy functional as well as independent numerical solutions of the problem. In particular, we find a certain critical radius below which a liquid droplet becomes unstable and evaporates.

A second topic of fundamental interest is the behavior of droplets on superhydrophobic substrates for the case where the droplet is of comparable size to the roughness scale. A simple analytical free energy model is presented that can explain all the essential results of our simulations. Most interestingly, we are able to observe a new generic metastable state of partial impalement that is different from the known Cassie/Baxter or Wenzel states. Furthermore, we study the stability of the Cassie/Baxter state and its dependence on the substrate geometry, contact angle and droplet size.

CPP 38.14 Thu 17:00 P3

Small droplets on superhydrophobic substrates — ●MARKUS GROSS^{1,2}, FATHOLLAH VARNIK^{1,2}, and DIERK RAABE¹ — ¹Max-Planck Institut für Eisenforschung, Düsseldorf, Germany — ²Interdisciplinary Center for Advanced Materials Simulation, Ruhr-Universität Bochum, Germany

We investigate the stability of liquid droplets on a regular superhydrophobic substrate for the case of droplets that are of comparable size to the surface asperities.

A simple analytic three-dimensional free energy model is proposed and compared to the results obtained from lattice Boltzmann computer simulations. Both approaches are found to be in good agreement. The

stability of the fakir state is shown to depend on the substrate geometry, contact angle and droplet size. Remarkably, we are able to observe a new metastable state of partial impalement that is different from the fakir or Wenzel state. We find that, due to this new state, an evaporating droplet can be saved from going over to the Wenzel state and instead remains close to the top of the surface texture.

CPP 38.15 Thu 17:00 P3

Mesoscopic dynamics of active media — ●ARTHUR V. STRAUBE and PHILIPP THOMAS — Department of Theoretical Physics, TU Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

We present a mesoscopic model describing nonequilibrium active media. We follow the ideas of the method of *stochastic rotation dynamics* and introduce a coarse-grained active field, which is modeled by discrete chemical particles coupled to the solvent. To validate our approach, we first look at the concentration dependence of the diffusion coefficient of passive chemical particles. Next we introduce birth and death rules and focus on population dynamics. Finally, we address the full problem of nonuniform active states produced by a source of the chemical field. The results are compared with the exact solution obtained within the continuum theory. We outline possible chemical and biological applications of the proposed approach.

CPP 39: POSTERS Colloids and Liquids

Time: Thursday 17:00–19:30

Location: P3

CPP 39.1 Thu 17:00 P3

Magnetfeldabhängige optische Transmission kolloidaler Suspensionen aus Nickelnanostäbchen — ●ALEKSEJ LAPTEV, ANDREAS TSCHÖPE and RAINER BIRRINGER — Technische Physik, Universität des Saarlandes, Saarbrücken, Germany

Kolloidale Suspensionen aus Nickelnanostäbchen wurden mit Hilfe eines dreistufigen Syntheseverfahrens präpariert. Im ersten Schritt wurden durch anodische Oxidation von Aluminiumfolien Template erzeugt, die lineare Porenstrukturen mit einem Durchmesser von etwa 9 nm enthielten. Im zweiten Schritt wurden die Porenkanäle durch AC-Abscheidung mit Nickel befüllt, wobei die Fülllänge je nach Abscheidendauer zwischen 30 und 100 nm variierte. Im letzten Syntheseschritt wurden die Nickelnanostäbchen durch Auflösen der Aluminiumoxidschicht freigelegt und zu einer stabilen wässrigen Suspension weiterverarbeitet. An diesen Nanostäbchen wurden Messungen der optischen Transmission in äußeren Magnetfeldern bis 35 mT durchgeführt. Insbesondere wurde die Abhängigkeit der Transmission von der relativen Orientierung zwischen Magnetfeld und Lichtpolarisation sowie die Feldabhängigkeit der Extinktion und die Relaxation der Partikelorientierung nach Abschalten des Feldes untersucht. Die Messergebnisse zeigen eine gute Übereinstimmung mit einem Modell, das die Anisotropie der Absorption und die Orientierungsverteilung der magnetischen Stäbchen im Magnetfeld berücksichtigt.

CPP 39.2 Thu 17:00 P3

The volume phase transition of thermoresponsive core-shell microgels investigated by small angle neutron scattering — ●MATTHIAS KARG¹, STEFAN WELLERT², YVONNE HERTLE³, and THOMAS HELLWEG³ — ¹TU Berlin, Germany — ²Helmholtz-Zentrum Berlin, Germany — ³Universität Bayreuth, Germany

Organic/inorganic hybrids attracted much interest within the last decade, since they can combine the properties of both components. Such composites can benefit e.g. from the thermoresponsive character of a polymer component and optical, catalytic or magnetic properties stemming from the inorganic material. Of special interest are hybrids with a core-shell structure, because they have a well-defined topology and hence are interesting for different physical investigations and applications like photonic materials.

We present here responsive core-shell microgels, with silica nanoparticles of different sizes as cores. Imaging techniques were used to study the structure of these hybrids regarding their core-shell topology. The volume phase transition (VPT) of the polymer shell was studied by dynamic light scattering and, focussing on the local length-scale, by small angle neutron scattering (SANS). SANS allowed to determine the correlation length of the polymer network. The scaling behavior of the correlation length was studied by SANS measurements in the vicinity of the VPT temperature. By contrast matching experiments

the core size and polydispersity was investigated in-situ[1].

[1] M. Karg, S. Wellert, I. Pastoriza-Santos, A. Lapp, L. M. Liz-Marzán, T. Hellweg, Phys. Chem. Chem. Phys., 2008, 10, 6708-6716

CPP 39.3 Thu 17:00 P3

Novel charge-induced protein interactions in solution studied by SAXS/SANS — ●FAJUN ZHANG¹, LUCA IANESELLI¹, MAXIMILIAN W. A. SKODA², ROBERT M. J. JACOBS³, OLIVER KOHLBACHER⁴, SOPHIE WEGGLER⁵, ANDREAS HILDEBRANDT⁵, and FRANK SCHREIBER¹ — ¹Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen, Germany — ²ISIS, Rutherford Appleton Laboratory, UK — ³CRL, University of Oxford, UK — ⁴Zentrum für Bioinformatik Tübingen, Tübingen — ⁵Zentrum für Bioinformatik Saar, Saarbrücken

Proteins can be considered as very complex *colloids*. Their interactions in solution challenge our understanding from conventional colloidal science. Using a model protein, BSA, we have studied the influence of ionic strength and the nature of salt on protein interactions by SAS. For simple salts, protein interactions can be described using a theoretical model based on a screened Coulomb potential [1]. By using multivalent counterions, a novel reentrant condensation behavior is observed, which is caused by short-ranged electrostatic interactions between ions and acidic residues, mechanistically different from the case of DNA. A short-ranged attraction arises between counterion-bound proteins in the reentrant regime. Monte Carlo simulations and zeta-potential measurements under these strong electrostatic coupling conditions support an effective inversion of charge on surface side chains through binding of the multivalent counterions [2]. These observations provide a new way for tuning protein interactions in solution. [1] F. Zhang, et al., J. Phys. Chem. B. 2007, 111, 251. [2] F. Zhang, et al., Phys. Rev. Lett. 2008, 101, 148101.

CPP 39.4 Thu 17:00 P3

Frequency dependent deformation of liquid crystal droplets in an external electric field — ●GÜNTER K. AUERNHAMMER, JINYU ZHAO, and DORIS VOLLMER — Max-Planck-Institut für Polymerforschung, Ackermannweg 10, 55128 Mainz

Nematic drops suspended in the isotropic phase of the same substance were subjected to alternating electrical fields of varying frequency. The system was carefully kept in the isotropic-nematic coexistence region, which was broadened due to small amounts of non-mesogenic additives. Whereas the droplets remained spherical at low (order of 10 Hz) and high frequencies (in the kHz range), at intermediate frequencies, we observed a marked flattening of the droplet in the plane perpendicular to the applied field. The deformation of the liquid crystal droplets occurred both in substances with positive and negative dielectric anisotropy. We show that this frequency dependent deformation can be modeled with a combination of the leaky dielectric model and

screening of the applied electric field due to the finite conductivity.

CPP 39.5 Thu 17:00 P3

A Simple and Robust Solver for the Poisson-Boltzmann Equation — MANUEL BAPTISTA, ROMAN SCHMITZ, and BURKHARD DUENWEG — Max-Planck-Institut fuer Polymerforschung, Mainz

A variational approach is used to develop a robust numerical procedure for solving the nonlinear Poisson-Boltzmann equation. Following Maggs et al., we construct an appropriate constrained free energy functional, such that its Euler-Lagrange equations are equivalent to the Poisson-Boltzmann equation. We then develop, implement, and test an algorithm for its numerical minimization, which is quite simple and unconditionally stable. The analytic solution for planar geometry is used for validation. Furthermore, some results are presented for a charged colloidal sphere surrounded by counterions. — See also arXiv:0810.0490v1

CPP 39.6 Thu 17:00 P3

Synthesis, characterization and cellular uptake of aminofunctionalized fluoresceine-labeled silica nanospheres — QI GAO¹, CHRISTINA GRAF², CYNTHIA KEMBUAN¹, FIORENZA RANCAN², STEFEN TROPPENS², SABRINA HADAM², ANNIKA VOGT², and ECKART RÜHL¹ — ¹Institut für Chemie und Biochemie, Freie Universität Berlin, Takustr. 3, 14195 Berlin — ²Department of Dermatology and Allergy, Charité - Universitätsmedizin Berlin, Charitéplatz 1, 10117

The understanding of the uptake mechanism of silica nanoparticles (NPs) by human cells is important for the development of NPs as novel therapeutic and diagnostic agents. Luminescent silica NPs are promising labeling reagents for various biomedical applications. We investigated the biological properties of 3-aminopropyltrimethylsilane (APS) functionalized and fluoresceine (FITC) labeled silica nanospheres. Nearly monodisperse FITC dye-labeled silica nanospheres with diameters of 30 - 300 nm are prepared by several modifications of the Stöber process. Surface functionalization of APS allows us to adjust the zeta potential of these nanospheres from highly negative to positive (-55 mV to +45 mV). Size and zeta potential of the NPs were characterized by transmission electron microscopy and dynamic light scattering. A positive zeta potential enhances the interaction of the nanoparticles with the negatively charged cell surface and hence, the cellular uptake. Toxicity experiments indicate that these FITC dye-labeled silica NPs are not toxic to human cells. Research on the uptake of the NPs to cells, especially human skin cells, is currently in progress.

CPP 39.7 Thu 17:00 P3

Studying mechanical microcontacts of fine particles with the quartz crystal microbalance — EWA ILSKA, MICHAEL KAPPL, and HANS-JÜRGEN BUTT — Max-Planck-Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

Micromechanical contacts are an important issue in a wide variety of applications. Although their significance is acknowledged and micromechanics is widely studied e.g. in pharmaceutical or electronics industry, fundamental knowledge is still limited. Within this work, we attempt to understand and describe the physics behind particles and polymer surface contacts. We apply therefore the quartz crystal microbalance (QCM) technique, supported by particles video tracking and atomic force microscopy (AFM) imaging of contact zones. Glass particles of several diameters were deposited onto a thick polystyrene film, which was spin-coated onto the QCM surface. The shift of the resonance frequency f_0 of the QCM signal depends in a complex manner on the mass loading but also on the coupling strength between surface and particles. Addition of small particles leads to a decrease of resonance frequency due to the added mass. Addition of larger particles leads to an f_0 increase, further enhanced by oscillation amplitude. After annealing, amplitude increase and particle detachment are found to strongly influence the resonance behaviour. These striking differences can be explained by the different coupling of particles to the PS film. This is also supported by AFM images of the contact zones after particle removal.

CPP 39.8 Thu 17:00 P3

Pt- and FePt- nanoparticles on the basis of emulsion techniques — ACHIM MANZKE¹, STEFAN WIEDEMANN¹, FABIAN ENDERLE¹, ALFRED PLETTL¹, PAUL ZIEMANN¹, EYK SCHREIBER², ULRICH ZIENER², KATHARINA LANDFESTER², JOHANNES BISKUPEK³, and UTE KAISER³ — ¹Institut für Festkörperphysik, Universität Ulm, D-89069 Ulm — ²Institut für Organische Chemie III, Universität Ulm, D-89069 Ulm — ³Materialwissenschaftliche Elektronenmikroskopie, Uni-

versität Ulm, D-89069 Ulm

Metal-precursor loaded colloidal polystyrene (PS) particles in aqueous solution are produced by an emulsion and miniemulsion technique, respectively [1]. We will report on colloids loaded with Pt- as well as with Fe- and Pt- complexes. After deposition of a hexagonally ordered monolayer of PS spheres on top of a silicon substrate, optimized plasma and temper sequences are applied to obtain metallic nanoparticles which still exhibit the original lateral order. The metal content within a colloid defines the size of the final particle, which could be varied between 6 and 14 nm, so far. The interparticle distance is determined by the diameter of the starting PS- particles and was varied between 80 and 250 nm. EDX- and ICP-OES- measurements were carried out to investigate the chemical composition of the colloids. For example, a ratio of Fe : Pt = 1 could be achieved with the miniemulsion technique. HRTEM- images demonstrate the crystalline structure of the Pt- and FePt- nanoparticles.

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

CPP 39.9 Thu 17:00 P3

Phase behaviour studies of novel smart microgels based on copolymers of NIPAM and N-substituted acrylamides — YVONNE HERTLE, CHRISTOPH HASENÖHRL, and THOMAS HELLWEG — Universität Bayreuth, Physikalische Chemie I, Universitätsstr. 30, 95447 Bayreuth, Germany

Microgels made of N-isopropyl-acrylamide (NIPAM) are the most studied water-swallowable microgel systems with a lower critical solution temperature (LCST) of $\sim 32^\circ\text{C}$ in water. This thermoresponsive behaviour can be strongly influenced by co-polymerisation with other organic comonomers. In this contribution thermoresponsive copolymer microgel networks made of N-isopropyl-acrylamide and other N-substituted acrylamides are presented. We use scattering techniques as light and neutron scattering to study the phase transition behaviour and the shape of the microgel particles in the swollen state. For characterisation of the particle shape in the totally collapsed state and their size distribution imaging methods such as transmission and scanning electron microscopy (TEM, SEM) are suitable.

CPP 39.10 Thu 17:00 P3

Investigating fluctuation and dissipation of optically trapped colloids — OLAF UEBERSCHÄR, CHRISTOF GUTSCHE, JÖRG REINMUTH, and FRIEDRICH KREMER — Universität Leipzig, Germany

Fluctuation and dissipation as the dominant mechanisms behind the well-observable Brownian motion of micron-sized particles are investigated and quantified on a single molecule level by means of optical tweezers technique. Using an outstandingly fast optical diffraction image analysis routine with a sampling frequency of 10 kHz combined with an automated data acquisition loop, we deduce the size of the colloid under study and the temperature of the heat bath interacting with it. Comparing blank and DNA-grafted colloids (DNA properties: molecular weight of 2800 base pairs, contour length of approximately 400 nm), the underlying mechanisms of dissipation are analyzed on a single colloid level. Bridging experiment and theory, we have adapted an experiment first carried out by Wang et al. in 2002 [1] in which the first experimental evidence for the validity of the fluctuation theorem (FT) was given. We find quantitative agreement with the FT being widely considered as the system-size and timescale independent generalization of the second law of thermodynamics. Eventually, we compare entropy production and consumption rates of blank and grafted colloids.

References: [1] G.M. Wang, E.M. Sevick, E. Mittag, D. J. Searles, and D. J. Evans, Phys. Rev. Lett. 89, 050601 (2002).

CPP 39.11 Thu 17:00 P3

Critical Casimir Forces in Colloidal Suspensions on Chemically Patterned Surfaces — OLGA ZVYAGOLSKAYA, FLORIAN SOYKA, DOMINIK VOGT, CHRISTOPHER HERTLEIN, LAURENT HELDEN, and CLEMENS BECHINGER — Universität Stuttgart, 2. Physikalisches Institut, Pfaffenwaldring 57, 70569 Stuttgart

We investigate the behavior of colloidal particles immersed in a binary liquid mixture of water and 2,6-lutidine in the presence of a chemically patterned substrate. Close to the critical point of the mixture, the particles are subjected to critical Casimir interactions with the force acting between the surfaces of the particles as well as between the particle and the wall. The strength and sign of these interactions depend on the surface properties and the mixture's temperature. Between equally coated surfaces an attractive force arise, a repulsive force

occurs between contrarily coated surfaces. Chemically patterned substrates are created by first coating the substrate with a layer of one adsorption preference which is then locally removed creating a pattern of an opposite adsorption preference [1]. In addition to a variation of the substrate properties we can also modify the particle's surface properties by adsorption of thiols with different terminal groups. Due to the interplay of lateral and vertical critical Casimir forces, we observed very different colloidal structures.

[1] Critical Casimir forces in colloidal suspensions on chemically patterned surfaces F. Soyka et al. Phys. Rev. Lett., 101, 208301 (2008)

CPP 39.12 Thu 17:00 P3

Wetting properties of sugar surfactant based microemulsions at solid surfaces — ●STEFAN WELLERT¹, RALF STEHLE², CHRISTOPH SCHULREICH², MATTHIAS KARG², ANDRE RICHARDT³, and THOMAS HELLWEG² — ¹Helmholtz-Zentrum Berlin f. Energie und Materialien, Glienicke Str. 100, D-14109 Berlin — ²Physikalische Chemie I, Universität Bayreuth Universitätsstr. 30, D-95447 Bayreuth — ³WIS f. ABC Schutztechnol. Munster, Humboldtstr.1 D-29623 Munster

Compared to many standard products, surfactants containing sugar components and fatty acids are advantageous with respect to applications where environmental compatibility or human health is important. In this context very often microemulsions are used to overcome solubilization problems also in the presence of various solid surfaces. For example, cleaning and extraction applications in sensitive environments like human skin or interior technical equipment can benefit from the green and soft performance of sugar surfactant based microemulsions. Although the interaction between the microemulsion and the surface is essential for the desired functionality, only a few works attributed to this can be found in the literature. In this contribution we discuss the wetting properties of sugar surfactant based microemulsions on surfaces of different hydrophobicity. In the microemulsion systems under investigation Pentanol and sugar surfactants were used to form the interface between water and oils of different polarity. The wetting properties in terms of contact angles were investigated with droplet and bicontinuous microemulsions at different oil-water ratios at hydrophilic, -phobic and partially hydrophobic surfaces.

CPP 39.13 Thu 17:00 P3

Shear stable colloidal crystals. — ROY GOLDBERG, JOSE MARQUEZ HUESO, ANA BARREIRA FONTECHA, and ●HANS JOACHIM SCHÖPE — Johannes Gutenberg-Universität Mainz, Institut für Physik, Staudinger Weg 7, 55099 Mainz, Deutschland

Colloidal crystals show interesting optical properties with potential application as new types of optical gratings or optical filters. For these applications it is necessary to prepare rigid and robust opaline materials where the crystalline order of the particles is maintained and can not be disturbed by thermal or mechanical forces. We here present several methods producing shear stable colloidal crystals and discuss their advantages and disadvantages. We present colloidal crystals with bcc, fcc and exotic crystal structure and characterize their optical properties. José Marqués-Hueso and Hans Joachim Schöpe, Progr. Colloid Polym. Sci. 134, 48*56 (2008) A. Barreira Fontecha, H. J. Schöpe, Phys. Rev. E. 77, Art. No. 061401(2008). R. Goldberg and H. J. Schöpe, Chem. Mat. 19, 6095-6100 (2007).

CPP 39.14 Thu 17:00 P3

Transport in micromodel porous media visualized by colloidal particles — ●YUJIE LI^{1,2}, MARIA ZVYAGOLSKAYA¹, and CLEMENS BECHINGER^{1,2} — ¹2. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany — ²Max-Planck-Institut für Metallforschung, Heisenbergstrasse 3, 70569 Stuttgart,

Porous structures are found extensively in nature from soils/rocks to biological tissues. Transport properties of molecules and particles in porous media are of significant interest for environmental remediation, drug delivery, oil recovery, composite material reinforcement, and chemical reactors.

In our work, transport processes in pore scale are modelled and visualized by colloidal solutions flowing through 2D micromodels, which were designed with different spatial statistic properties. Reynolds number and Péclet number were varied in two orders of magnitude. The influences of the ratio of particle/structure sizes were studied as well. We analyzed particle trajectories by taking into account both coherent and incoherent particle movement. Streamlines of the flow field were reconstructed from the coherent part of particle velocities. Interesting phenomenon like bifurcation of the flow pathway, slowing-down, and trapping of particles at stagnant parts in the flow field were observed

and could be attributed to the incoherent movement.

CPP 39.15 Thu 17:00 P3

Soft X-ray induced modifications & quantitative Analysis of PVA-based Microballoons (MBs) — ●BIRGIT GRAF-ZEILER¹, GEORGE TZVETKOV¹, PAULO FERNANDES², ANDREAS FERY³, and RAINER FINK¹ — ¹Universität Erlangen, Physikal. Chemie II, Erlangen — ²MPI for Colloids & Interfaces, Potsdam — ³Universität Bayreuth, Physikal. Chemie II, Bayreuth

We describe the characterization of poly(vinyl alcohol) (PVA) based gas-filled MBs in water using scanning transmission X-ray microscopy (STXM)[1]. The PolLux-STXM (SLS) combines NEXAFS with high-resolution microscopy, thus providing high chemical sensitivity and spatial resolutions <40 nm. The different absorption contrast below and above the O K-edge can provide unique information on the interior of the MBs. Soft x-ray illumination leads to the shrinking of the MBs. Nearly no change in the shell thickness can be verified, but the degradation of the PVA network and formation of carbonyl- and carboxyl-containing species could be detected. Based on existing theoretical models the radial transmittance profiles were evaluated[2]. These models are based on an ideal system of perfectly spherical MBs where the density gradient of the stabilizing shell and the finite beam width of the focused X-ray beam are taken into account. We have recently extended the existing models in order to explore the chemical composition of the stabilizing shell in greater detail with particular emphasis to quantify the gradient of water within the shell. Funded by the BMBF, project 05KS7WE1. [1]Tzvetkov et al., Soft Matter, 2008, 4, 510. [2]Fernandes et al., Langmuir, 2008, 24, 13677.

CPP 39.16 Thu 17:00 P3

Modifications in torsional resonance spectroscopy of charged sphere colloids — ●ALEXANDER REINMÜLLER, NINA LORENZ, LUCAS CHANCHETTI, THOMAS TODD, HANS-JOACHIM SCHÖPE, and THOMAS PALBERG — Institut für Physik der Universität Mainz, Staudingerweg 7, D-55099 Mainz, Germany

Morphological changes in colloidal crystals may have strong effects on the elastic properties of the corresponding solids. A modified experimental setup for measuring the shear moduli of torsionally oscillating charged sphere colloidal crystals by light scattering [1] [2] is presented: On the detection side a frequency analyzer is used instead of the conventional lock-in-amplifier. On the excitation side a white noise generator can be used instead of a simple sine generator. A comparison with the older method shows the following advantages: The measurement times can be reduced, structural changes can be controlled more precisely and coupling of resonance modes can be observed. Particular attention is paid to keeping the excitation amplitude small enough to leave the sample uninfluenced during thermal annealing.

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CPP 39.17 Thu 17:00 P3

Synthesis, characterization and cellular uptake of aminofunctionalized fluoresceine-labeled silica nanospheres — ●QI GAO¹, CHRISTINA GRAF¹, CYNTHIA KEMBUAN¹, FIORENZA RANCAN², STEFEN TROPPENS², SABRINA HADAM², ANNIKA VOGT², and ECKART RÜHL¹ — ¹Institut für Chemie und Biochemie, Freie Universität Berlin, Takustr. 3, 14195 Berlin — ²Department of Dermatology and Allergy, Charité-Universitätsmedizin Berlin, Charitéplatz 1, 10117 Berlin

The understanding of the uptake mechanism of silica nanoparticles (NPs) by human cells is important for the development of NPs as novel therapeutic and diagnostic agents. Luminescent silica NPs are promising labeling reagents for various biomedical applications. We investigated the biological properties of 3-aminopropyltrimethylsilane (APS) functionalized and fluoresceine (FITC) labeled silica nanospheres. Nearly monodisperse FITC dye-labeled silica nanospheres with diameters of 30 - 300 nm are prepared by several modifications of the Stöber process. Surface functionalization by APS allows us to adjust the zeta potential of these nanospheres from highly negative to positive (-55 mV to +45 mV). Size and zeta potential of the NPs were characterized by transmission electron microscopy and dynamic light scattering. A positive zeta potential enhances the interaction of the nanoparticles with the negatively charged cell surface and hence, the cellular uptake. Toxicity experiments indicate that these FITC dye-labeled silica NPs are not toxic to human cells. Research on the uptake of the NPs to cells, especially human skin cells, is currently in progress.

CPP 39.18 Thu 17:00 P3

Modeling effective single-particle dynamics by the harmonic chain method — JÖRG R. SILBERMANN, MICHAEL MELLE, and MARTIN SCHOEN — Stranski-Laboratorium für Physikalische und Theoretische Chemie, Technische Universität Berlin, D-10623 Germany

We consider the dynamics of a single tagged particle in a Lennard-Jones (LJ) system. Based on the equivalent harmonic chain method introduced by Adelman [1] a coarse grained description of the full many body system is generated. In this description the influence of the 'bath' surrounding the tagged particle is captured by means of a N -atom nearest neighbour harmonic chain. This chain is completely defined by a set of Einstein frequencies $\{\omega_{c_n}^2\}$ and coupling constants $\{\omega_{c_n}^2\}$ that can be determined from the memory function $M(t)$ linked to the velocity autocorrelation function (VACF) of the tagged particle in the LJ system [2]. In our work we assume $M(t)$ to be Gaussian. While this ansatz completely neglects long-time collective effects, $M(t)$ is then completely defined by static properties of the full LJ system that can be easily obtained from short Molecular Dynamics simulation runs. We study the influence of chain-length N on the dynamics of the tagged particle. Moreover, we investigate systematically the impact of the specific thermodynamic conditions (i.e., temperature and density) on the performance of our approach.

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CPP 39.19 Thu 17:00 P3

Colloidal particles in microchannels — CHRISTIAN KLIX and CHRISTIAN KREUTER — Universität Konstanz

Transport behavior of interacting particles through narrow constrictions is of high importance for many processes, e. g. for the size selectivity in ion channels. Due to the fact that these systems are very complex, only hypotheses of the underlying physics can be made. Experimentally easily accessible model systems can reveal the processes governing such phenomena. Over the last years colloidal systems have become a standard approach to model and simulate real systems. In our experiments, we use either superparamagnetic particles or particles with metallic caps. These latter particles can exhibit permanent magnetic dipole moments. We investigate the transport behavior of such interacting particles, gravitationally driven through narrow channels defined by optical lithography. Various potential shapes can be defined by crossings of channels or by channels with structured walls. Furthermore, we modify the transport behavior through realisation of barriers perpendicular to the particle flow.

CPP 39.20 Thu 17:00 P3

Controlled optical heating of single metal nanoparticles in an optical trap — SPAS NEDEV, ROMY RADÚNZ, and FRANK CICHOS — Molecular Nanophotonics Group, Institute of Experimental Physics I, University Leipzig, Linnéstraße 5, 04103 Leipzig

Recently a technique called photothermal correlation spectroscopy has been developed by our group. This technique is based on a heterodyne photothermal detection of gold nanoparticles, where a laser heats a particle periodically and a probe laser detects the light scattered by the refractive index gradient caused by the local temperature field around the particle. If these particles are suspended in a liquid and freely diffusing, the heating will cause an enhanced Brownian motion in a local viscosity and temperature field. Within this study we are trying to disentangle all different contributions to the mobility of the particle by trapping gold nanoparticles in an optical tweezer and heating them in a controlled way with a second laser at the plasmon resonance. The positional fluctuations of the particle are studied as a function of the heating laser intensity to yield an effective trap stiffness due to the modified temperatures and viscosities. As a result of these experiments we hope to shine light on hot particle diffusion as well as on thermal boundary resistances between the nanoparticle and the liquid.

CPP 39.21 Thu 17:00 P3

Integral equations study of the depletion interaction between large colloids and a planar wall — MARTIN OETTEL and VITALIE BOTAN — Johannes-Gutenberg-Universität Mainz, Mainz, Germany

The integral equation theory, which is based on the full set of coupled inhomogeneous Ornstein-Zernike integral equations, has been developed for studying the depletion forces in colloidal suspensions containing a binary mixture of spheres close to a planar wall. Recent simulations pointed to a lack of sufficient theoretical understanding of the

depletion force in hard systems with large asymmetry [1]. Our investigations of the wall-sphere depletion force in a purely hard system seem to be in good agreement with the recent Monte-Carlo simulation and density functional studies as well as predictions from morphological theory [2], which offers better insight into the regime of large asymmetry. The hard-sphere model captures the essence of the depletion phenomenon and can be mimicked experimentally by suitable choices of colloidal solutions [3]. However, a quantitative comparison between theory and experiment only appears possible if residual interactions are taken into account. We discuss the influence of effective electrostatic interactions among both species and the wall as well as the effect of gravity and tweezer forces in a model TIRM setup [4].

[1] A. R. Herring et al., Phys. Rev. Lett. **97** (2006), 148302.

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[3] A. D. Dinsmore et al., Phys. Rev. Lett. **80** (1998), 409.

[4] D. Kleshchanok et al., J. Phys.: Cond. Matter **20** (2008), 073101.

CPP 39.22 Thu 17:00 P3

Aggregation of cationic surfactants with different counterions in the presence of poly(methacrylic acid) — DAN F. ANGHEL, SHUJI SAITO, ALINA IOVESCU, ADRIANA BARAN, and GABRIELA STINGA — Department of Colloids, "Ilie Murgulescu" Institute of Physical Chemistry, Spl. Independentei 202, Bucharest, Romania

Counterions effect of a cationic surfactant upon its interaction with poly(methacrylic acid) (PMA) was investigated and compared with the analogous in poly(acrylic acid) (PAA) systems. Decylammonium (DeA+) with different counterions (Cl-, SCN-, acetate (Ac-) and butyrate (Bu-)) were employed. The interaction critical points, determined from surface tension measurements, indicated the concentrations at which primary and secondary aggregates were formed. For each counterion, T1 with PMA was higher than the respective T1 with PAA. In aqueous solution, PMA was compactly coiled up forming hydrophobic microdomains (HMD) in the chain. The surfactants were first bound to the HMD, and at T1 the free ones cooperatively formed primary aggregates on the other parts of PMA. Different from PAA systems, T1 with PMA was the sum of the surfactant amount bound to HMD and the ordinary cac. For both polymers, T1 raised in the order DeA-Ac < DeA-Bu < DeA-Cl < DeA-SCN, which was opposite to the order of the respective critical micellar concentration (cmc). The formation of hierarchical polymer-surfactant super-structures was highly influenced by the cationic surfactant concentration and counterion nature and by the polymer hydrophobic character.

CPP 39.23 Thu 17:00 P3

Flux Forward Sampling Study of Homogeneous Nucleation in Hard Spheres — DOROTA NIEDZIALEK and TANJA SCHILLING — Johannes-Gutenberg University of Mainz, Germany

As nucleation is an activated process, its study requires special rare event simulation techniques. We applied Flux Forward Sampling to a simple model problem: crystallization of hard spheres. We present results on the morphology of the crystalline aggregates and an estimate of the nucleation rate. We compare our results to a phase field model and to previous simulations which were based on umbrella sampling, and hence required an preliminary guess of the reaction coordinate.

CPP 39.24 Thu 17:00 P3

Quadratic electroclinic effect in bent-core liquid crystals — STEPHAN STERN, ALEXEY EREMIN, and RALF STANNARIUS — Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, D-39106 Magdeburg

We report an electric-field induced SmA-SmC transition in a liquid crystal formed by achiral bent molecules. The steric moment of such molecules is too small to spontaneously induce the phases characteristic to the bent-core mesogens. On the other hand, its contribution to the thermodynamical properties of the mesophases make it possible to induce tilt and polar order by the action of the external electric field. This effect is unique for bent mesogens and its physical nature differs from an electroclinic effect observed in the SmA* phase of chiral liquid crystals.

CPP 39.25 Thu 17:00 P3

Step-Emulsification Microfluidics for the Generation of Spherical Mesoporous Silica Particles — VENKATACHALAM CHOKKALINGAM¹, BORIS WEIDENHOF², WILHELM MAIER², STEPHAN HERMINGHAUS¹, and RALF SEEMANN^{1,3} — ¹Max Planck Institute for Dynamics and Self-Organization, Goettingen 37073, Germany — ²Technical Chemistry, Saarland University, Saarbruecken 66123, Ger-

many. — ³Experimental Physics, Saarland University, Saarbrücken 66123, Germany

We explore two phase microfluidics for complex chemical reactions. By dispersing different reagents into droplets and subsequently merging the droplets containing the different reagents, we realize chemical reactions, which are neither possible in single phase microfluidics, nor in droplet based microfluidics if the reagents are already mixed before being dispersed into droplets. We explore this explicitly for the production of porous silica particles from sol-gel chemistry. Regular pairs of aqueous droplets containing tetramethoxysilane (TMOS) and ammonia, respectively, are formed. The sol-gel reaction is started by merging the individual droplets using either electrocoalescence or a geometrical constriction. The concentration of the solutions is adjusted such, that the gel is fully developed when the coalesced droplets are collected outside of the microfluidic device for subsequent drying and heat treatment. The resulting silica particles have a diameter of a few micrometers, only. Further BET surface area analysis yields the chemical properties of the silica particles obtained. Particles obtained have a pore radius of about 4.5 nm and a surface area of about 600 sq.m/g.

CPP 39.26 Thu 17:00 P3

Directed Growth of Metal Organic Frameworks — ●FLORIAN WIELAND¹, MICHAEL PAULUS¹, CHRISTIAN STERNEMANN¹, FLORIAN EVERS¹, OSAMA SHEKHAH², HUI WANG², METIN TOLAN¹, and CHRISTOF WÖLL² — ¹Fakultät Physik/Delta, TU Dortmund, D-44221 Dortmund, Germany — ²Ruhr-Universität Bochum, Physikalische Chemie I, D-44780 Bochum Germany

Metal organic frameworks (MOFs) are a new class of advanced materials which may be used for various applications. In contrast to the usual synthesis protocol a new approach for the synthesis of MOFs was developed in order to investigate the dynamics and the process of the structural formation. Thin films of the MOF [Cu₃BTC₂(H₂O)_n] (HKUST-1) are grown by layer-by-layer deposition on top of functionalized organic surfaces which serve as a two dimensional nucleation site [1]. The samples were investigated by x-ray diffraction at the synchrotron source DELTA. Two dimensional scattering patterns were obtained giving information about the structural order of the films. Comparing x-ray diffraction data of the corresponding bulk material with our data we find that layers of HKUST-1 grow in different preferred directions depending on the functional group of the self-assembled monolayer. The structural behavior under temperature load was investigated up to a temperature of 250°C. The data shows a change of the HKUST-1 orientation.

[1] O. Shekhah et al, J.AM.CHEM.SOC. 2007,129,15118-15119

CPP 39.27 Thu 17:00 P3

Adhesion Properties of Polymer Microbubbles studied by AFM and RICM — ●MELANIE PRETZL, PAULO FERNANDES, and ANDREAS FERY — Universitätsstraße 30, Universität Bayreuth

Air filled polymer microbubbles are interesting devices for medical applications, they can be used as ultrasound contrast agents and for local drug delivery [1]. To improve their diagnostic and therapeutic properties it is important to understand and control their interactions with the surrounding tissue.

We investigated the adhesion properties of these novel medical devices in detail with a colloidal probe-AFM set up, that was used in combination with an inverted optical microscope. The optical microscope was used during the measurements in the RICM mode, reflection interference contrast microscopy mode. This technique enabled us to determine the change in the contact area between individual microbubbles and test substrate in dependence on varying applied external forces [2]. First results indicate that the increase of the contact area with rising external forces is also dependent on the microbubble size, the shell thickness and the air/water content of the particles. We analyzed the system also in terms of temperatures and pH.

[1]*F. Cavaliere, I. Finelli, M. Tortora, P. Mozetic, E. Chiessi, F. Polizio, T. Brismar, G. Paradossi, Chemistry of Materials 2008, 20, (10), 3254-3258.

[2]*Dubreuil, F.; Elsner, N.; Fery, A., European Physical Journal E 2003, 12, (2), 215-221.

CPP 39.28 Thu 17:00 P3

Investigations of the Molecular Structure of Bent-Core Liquid Crystals by NMR — ●GÜNTER HEMPEL — Martin-Luther-Universität, Institut für Physik, D-06099 Halle, Germany

Liquid crystals consisting of molecules with bent cores exhibit an inter-

esting phase behaviour. For example, ferroelectricity is observed even if the molecules are achiral. The phase structure depends strongly on the geometry of the molecules, particularly on the angle by which the mesogenic core is bent. Because of absence of long-range periodicity, a non-scattering method was needed for estimating the structure directly in the nematic phase.

In our NMR experiments, the dipolar coupling among nuclear spins was explored. For monitoring the 1H-13C interaction we applied the cross-polarization procedure. It relies on the exchange of polarization between 1H and 13C spin systems which can take place as oscillation. Its frequency is proportional to the dipolar coupling. Furthermore the interaction among the 1H spins was investigated by means of the decay of the proton magnetic resonance signal (WISE experiment). In both cases a two-dimensional Fourier transformation was performed which gives two frequency axes: One related to chemical-shift scale, the other related to the interaction frequency scale. The interaction between two magnetic moments depend on the angle between the connection line and the magnetic field. At this way it was possible to calculate intramolecular angles from the coupling constants.

CPP 39.29 Thu 17:00 P3

Tetrahydrofuran clathrate hydrate formation studied by x-ray Raman scattering — ●HEIKO CONRAD¹, FELIX LEHMKÜHLER¹, CHRISTIAN STERNEMANN¹, ARTO SAKKO², Omid FERUGHI¹, LAURA SIMONELLI³, SIMO HUOTARI³, DIETMAR PASCHEK⁴, KEIJO HÄMÄLÄINEN², and METIN TOLAN¹ — ¹TU Dortmund, Fak. Physik/DELTA, Dortmund, Germany — ²Div. Mat. Phys., Dep. of Physics, U Helsinki, Finland — ³ESRF, Grenoble, France — ⁴Rensselaer Polytechnic Institute, Troy, NY, USA

The formation of clathrate hydrates in the system water-Tetrahydrofuran (THF) was studied by means of non-resonant x-ray Raman scattering (XRS). Hydrates are ice-like inclusion compounds where guest molecules are embedded in water nano-cages. A possible future application of hydrates is the storage of gases, in particular H₂ in THF hydrate for fuel cells. Therefore, a detailed knowledge of the hydrate formation process is important.

XRS is an energy loss spectroscopy which allows to measure light element x-ray absorption using hard x-rays. In the dipole limit XRS directly corresponds to x-ray absorption spectroscopy (XAS). XRS spectra are sensitive to possible hydrate precursors in a supercooled state and thus yield unique information about the hydrate formation process. X-ray Raman spectra of the oxygen K-edge were measured of the hydrate, of a supercooled liquid THF/water mixture, and of a mixture at a temperature above the region of hydrate stability. The measurements were compared with DFT calculations employing local structures obtained from molecular dynamics simulation snapshots.

CPP 39.30 Thu 17:00 P3

Stability of free flying liquid films — ●PASCAL FRANK, JOHANNES BONEBERG, and PAUL LEIDERER — Universität Konstanz, Deutschland

A 10 ns laser pulse is used to rapidly heat the surface of a silicon substrate, where a thin (100-500nm) liquid film is deposited on top. The subsequent phase transition of the first ten nanometers at the interface leads to desorption and acceleration of this film. Ns-time resolved reflectometry allows to determine the actual position of the free flying liquid film. The measurements show that under ambient conditions the flight is parabolic and the film returns to the substrate after some hundred nanoseconds as the accelerating pressure rapidly decreases below the ambient pressure with increasing distance to the substrate. The maximal distance of the film is up to a few micrometers. The liquid remains stable during the time of flight of several hundred nanoseconds. If the exciting laser pulse is modulated via laser interference with periods exceeding thermal conduction length during the pulse, the film thickness can be modulated as well. Investigation of the diffraction provides insights to the stability of this modulation and the whole film.

CPP 39.31 Thu 17:00 P3

Changes of the Near-Surface Chemical Composition of the [EMIM]Tf₂N Room Temperature Ionic Liquid under the Influence of Irradiation — ●ANGELA KEPPLER¹, MARCEL MARSCHEWSKI², MARCEL HIMMERLICH¹, SYED IMAD-UDDIN AHMED¹, JUERGEN A. SCHAEFER¹, EVGENIJ PACHOMOW², WOLFGANG MAUS-FRIEDRICHS², OLIVER HÖFFT³, FRANK ENDRES³, and STEFAN KRISCHOK¹ — ¹Institut für Physik and Institut für Mikro- und Nanotechnologien, TU Ilmenau, P.O. Box 100565, 98684 Ilmenau, Germany — ²Institut für Physik und Physikalische Technologien, TU

Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld, Germany — ³Institut für Mechanische Verfahrenstechnik, TU Clausthal, Robert-Koch-Str. 42, 38678 Clausthal-Zellerfeld, Germany

In some applications room temperature Ionic Liquids (RT-ILs) are exposed to different kinds of irradiation. Using the low vapour pressures of RT-ILs, we studied the influence of irradiation on the surface properties under UHV conditions by photoelectron spectroscopy and Metastable Induced Electron Spectroscopy. We present the effect of irradiation by electrons and photons with energies ranging from a few eV to several keV on the surface composition of [EMIM]Tf₂N and its valence band structure. Our results indicate a strong reduction of the carbon content during keV-electron irradiation as well as other compositional changes. The changes of the film composition are correlated with changes in the valence band structure as a function of irradiation energy. X-ray irradiation with high exposures cause also variations in chemical composition of the [EMIM]Tf₂N.

CPP 39.32 Thu 17:00 P3

The Fréedericksz transition in thermoreversible nematic liquid-crystal gels — ●FLORIAN HEYM¹, ACHIM SACK¹, WOLFGANG SCHÖPF¹, INGO REHBERG¹, ROBIN PETTAU², and HANS WERNER SCHMIDT² — ¹Experimentalphysik V, Universität Bayreuth — ²Makromolekulare Chemie I, Universität Bayreuth

Liquid crystals like '5CB' are often gelified in order to increase the relaxation speed and to influence the liquid crystals' orientation and mechanical properties. As a gelator we use new ABA triblockcopolymers with a midblock containing Cyanobiphenyl. The properties of these nematic liquid-crystal gels are investigated and compared with ordinary nematics and nematics gelified by low molecular weight organogelators. We measure the dependency of the relaxation time of the Fréedericksz transition on the sample thickness using polarisation microscopy.

CPP 39.33 Thu 17:00 P3

Time-resolved optical measurement of director dynamics in electroconvection — ●STEPHAN MESSLINGER, ACHIM SACK, WOLFGANG SCHÖPF, and INGO REHBERG — Experimentalphysik V, Universität Bayreuth, Bayreuth, Germany

We investigate the time-dependent behavior of electroconvective patterns in liquid crystal cells [1-3] with a shadowgraph setup. Time resolution is achieved by a stroboscopic illumination [4], phase-locked to the periodic driving voltage applied to the cell. By varying the illumination phase relative to the driving voltage, the temporal modulation of the electroconvective patterns can be visualized. We present a harmonic analysis of the temporal behaviour near the convection onset, both in the dielectric and in the conductive regime.

[1] I. Rehberg, B. L. Winkler, M. de la Torre Juárez, S. Rasenat and W. Schöpf, *Adv. Solid State Phys.* **29**, 35 (1989).

[2] P. G. de Gennes and J. Prost, *The Physics of Liquid Crystals* (Clarendon Press, Oxford, 1993).

[3] A. Buka and L. Kramer, *Pattern Formation in Liquid Crystals* (Springer, New York, 1996).

[4] U. Schneider, M. de la Torre Juárez, W. Zimmermann and I. Rehberg, *Phys. Rev. A* **46**, 1009, (1992).

CPP 39.34 Thu 17:00 P3

Planar and curved electrolytic liquid-liquid interfaces — ●MARKUS BIER — MPI f. Metallforschung, Heisenbergstr. 3, 70569 Stuttgart

The interfacial tension of a liquid-liquid interface in the presence of microscopic ions is studied for the cases of planar as well as curved interfaces. Unequal partitioning of the ions between the two liquid phases is identified as the mechanism dominating the planar interfacial tension at low ionic strengths. Several scaling regimes of the curved interfacial tension are found which allows, e.g., to assess the range of validity of low-curvature expansions.

CPP 40: POSTERS Electronic and Optical Properties

Time: Thursday 17:00–19:30

Location: P3

CPP 40.1 Thu 17:00 P3

Optimization of the Photochromic Response of Photo-Addressable Polymers with Azobenzene-Containing Molecular Glasses — ●HUBERT AUDORFF¹, LOTHAR KADOR¹, ROLAND WALKER², and HANS-WERNER SCHMIDT² — ¹University of Bayreuth, Institute of Physics and BIMF, D-95440 Bayreuth, Germany — ²University of Bayreuth, Macromolecular Chemistry I and BIMF, D-95440 Bayreuth, Germany

A new series of photochromic molecular glasses has been synthesized and investigated as blending materials for improving the photochromic response of photoaddressable diblock copolymers. We performed a detailed study of the optical properties of the new materials in correlation with their structural properties. Various end groups as well as different core compounds are employed to achieve a combination of high thermal stability, good sensitivity, and high refractive index modulation. To obtain a better understanding of the photochromic response behavior of our materials, we performed the holographic experiments under a variety of conditions, e.g. at elevated temperatures and on blends with polystyrene and an azobenzene-containing homopolymer. In a blend of the molecular glass with polystyrene, 20 plane-wave holograms were recorded at the same spot by angular multiplexing. By doping the photochromic molecular glass into photoaddressable diblock copolymers, we accomplished an increase of the comparably low sensitivity of the latter, which is the biggest drawback of polymer materials. To increase the sensitivity even further, the holographic grating can be inscribed at elevated temperatures.

CPP 40.2 Thu 17:00 P3

High resolution single molecule spectroscopy of dye in different environments. — ●STEFAN KRAUSE, JÖRG SCHUSTER, and CHRISTIAN VON BORCZYKOWSKI — Center of nanostructured materials and analytics, TU Chemnitz, 09107 Chemnitz

The use of functionalized dyes for fluorescence labelling has introduced a lot of new branches especially in the fields of physics, medicine and biology. Thus, investigating orientation and conformation of bound functionalized molecules is the key to various new applications. Ac-

ording to recent publications on perylene-dyes their spectral properties are very sensitive to conformations of the dye backbones. Hence more detailed single molecule investigations by high resolution fluorescence spectroscopy at low temperature with narrow band dye lasers are a first step to understand the physical processes within these complex systems. Especially the influence of different environments given by the binding of the label on the target surface or the interaction with quantum dots on spectral positions and line widths are of interest [1]. Here we present first results we obtained on surface bound perylene using a home built low temperature single molecule microscopy and spectroscopy setup.

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

CPP 40.3 Thu 17:00 P3

Lowest ionization energies of transition metal ions in aqueous solutions investigated by photoelectron spectroscopy — ●ROBERT SEIDEL¹, MANFRED FAUBEL², WOLFGANG EBERHARDT¹, and BERND WINTER¹ — ¹Helmholtz Zentrum Berlin/BESSY II, Albert-Einstein-Strasse 15, 12489 Berlin, Germany — ²Max-Planck-Institut für Dynamik und Selbstorganisation, Bunsenstrasse 10, 37077 Göttingen, Germany

Hydration structure and electron energies of solvated ions are crucial for their reactivity in aqueous solutions. Here we report photoemission spectra from aqueous transition metal ions, which serve as homogeneous and heterogeneous catalysts. From the spectra the experimental vertical ionization energies of Ag⁺, Fe²⁺, Fe³⁺, and Cu²⁺ in water are obtained for the first time. The experiments were performed at the soft X-ray U41 PGM undulator beamline at BESSY II. A specially designed liquid microjet, providing a free liquid surface in vacuum, enables the detection of photoelectrons from the highly volatile solutions. A number of inorganic salt solutions are systematically investigated. One focus is on correlating measured electron binding energies, obtained for different counter ions and concentrations, with solvation shell structural details. Experimental binding energies are compared with theoretical calculations.

CPP 40.4 Thu 17:00 P3

Increasing conjugated polymer film conductivity by charge transfer complexes — ●FATEMEH GHANI¹, JÖRN-OLIVER VOGEL¹, GEORG HEIMEL¹, JÜRGEN P. RABE¹, NORBERT KOCH¹, SEYFULLAH YILMAZ², SYBILLE ALLARD², and ULLRICH SCHERF² — ¹Institut f. Physik, Humboldt-Universität zu Berlin, 12489 Berlin, Germany — ²Fachgebiet Makromolekulare Chemie, Fachbereich C - Mathematik und Naturwissenschaften, Bergische Universität Wuppertal, 42119 Wuppertal, Germany

Charge transfer complexes formed by mixing the molecular acceptor tetrafluoro-tetracyanoquinodimethane (F4TCNQ) with different donor materials (based on oligothiophene/quinoxaline copolymers) in thin films were investigated. Infrared absorption spectroscopy was used to quantify the donor-acceptor charge transfer as function of acceptor concentration. Furthermore, current/voltage curves of such thin films were measured, and a pronounced increase of the conductivity was found for increasing acceptor concentration (up to three orders of magnitude). However, the dependence of the conductivity on acceptor concentration was sub-linear, implying that the charge carrier mobility was reduced upon charge transfer complex formation.

CPP 40.5 Thu 17:00 P3

Influence of electrochemical cell construction at impedance spectroscopy measurements — MATTHIAS HAASE, ●PATRYK HALLEK, and VOLKER BUCK — University Duisburg-Essen, Department of Technical Physics, Germany

The degradation of materials which follow-up to corrosion is one of the most important problems. Particular identification of processes, which take place at the surface of materials, helps to improve the properties of anticorrosion coatings. One of the best method to study corrosion processes is the Electrochemical Impedance Spectroscopy (EIS). This method gives the possibility to recognize very well the change of the surface properties through corrosion products, but a wrong layout of the electrochemical cell can take strong influence at the results.

This work describes the influence of the construction of an electrochemical cell at the measured impedance spectra. For the measurements a three electrode system was established by using either a glass and a plastic chamber. A platinum foil was used as a counter electrode. As a reference electrode and pseudo-reference electrode we took a silver chloride electrode or a platinum rod, respectively.

The measured spectra show a strong interaction between the three electrodes. The impedance plots contain several artifacts in form of capacitive and inductive arcs. This arcs are not correlated with the corrosion process, but they influence on the correct interpretation of the results and choice of an equivalent electric network. The experiments shows that this effects can be minimized by the optimization of the electrochemical cell construction.

CPP 40.6 Thu 17:00 P3

Chemical etching of the tips for SNOM-Raman Microscope — ●DARIA KOVALENKO, MARTIN KÜTTNER, and JÖRG OPITZ — Fraunhofer Institut IZFP Dresden Deutschland

In this paper we will present our results concerning tip preparation for an instrument combining the SNOM and the Raman techniques of probe analysis. Like in SNOM and other kinds of optical microscopy, the resolution depends on the shape and properties of the tip. There are different ways of the tip preparation. In our case the etching is used. The tip etching was held in a two-layer solution: the lower layer consisted of 40 % hydrofluoric acid (HF), the upper layer was an organic solvent, such as toluol or cyclohexane. The time and the temperature of etching were varied. The dependences between the tip shape and the parameters of the etching were carried out. The optimal time of etching the fiber ranges from 90 to 120 min. The temperature of the etching depends strongly on the physical properties of the solvent. Typically a temperature of about 15-25 oC is used. For higher temperatures of the etching solution a faster etching is observed. The density of the solvent influences the lubricity of the surface and also the tip angle. The best results (tip angle equals 90o) are able to obtain in the solvent with density of about 0,90 * 1,05 g/cm3.

CPP 40.7 Thu 17:00 P3

A tunable subwavelength microresonator design for investigation of single quantum emitters — ●RAPHAEL GUTBROD¹, ALEXEY CHIZHIK¹, ANNA CHIZHIK¹, DMITRY KHOPTYAR², and ALFRED J. MEIXNER¹ — ¹Institute of Physical and Theoretical Chemistry, University of Tübingen, Auf der Morgenstelle 8, 72076 Tübingen, Germany — ²Department of Physics, Lund University, Box 118, S-221 00

Lund, Sweden

Optical microresonators are structures which confine light to a small volume in the range of one wavelength. Our system is based on a Fabry-Perot $\lambda/2$ -microresonator and can be reversibly tuned across the whole visible spectral range. This has great potential for intra-cavity studies and can be used to modify the optical properties of a definite single quantum emitter. We present here experimental and theoretical results on modification of the fluorescence emission spectrum as well as the spontaneous emission rate of a single molecule embedded in the microresonator. Additionally, a single fluorescent bead is used to probe the change of the intra-cavity excitation field during resonator tuning. We use radially and azimuthally polarized doughnut mode laser beams for excitation and compare the result with calculated patterns. These beams show an excitation pattern which has distinct features in different parts of the microresonator. This allows us to determine the position of the fluorescent bead with an accuracy of a few nanometres. Furthermore, we also use these beams to determine the orientation of single molecules in the microresonator.

CPP 40.8 Thu 17:00 P3

Dynamical screening of an endohedral atom — ●STEPHANIE LO¹, ANDREI KOROL^{1,2}, and ANDREY SOLOV'YOV¹ — ¹FIAS, JW Goethe University, Frankfurt am Main, Germany — ²Department of Physics, St. Petersburg State Maritime Technical University, St. Petersburg, Russia

The present work is a generalisation of the dynamical screening factor presented in [1] to consider an atom located at an arbitrary position within the fullerene. A more elaborated investigation into the case where the atom is located at the centre is performed and compared with quantum mechanical calculations for dynamical screening factor of Ar@C₆₀ [2] and Mg@C₆₀ [3]. The π and σ plasmons of the fullerene are accounted for in a modified screening factor to improve correspondence with the quantum calculations. The spatial dependence of the screening factor was explored with Ar@C₆₀ and Ar@C₂₄₀ and found to depend significantly on the radial distance of the atom from the centre of the fullerene. A spatial averaging of the screening factor is presented. The dynamical screening of an endohedral molecule is also being considered.

References

- [1] Lo S, Korol A V and Solov'yov A V 2007 *J. Phys. B: At. Mol. Opt. Phys.* **40** 3973-81
- [2] Madjet M E, Chakraborty H S and Manson S T 2007 *Phys. Rev. Lett.* **99** 243003
- [3] Chakraborty H S, Madjet M E, Rost J-M and Manson S T 2008 *Phys. Rev. A* **78** 013201

CPP 40.9 Thu 17:00 P3

About the molecular weight and temperature dependence of the microstructure of regioregular poly(3-hexylthiophene) — ●ZHIYONG WU¹, ALBRECHT PETZOLD¹, THOMAS THURN-ALBRECHT¹, RUTH LOHWASSER², MICHAEL SOMMER², and MUKUNDAN THELAKKAT² — ¹Institut für Physik, Martin-Luther-Universität Halle-Wittenberg — ²Makromolekulare Chemie I, Universität Bayreuth

We report about structural investigations of a series of regioregular poly(3-hexylthiophene) (P3HT) with different, well defined molecular weight using a combination of x-ray scattering techniques (WAXS, SAXS) and calorimetry (DSC). The semicrystalline structure of P3HT shows a complex temperature dependence. It undergoes a solid-to-solid phase transition at around 60°C and melting occurs in two steps with an intermediate layered structure with smectic symmetry. Wide angle x-ray diffraction (WAXD) experiments give evidence for an orthorhombic crystal unit cell consistent with previous reports in the literature. We propose a structure at room temperature with polyethylene-like packing of the side chains tilted with respect to the main chains and without interdigitation. At the phase transition side chain melting occurs and the side chains acquire a disordered state. The corresponding ordering process during cooling is kinetically hindered for higher molecular weight. DSC measurements show, that the melting temperature as well as the enthalpy of melting strongly increase with increasing molecular weight, indicating an increase both of the thickness of the crystallites and of the crystallinity. This result is confirmed by direct structural analysis using small angle x-ray scattering.

CPP 40.10 Thu 17:00 P3

Femtosecond Transient Absorption of a Polyfluorene Copolymer at High Hydrostatic Pressure — ●SEBASTIAN ALBERTSEIFRIED — Cavendish Laboratory, University of Cambridge, J. J.

Thompson Avenue, Cambridge CB3 0HE, United Kingdom

Organic light emitting diodes (OLED) are currently considered low-cost alternatives to established illumination and display technologies. However, the two main problems faced by OLED technologies are short device lifetime and low energy efficiency. To address these shortfalls, it is critical to understand the photophysics of conjugated polymers in the solid state, which are often more complex than in their inorganic counterparts due to the ill-defined interaction of neighbouring molecules.

Applying high pressure is a clean reversible way to increase the inter-chain interactions and thus study their effects on conjugated polymers. For this purpose, a technique was developed to study ultrafast dynamics of excitation under hydrostatic pressure up to 90 kbar by transient absorption over the whole visible spectrum. In thin films of poly(9,9-di-n-octylfluorene-*alt*-benzothiadiazole) (F8BT) at high hydrostatic pressure, a strong dynamic relaxation of the stimulated emission by around 200meV was found after excitation. Further, a sharp decline of stimulated emission and photoluminescence with increasing pressure was measured. The pressure dependent spectroscopy is interpreted in terms of interchain and intrachain effects on radiative and nonradiative processes.

CPP 40.11 Thu 17:00 P3

Terahertz Time Domain Spectroscopy of PEDOT:PSS conducting polymer for photovoltaic devices — ●MONIKA WEBER¹, KONRAD VON VOLKMAN¹, TOBIAS KAMPFRATH³, MARTIN SCHEUCH¹, INGO SALZMANN², CHRISTIAN FRISCHKORN¹, NORBERT KOCH², and MARTIN WOLF¹ — ¹Institute of Experimental Physics, Freie Universität Berlin — ²Physics Institute, Humboldt-University Berlin — ³FOM Institute for Atomic and Molecular Physics [AMOLF], Amsterdam

The number of polymer based devices grows very fast. Almost all of them, like organic field effect transistors, electro luminescent panels, LEDs or photovoltaic cells, use conducting layers. One of widely used intrinsic conducting polymers is poly-(3,4-ethylenedioxythiophene) complex with sulfonic acid also known as PEDOT:PSS. Understanding of charge transfer in PEDOT:PSS is still lacking.

Here, we present first measurements of PEDOT:PSS thin films measured with terahertz time domain spectroscopy in a frequency range between 8 THz and 32 THz. THz TD spectroscopy allows us to determine the complex dielectric function and conductivity. Temperature-dependent measurements give information about charge transfer.

CPP 40.12 Thu 17:00 P3

Charge Trapping and Color Stability in a White-Emitting Copolymer — ●SEBASTIAN BANGE and DIETER NEHER — Universität Potsdam, Institut für Physik und Astronomie, Karl-Liebknecht-Str. 24–25, 14476 Potsdam-Golm, Germany

Organic white light-emitting devices are of considerable interest as a technology capable of providing low-cost, potentially highly efficient lighting. Precise control over the emission color is especially difficult for polymeric devices, where several chromophores compete for excitations within a single active layer.

We investigate the role of charge trapping for the emission color of polymeric light-emitting devices comprising a copolymer based on polyspirofluorene with additional hole transporting units and blue, green and red singlet emitting moieties. Strong influence of drive parameters on the emission spectrum are observed and explained by an analytic model accounting for charge trapping on the red dye. Contrary to purely kinetic arguments[1], this model allows to understand the effects of electrode modifications and provides insight into interface conditioning effects[2] during operation.

[1] Gather et al., *Advanced Materials* 19, 4460 (2007)

[2] Bange et al., *Journal of Applied Physics* 104, 104506 (2008)

CPP 40.13 Thu 17:00 P3

Hydrogen storage in charge compensated organic molecular crystals — ●MINA YOON^{1,2} and MATTHIAS SCHEFFLER¹ — ¹Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — ²Oak Ridge National Laboratory, USA

We propose charge compensated organic molecular crystals as a promising class of materials for hydrogen storage. Using quantum mechanical first-principles calculations based on numerical atom-centered orbitals as all-electron basis functions [1] we study the basic structural properties of molecular crystals consisting of parallel sheets of cations and anions (such as DMPH and TCNQ) stacked alternately.

The long range dispersion interactions between the cations and anions, which are important for the stability of the crystals, were studied and compared using various DFT xc functionals, semi-empirical approach [2], and Møller-Plesset perturbation theory. The molecular configuration causes accumulation of electrons at acceptors and depletion at donors, which results in finite dipolar fields. Our study indicates that these fields make it possible to use charge compensated organic molecular crystals for hydrogen storage.

[1] V. Blum *et al.*, FHI ab initio molecular simulations (FHI-aims) project. [2] A. Tkatchenko and M. Scheffler, to be published.

CPP 40.14 Thu 17:00 P3

Surface and structure analysis of thin MEH-PPV:PVK polymer blend films — ●ROBERT MEIER¹, MATTHIAS A. RUDERER¹, GUNAR KAUNE¹, ALEXANDER DIETHER¹, STEPHAN V. ROTH², and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik Department LS E13, James-Frank-Straße 1, 85747 Garching — ²HASYLAB at DESY, Notkestraße 85, 22603 Hamburg

The surface and inner structure of novel thin blend films of photoactive conjugated polymers are investigated. Conjugated polymers in thin films become of great interest for versatile applications such as organic thin film transistors, light emitting diodes or photovoltaics. We focus on blend films based on MEH-PPV (poly[2-methoxy-5-(2-ethylhexyloxy)-1,4-phenylenevinylene]) and PVK (poly N-vinylcarbazole) which are prepared with spin coating. It has been shown that, due its charge transfer properties, MEH-PPV is a very promising candidate for applications [1]. The thin films show phase separation at the microscale, which turned out to be very well tuneable via the polymer concentrations in their solution used for preparation. The film surface is characterized by using atomic force microscopy and imaging ellipsometry and the inner film structure is analysed with GIUSAXS and GISANS measurements. The investigation is complemented by probing the conducting properties of the polymer blend films and their light absorbing abilities using UV-Vis spectroscopy.

[1] R. Meier *et. al.*, *Physical Review B* 77, 195314 (2008)

CPP 40.15 Thu 17:00 P3

The role of exciplexes in phosphorescent host-guest systems — ●BIANCA HÖFER¹, MANUEL THESEN², HARTMUT KRÜGER², SILVIA JANETZ², and ANNA KÖHLER¹ — ¹Department of Physics, University of Bayreuth, 95440 Bayreuth, Germany — ²Fraunhofer Institute of Applied Polymer Research, 14476 Potsdam, Germany

Efficient organic white light emitting diodes (OLEDs) can be produced using several organometallic phosphorescent dyes embedded in an organic matrix. We recently demonstrated that steric shielding can be employed to avoid cascading energy transfer from blue to red emitting dyes in a blend of Ir-complexes using polymeric oxadiazole- and triphenylamine-derivatives as electron and hole transporting materials.* Here we investigate the dynamics of energy transfer between the emissive dyes and the host materials. We address the issue how non-emissive exciplexes in the host materials may control the efficiency of the white OLEDs.

CPP 40.16 Thu 17:00 P3

Intermolecular coupling in low polydispersity poly(3-hexylthiophene)s — ●CHRISTINA HACKE¹, BIANCA HÖFER¹, RUTH LOHWASSER², MUKUNDAN THELAKKAT², and ANNA KÖHLER¹ — ¹Department of Physics, University of Bayreuth, 95440 Bayreuth, Germany — ²Department of Chemistry, University of Bayreuth, 95440 Bayreuth, Germany

The optical and electronic properties of regioregular poly(3-hexylthiophene) (P3HT) are of great interest for many applications in the field of organic semiconducting materials such as solar cells and field-effect transistors (OFETs). Recent research has highlighted the strong dependence of charge carrier mobility in the conformation of the P3HT backbone and the resulting intermolecular interactions. The formation of weakly interacting aggregates in P3HT depends strongly on molecular weight. Here we use P3HT with a very low polydispersity to study the molecular weight dependence in the formation of such aggregates. To assess the intermolecular interaction and the resulting morphology of the film, we use absorption measurements in solutions and films in combination with atomic force microscopy.

CPP 40.17 Thu 17:00 P3

The oligomer length dependence of triplet excitation diffusion in polyfluorenes — ●SEBASTIAN T. HOFFMANN¹, LEKSHMI SUDHA DEVI¹, IRENE BAUER¹, ESTHER SCHELER², PETER STROHRIEGL², and

ANNA KÖHLER¹ — ¹Department of Physics, University of Bayreuth, 95440 Bayreuth, Germany — ²Department of Chemistry, University of Bayreuth, 95440 Bayreuth, Germany

Triplet excitons play an important role in organic light emitting diodes and solar cells. However, very little is known about the mechanism by which the triplet excitons move and the microscopic parameters which govern triplet (Dexter) energy transfer in conjugated polymers. For a heavy metal containing conjugated polymer and its associated monomer, we have recently shown that triplet diffusion occurs by quantum mechanical tunneling at low temperatures and by thermally activated hopping above a transition temperature. [1,2]. In the present study, we extend our investigation to a PF2/6 polymer, trimer and dimer. We find that for the polyfluorene compounds, triplet diffusion can be described by the same model. As theoretically predicted², the activation energy in the hopping regime and the transition temperature between the hopping and the tunnelling regime decreases with oligomer length. We discuss the influence of disorder on the transport process.

References [1] L. S. Devi, M. K. Al-Suti, C. Dosche, M. S. Khan, R. H. Friend, and A. Kohler, *Physical Review B* 78 (2008). [2] I. I. Fishchuk, A. Kadashchuk, L. S. Devi, P. Here-mans, H. Bassler, and A. Kohler, *Physical Review B* 78 (2008).

CPP 40.18 Thu 17:00 P3

A model for triplet exciton diffusion in poly(para-phenylene) derivatives — ●ANNA KÖHLER¹, SEBASTIAN HOFFMAN¹, LEKSHMI SUDHA DEVI¹, MICHAEL FORSTER², JAN-MORITZ KOENEN², and ULLRICH SCHERF² — ¹Department of Physics, University of Bayreuth, 95440 Bayreuth, Germany — ²Department of Chemistry, Bergische Universität Wuppertal, Wuppertal, Germany

Efficient triplet exciton emission has allowed improved operation of organic light-emitting diodes (LEDs). To enhance the device performance, it is necessary to understand what governs the motion of triplet excitons through the organic semiconductor. We have recently shown that, for an organometallic polymer with low energetic disorder, triplet diffusion can be described in the framework of the Holstein small polaron model.^(1,2) It predicts a tunnelling process at low temperatures followed by a thermally activated hopping process above

a transition temperature. Using phosphorescence measurements, we have here investigated the dynamics of triplet diffusion in the polyfluorene PF2/6 and the ladder-type poly(para-phenylene) MeLPPP. We find this model is suited to describe the dynamics of triplet diffusion in these organic polymers and oligomers. The dominant parameter that controls the triplet transfer rate is the relative size of polaronic effects to energetic disorder. Experimentally, we show that the triplet diffusion rate increases with decreasing geometric relaxation energy and disorder.

(1) L. Sudha Devi et al, *PRB* 78, 45210, 2008. (2) I. I. Fishchuk et al, *PRB* 78, 45211 2008.

CPP 40.19 Thu 17:00 P3

Electroactive Polymers for Flexible and Conformable Touchpads and Keyboards — ●GERDA BUCHBERGER, REINHARD SCHWÖDIAUER, NIKITA ARNOLD, and SIEGFRIED BAUER — Johannes Kepler Universität, Linz, Österreich

Cellular polypropylene ferroelectrets are flexible, lightweight and piezoelectric transducer materials, which are used in a wide range of sensing applications. We fabricated and characterized a ferroelectret touchpad of 10x10 cm². It consists of a ferroelectret film that is placed between two large area electrodes. Electrical ports are fixed to the corners of the device. If a force is applied, transient voltage signals can be measured due to the piezoelectric effect. The voltage amplitudes depend on the touch position. In addition to the touchpad we fabricated keyboards using a binary coding technique profiting from the polarization states of the ferroelectret. Functional layers with a polarization pattern are covered by large area electrodes and stacked afterwards. The keys are encoded by the sequence of the polarization states. If a force is applied to a key, the corresponding transient voltage signals are measured at the edges of the device for every layer. As the polarization pattern and therefore the signal sequence is characteristic for every key it can be determined unambiguously. As we use large area electrodes combined with contacts only at the edges, sensor matrices are avoided. The concepts can be further extended to flexible transparent devices using polyvinylidene fluoride and transparent electrodes. The devices may be used for rollable touchpads and keyboards, for consumer goods as intelligent price tags and for whole body tactile sensors.

CPP 41: Organic Photovoltaics III

Time: Friday 10:30–13:15

Location: ZEU 222

CPP 41.1 Fri 10:30 ZEU 222

Characterization of electroactive polymers and block copolymers with potential application in organic solar cells — ●SABINE LUDWIGS — Freiburg Institute for Advanced Studies & Freiburg Materials Research Center, Stefan-Meier-Str. 21, 79104 Freiburg

Organic solar cells represent a new type of solar cells based on composites of an electron-donor (p-type) and an electron-acceptor (n-type) material. The low consumption of material and the application of efficient production techniques offer great potential for cost-efficient production of these solar cells.

In my talk I will show results on the electrochemical characterization of redox polymers bearing triarylamine as pendant electroactive units and on conjugated polymers, e.g. poly(para-phenylene vinylenes). We use electrochemically-gated transistors to study the electronic properties of these p-type polymers, in particular the potential of doping and the intrinsic conductivity.

Block copolymers consisting of the above-mentioned polymers and neutral, sacrificial poly(lactides) were further polymerized and characterized. Block copolymers are particularly interesting because they typically self assemble into ordered microdomain morphologies with length scales of about 5-50 nm. Upon degradation of the sacrificial block after structure formation polymer films with nanopores can be obtained. Ultimately these nanoporous polymer films shall be employed as templates for the deposition of semiconducting inorganic materials.

CPP 41.2 Fri 10:45 ZEU 222

Bipolar substituted spiro-bifluorenes for organic solar cells? — ●CORNELIA M. BRENDEL¹, FERNANDO DIAS², ANDY P. MONKMAN², and JOSEF SALBECK¹ — ¹Macromolecular Chemistry and Molecular

Materials, University of Kassel, Heinrich-Plett-Strasse 40, 34132 Kassel, Germany — ²Durham Photonic Materials Institute, Department of Physics, Durham University, South Road, Durham DH1 3LN, U.K. Substituted spiro-bifluorenes are frequently being employed in optoelectronic devices due to their tendency to build amorphous layers. Donor-acceptor compounds with a spiro-bifluorene unit as bridge have already been employed in phototransistors and have potential for application in organic solar cells.

To test their suitability for organic solar cells and clarify the role bipolar substituted spiro-bifluorenes play in phototransistors we investigated these compounds more closely by spectroscopic methods. Bipolar substituted spiro-bifluorenes show strong solvatochromism of about 100 nm when cyclohexane is exchanged by more polar solvents, e. g. methyl-THF or acetone, indicating charge-transfer emission. Charge separation by photoexcitation happens within some hundred picoseconds and has a lifetime of up to 50 ns.

We will discuss the interplay of the locally excited and the charge-transfer state on the basis of temperature dependent measurements of fluorescence and absorption as well as measurements of the fluorescence lifetime. We will also go into detail about the origin of triplet emission and its connection with the charge transfer state.

CPP 41.3 Fri 11:00 ZEU 222

Tuning the ionization energy of organic-semiconductor films: The role of intramolecular polar bonds — ●INGO SALZMANN¹, STEFFEN DUHM¹, GEORG HEIMEL¹, MARTIN OEHZELT², ROLF KNIPRATH¹, ROBERT L. JOHNSON³, JÜRGEN P. RABE¹, and NORBERT KOCH¹ — ¹Institut für Physik, Humboldt-Universität zu Berlin, Berlin, Germany — ²Institut für Experimentalphysik, Johannes Kepler Universität, Linz, Austria — ³Institut für Experimentalphysik, Universität Hamburg, Hamburg, Germany

For the prototypical conjugated organic molecules pentacene and perfluoropentacene, we demonstrate that the surface termination of ordered organic thin films with intramolecular polar bonds (e.g., -H versus -F) can be used to tune the ionization energy. The collective electrostatics of these oriented bonds also explains the pronounced orientation dependence of the ionization energy. Furthermore, mixing of differently terminated molecules on a molecular length scale allows continuously tuning the ionization energy of thin organic films between the limiting values of the two pure materials. Our study shows that surface engineering of organic semiconductors via adjusting the polarity of intramolecular bonds represents a generally viable alternative to the surface modification of substrates to control the energetics at organic/(in)organic interfaces.

CPP 41.4 Fri 11:15 ZEU 222

Textile electrodes as substrates in the electrochemical growth of porous ZnO for application in dye-sensitized solar cells — ●THOMAS LOEWENSTEIN¹, MARKUS MINGEBACH¹, MELANIE RUDOLPH¹, KERSTIN STRAUCH¹, YVONNE ZIMMERMANN², ANDREAS NEUDECK², and DERCK SCHLETTWEIN¹ — ¹Justus-Liebig-Universität Gießen, Institut für Angewandte Physik, D-35392, Gießen. — ²Textilforschungsinstitut Thüringen-Vogtland e.V., D-07973, Greiz.

The use of textile substrates for solar active electrodes is of interest in view of future applications of textile based electronics. Active structures prepared below 150 °C are needed. An approach using dye sensitized solar cells is useful for the achievable electrode distances in the micrometer range. Deposition of semiconductor films from solutions appears as an optimum technique. We will discuss the results of cathodic electrodeposition of porous ZnO films from aqueous zinc salt solutions with a structure directing agent (SDA) on metal-coated polyamide fibers leading to well-oriented single crystalline particles of ZnO with a high internal surface area. Individual fibers showed characteristics of microelectrodes and hence increased deposition rates were obtained relative to traditional planar electrodes. The modification of the diffusion layer by hydrodynamic flow or pulsed deposition had a strong effect on the morphology of the grown ZnO. Following the dissolution of the SDA in aqueous KOH, a porous ZnO structure was obtained. Sensitization studies will be presented to show the feasibility of the chosen approach. Lit.: T. Loewenstein et al. *Phys.Chem.Chem.Phys.*, 10, 1844 (2008)

CPP 41.5 Fri 11:30 ZEU 222

Doping of organic absorbers for application in solar cells — ●CORINNA HEIN, ERIC MANKEL, THOMAS MAYER, and WOLFRAM JAEGERMANN — Technische Universität Darmstadt, Materials Science Institute, Surface Science Division, 64287 Darmstadt, Germany

The band alignment of the absorbing layers of an organic bilayer heterojunction solar cell was determined by synchrotron induced photoemission (SXPS). As donor type material copper phthalocyanine (CuPc) was used, the acceptor layer consists of BPE-PTCDI (a perylene derivative). At the CuPc/BPE-PTCDI interface a band bending is induced that retains the generated charge carriers leading to recombination and a low photo current of 2.4 mA/cm². P-doping is suggested to reverse the electric field. As dopant WO₃ was used, known to be a strong electron acceptor. Doping was successfully performed by co-evaporation of the CuPc matrix and the dopant showing high doping efficiency and limit. The Fermi level shifts gradually with the concentration of dopant up to 690 meV. The doping mechanism was additionally investigated by layer by layer photoemission studies. Assuming phase separation the doping limit can be explained by an interface dipole. Using the doped CuPc the field at the bilayer heterojunction was reversed to the beneficial direction.

CPP 41.6 Fri 11:45 ZEU 222

LEEM and X-PEEM investigations of diindenoperylene on Au(100) — ●MARIA BENEDETTA CASU¹, BRITT-ELFRIEDE SCHUSTER¹, TEVFIK ONUR MENTES², MIGUEL ANGEL NINO², ANDREA LOCATELLI², and THOMAS CHASSÉ¹ — ¹ITPC, University of Tuebingen, Auf der Morgenstelle 8, 72076 Tuebingen, Germany — ²Sincrotrone Trieste S.C.p.A., 34012 Basovizza, Trieste, Italy

Diindenoperylene (DIP) thin films can give rise to different film phases depending essentially on the substrate, including its local morphology, and preparation conditions. By using a combination of microscopic imaging and diffraction techniques with structural and chemical sensitivity, we studied the growth of DIP on Au(100), willing to compare the results with what previously obtained on polycrystalline gold. DIP thin films were grown on Au(100) by organic molecular beam deposi-

sition at room temperature (RT) and at very low evaporation rate ($\sim 0.1 \text{ \AA}/\text{min}$). The growth and structure of DIP films of different thickness was monitored in situ and in real time by LEEM. Our investigations showed the occurrence of a Stranski-Krastanov growth mode, also establishing the influence of the local substrate morphology. Micro-LEED evidenced the different structure of the wetting layer and the islands, confirming a different molecular arrangement depending on the film thickness. Domains of different molecular orientation were identified by dark-field LEEM, following their evolution during growth. In parallel, XPEEM and micro-XPS provided information about the bond between the molecule and the substrate as well as the chemical environment.

CPP 41.7 Fri 12:00 ZEU 222

Growth of metal thin films on conductive polymer surfaces — ●GUNAR KAUNE¹, MATTHIAS A. RUDERER¹, EZZELDIN METWALLI¹, ROBERT MEIER¹, WEINAN WANG¹, SEBASTIEN COUET², KAI SCHLAGE², STEPHAN V. ROTH² und PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik Department LS E13, James-Franck-Straße 1, 85747 Garching — ²HASYLAB at DESY, Notkestraße 85, 22603 Hamburg

Type and structure of the metal electrode deposited on top of the active layer of an organic photovoltaic cell have a strong influence on the performance of the device. Therefore it is necessary to understand the structural growth and the interaction with the photoactive polymer layer. We investigate the formation of a metal/polymer interface by deposition of gold on a poly(N-vinylcarbazole) surface [1]. The growth of the gold film is investigated in-situ with grazing incidence small angle x-ray scattering (GISAXS). In-situ GISAXS allows us to follow the spatial growth of the gold clusters from the initial stage to the formation of a continuous layer and to determine the temporal evolution of the cluster morphology. From these observations a growth model is derived, explaining the cluster growth in four steps, with a characteristic process being attributed to each step. Metal incorporation inside the semi-conducting polymer film is revealed with x-ray reflectivity measurements [1]. Finally, the results are compared with the growth of an aluminium layer on a poly(3-hexylthiophene) surface.

[1] G. Kaune et al., ACS Applied Materials and Interfaces, at press

CPP 41.8 Fri 12:15 ZEU 222

Growth and morphology of photoactive small organic molecules on device-relevant substrates — ●JONATHAN HEIDKAMP¹, AYSE TURAK², FELIX MAYE^{1,2}, and HELMUT DOSCH^{1,2} — ¹Universität Stuttgart — ²Max-Planck-Institut für Metallforschung Stuttgart

Indium-Tin-Oxide (ITO) is a commonly used electrode in organic solar cells. However, the performance of these devices depends crucially on the characteristics of the interface between the ITO and the photoactive organic layer.

To study the interface characteristics, we investigated the growth, morphology, structure and ordering of small organic molecules, diindenoperylene (DIP) and perylene tetracarboxylic di-imide (PTCDI), on SiO₂, ITO and modified ITO substrates by atomic force microscopy and x-ray measurements.

Both molecules formed well ordered multilayer structures on all investigated substrates. However, only DIP showed a substrate dependence in the growth behaviour and stability, indicating different interfacial interactions for the two molecules. These differences in growth and especially in stability for different substrates can have significant implications for the use of DIP and PTCDI in organic devices.

CPP 41.9 Fri 12:30 ZEU 222

Excitons in Conjugated Polymers - Do we need a Paradigma Change — ●WICHARD J. D. BEENKEN — Technische Universität Ilmenau, Institut für Physik, FG Theoretische Physik I, Germany

We have previously shown that both, polymer conformation and dynamics are crucial for the exciton transport in conjugated polymers. Thereby we found that the usual Förster-type hopping transfer model – even if one applies the line-dipole approximation – fall short in two respects: (i) It is still unclear of what kind the site the excitons are transferred between is. We found that the simple model of spectroscopic units defined as segments of the polymer chains separated by structural defects breaking the π -conjugation is only justified for chemical defects like hydrogenated double bonds, or extreme gauche (90°) torsions between the monomers. Both defects are far too rare in a well prepared conjugated polymer to explain the mean spectroscopic unit length of typically 6-7 monomers. In the meanwhile, also the concept of

dynamical formation of the spectroscopic units, we had previously suggested, has turned out to fail. (ii) For the ultra-fast anisotropy decay observed in films of polythiophenes, the Förster-rates are far too low. Therefore, the mechanisms resulting in initial turns of the transition-dipoles have to be different from the excitation energy transfer valid on longer time-scales. In the present talk several possible ways out of these problems will be pinpointed. It will turn out that these considerations may lead to simplified concepts for the design of polymer-based organic solar cell, with possibly higher efficiencies and longer life-times than the common polymer-fullerene blends.

CPP 41.10 Fri 12:45 ZEU 222

The nature of charge transfer excitons in conjugated polymer-fullerene blends — ●ILKA KRIEGEL, ENRICO DA COMO, MARKUS HALLERMANN, STEPHAN HANEDER, and JOCHEN FELDMANN — Photonics and Optoelectronics Group, Department of Physics and CeNS Ludwig-Maximilians-Universität, 80799, Munich (Germany)

Blends of conjugated polymers and fullerene derivatives are one of the most promising systems for organic photovoltaics. We have focussed our attention on the nature of the electronic interactions taking place at the heterojunction between the polymer MDMO-PPV and the fullerene PCBM. The presence of charge transfer excitons in these materials has been recently considered and it appears to have important implications for the solar cell efficiency [1]. Here we demonstrate the presence of hybrid ground- and excited-states at the MDMO-PPV:PCBM heterojunction. Evidence for such states is provided by photoluminescence (PL) spectroscopy, where a red-shifted emission is detected in the blend film, in addition to the MDMO-PPV excitonic emission. A comparison with the spectra of the pristine polymer or PCBM indicates that the new emission originates exclusively from a charge transfer exciton forming between the two materials in the blend. In contrast to exciplexes reported in polymer/polymer blends,

the emission at 1.4 eV can be directly excited below the gap of the two materials, demonstrating the presence of a ground state [1].

[1] M. Hallermann, S. Haneder, E. Da Como, Applied Physics Letters 93, 053307 (2008)

CPP 41.11 Fri 13:00 ZEU 222

Electronic properties of pristine FePc and CoPc thin films: experiment and calculations — OLGA MOLODTSOVA¹, MARTIN KNUPFER¹, VOLODYMYR MASLYUK², YURI OSSIPIYAN³, ALEXANDER CHAIKA³, THOMAS BREDOW⁴, INGRID MERTIG², and ●VICTOR ARISTOV^{1,3} — ¹IFW Dresden, D-01069 Dresden, Germany — ²Martin-Luther-Universität Halle-Wittenberg, Fachbereich Physik, D-06099 Halle, Germany — ³ISSP RAS, Chernogolovka, 142432, Russia — ⁴Institute for Physical and Theoretical Chemistry, Bonn University, D-53115 Bonn, Germany

Magnetic transition metal (MTM) phthalocyanines are regarded as objects for the development of low dimensional molecular magnets because they are assumed as possible candidates for potential applications in high-density information storage and quantum computers that gives a strong motivation to characterize and study the electronic structure of MTM phthalocyanine thin films. Moreover this determines also the performance of devices. In this presentation we report the results of extensive investigations of the electronic structure: core-levels and valence band of the organic semiconductors CoPc and FePc in situ grown on Au(001) surface under UHV conditions. The studies were performed by means of direct and resonant photoemission, NEXAFS and DFT calculations. The experimentally obtained electronic states appeared to be in very good agreement with DFT calculations. This work was supported by the DFG under grant no. 436RUS17/52/06 and through the DFG Priority Program 1165., by the SMWK and by RFBR (grant no. 08-02-01170).

CPP 42: Polymer Physics IV

Time: Friday 10:30–13:00

Location: ZEU 160

CPP 42.1 Fri 10:30 ZEU 160

A Molecular Dynamics Study of Polymers in Confinement — ●JULIA ZABEL and ALEXANDER BLUMEN — Albert-Ludwigs-Universität Freiburg, Deutschland

The spin coating technique is a common method to produce thin polymer films. Experimental physicists are concerned that the extremely fast evaporation of the solvent leaves the polymers in an unequilibrated state. The behavior of these films in dewetting experiments leads to the assumption that the chains are under residual stress. Using Molecular Dynamics simulations we study the effects of confinement on polymer entanglement and the interdiffusion for two chains in a box. We also look at different geometric confinements such as pores and study the influence of the geometry on the dynamics. These results grant us a deeper understanding of the residual stress postulated by dewetting experiments with spin coated films.

CPP 42.2 Fri 10:45 ZEU 160

Investigations of Chain Dynamics of Polymers Confined into Nanopores — ●SALIM OK¹, FABIAN VACA CHAVEZ², MARTIN STEINHART¹, and KAY SAALWÄCHTER² — ¹Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle, Germany — ²Institute of Physics - Martin-Luther-University Halle-Wittenberg, Betty-Heimann-Str.7, 06120 Halle, Germany

Gaining better understanding of the nature of polymeric interphases in nanocomposites is still challenging. We show that self-ordered nanoporous anodic aluminum oxide (AAO) containing arrays of cylindrical channels with high aspect ratio and sharp diameter distribution is an ideal model system for the study of polymeric interphases in a well-defined anisotropic geometry. The chain dynamics of polybutadiene infiltrated into AAO was probed by Nuclear Magnetic Resonance (NMR) [1]. The mobility of polymer chains in nano-pores increased as a function of temperature systematically. However, comparing the bulk transverse relaxation (T_2) data with T_2 data in confined geometry shows that the mobility of the polymer molecules in the nano-pores is lower than the ones in the bulk. The less mobility is attributed to the smaller volume of the AAO nano-pores, restricting motion and entanglement of the polymer chains. The explanation is *corset effect*,

defined as combined effect of impenetrable pore walls, the mutual uncompressibility of polymer chains and the low compressibility of polymer chains [2].

[1] Saalwachter, K., *Prog. NMR Spectroscopy*, **51**, 1 (2007) [2] Fatkullin, N. *et al.*, *New Journal of Physics*, **6**,1 (2004)

CPP 42.3 Fri 11:00 ZEU 160

Determination of local mobilities in polymer electrolytes - concepts and simulations — ●DIDDO DIDDENS^{1,2}, ANDREAS HEUER^{1,2}, and ARIJIT MAITRA^{1,2} — ¹Institut für physikalische Chemie, Westfälische Wilhelms-Universität Münster, Corrensstraße 30, 48149 Münster, Germany — ²NRW Graduate School of Chemistry, Corrensstraße 36, 48149 Münster, Germany

In polymer electrolytes based on poly(ethylene oxide) (PEO) one observes a local slowing down of the polymer motion due to attached ions. We study this effect by MD simulations of an electrolyte composed of PEO and LiBF₄. It is, however, difficult to quantify locally slowed down polymer dynamics in MD simulations within established polymer theories like the Rouse model, as it describes the motion by nonlocalized modes. Additionally the short timescale dynamics in MD simulations do not obey the Rouse model but are strongly influenced by the local chemical structure. We provide a new statistical method to determine the relative mobilities of slow and fast regions from MD simulation data using the Langevin equation. In addition, Brownian dynamics simulations of various model chains that resemble polymer chains with heterogeneous friction coefficients are analyzed. By comparing molecular dynamics with the ideal Rouse dynamics the timescale for the validity of the Rouse model can be extracted.

CPP 42.4 Fri 11:15 ZEU 160

Coexistence of Melting and Growth during Heating a Semi-crystalline Polymer: a MD simulation — ●CHUANFU LUO and JENS-UWE SOMMER — Leibniz Institute of Polymer Research Dresden, Dresden, Germany

We present molecular dynamics (MD) simulations of the cooling/heating of semi-crystalline polymers. Using a highly parallelized code we are able to study chains up to a length of 1000 repeat units us-

ing a coarse grained polymer model [1,2]. It is the first time that a clear multi-stage melting process during the heating of a semi-crystalline polymer is analyzed by MD simulations. The step-by-step melting of different sized micro-crystalline-domains (MCDs) can explain the multiple peaks in the curve of specific heat (c_p -T). However, melting is not a simple stepwise ‘melting-recrystallization-melting’ process. The averaged stem length (lamella thickness) is increasing during the melting of smaller MCDs, and the main contribution originates from orientational correlations in the semi-melted regions and not only from local trans-trans conformations. We can interpret this a slackening of the stems which increases their mobility in reorganization processes.

- [1] H. Meyer and F. Müller-Plathe, J. Chem. Phys. 115, 7807 (2001).
 [2] C. Luo and J.-U. Sommer, Comp. Phys. Comm. (in press)

CPP 42.5 Fri 11:30 ZEU 160

Solid-solid transitions of flexible polymers — ●STEFAN SCHNABEL, MICHAEL BACHMANN, and WOLFGANG JANKE — Institut für Theoretische Physik, Universität Leipzig, Postfach 100920, D-04009 Leipzig, Germany

Solid-solid transitions of Lennard-Jones clusters including non-icosahedral conformations are a challenging subject for computational research [1]. Applying a new extension to the multicanonical method we successfully analyzed similar transitions for a flexible off-lattice homopolymer model with FENE (finitely extensible nonlinear elastic) bond potential and intramonomeric Lennard-Jones interaction [2,3]. As a result we gain a detailed insight into the polymer crystallization process and the behavior within the solid phase. The transition between icosahedral and decahedral conformations was investigated for different system sizes (e.g. $N = 75, 102$) as well as the transition to the tetrahedral ground state for $N = 98$. Small peaks in the specific heat as well as changes in geometrical quantities indicate the cross-over.

- [1] V. A. Sharapov and V. A. Mandelstam, J. Phys. Chem. A 111, 10284 (2007).
 [2] S. Schnabel, T. Vogel, M. Bachmann, and W. Janke, *to be published*.
 [3] S. Schnabel, M. Bachmann, and W. Janke, *to be published*.

CPP 42.6 Fri 11:45 ZEU 160

Scaling and scattering analysis for bottle-brush polymers in solutions — ●HSIAO-PING HSU, WOLFGANG PAUL, and KURT BINDER — Institut für Physik, Johannes Gutenberg-Universität Mainz, Staudinger Weg 7, D-55099 Mainz, Germany

Bottle-brush polymers with a rigid backbone and flexible side chains are studied in a good solvent and a theta solvent by extensive Monte Carlo simulations. Varying the side chain length, backbone length, and the grafting density, the scaling behavior of the radius of gyration, end-to-end distance, radial density profiles of monomers and side chain ends are estimated and checked with the previous theoretical predictions [1]. In order to compare our results with experimental scattering data, the structure factors describing the scattering from a single side chain and from the total bottle-brush polymer are also estimated. Our simulations include two sets of data: (1) To describe the structure of a very long bottle-brush polymer, a periodic boundary condition along the backbone is used. (2) To describe effects due to the finiteness of the backbone, free ends of the backbone are considered in our simulations. In the latter case, the inhomogeneity of the structure in the direction along the backbone is carefully investigated. A detailed analysis of radial density profile and the total scattering of a bottle-brush are given [2].

- [1] H.-P. Hsu, W. Paul, and K. Binder, Macromol. Theory & Simul. 16, 660 (2007).
 [2] H.-P. Hsu, W. Paul, and K. Binder, J. Chem. Phys. 129, 204904 (2008).

CPP 42.7 Fri 12:00 ZEU 160

Monte Carlo simulations of dendrimers — ●JAROSLAW KLOS and JENS-UWE SOMMER — Leibniz Institute of Polymer Research, Dresden, Germany

We inspect star-burst dendrimers by means of Monte Carlo simulations based on the Bond Fluctuation Model. Each molecule is modeled as a collection of monomers connected with bonds so as to form a tree-like structure on a cubic lattice. The simulations are athermal since merely the excluded volume interactions between the monomers and bond constraints are considered. Through a variation of dendrimers’ generation number G and spacer length S we focus on their mean instantaneous shape, size and radial distributions of monomers and terminal groups. The calculations show that the shape of dendrimers

changes monotonously from oblate to spherical as the increase in their molecular weight N is caused by an increase in G , while for fixed G it is hardly affected by variations of S . The obtained data lead to the conclusion that the radius of gyration obeys satisfactorily the scaling prediction $R_g \sim (SG)^{2/5} N^{1/5}$ with G and S treated as two independent variables. Moreover, our simulations support the dense-core picture of dendrimers due to a substantial decrease of monomer densities with the radial distance from the dendrimers’ centre of mass. The decrease is strictly monotonous for low generation molecules, whereas for ones with higher G there is either a local maximum or relatively broad plateau in the density profiles that correspond to the dendrimers’ domain. The interior of dendrimers is also penetrated by the terminal groups due to finite values of the end-group densities in that area.

CPP 42.8 Fri 12:15 ZEU 160

Chain conformations in bidisperse blends of linear chains — ●MICHAEL LANG and JENS-UWE SOMMER — Leibniz Institut für Polymerforschung Dresden

Bidisperse polymer melts containing a small fraction of N -mers in a matrix of P -mers were studied using the bond fluctuation model. For mono-disperse melts ($N = P$) we find deviations from ideal chain conformations in melt similar to previous studies [e.g. J.P. Wittmer, P. Beckrich, H. Meyer, A. Cavallo, A. Johner, J. Baschnagel, PhysRevE 76, 011803 (2007)] including long range correlations of bond vector orientations. The excluded volume screening in a dense melt according to the random phase approximation is controlled by the scaling variable $N^{1/2}/P$. For the case $N^{1/2} > P$, the N -mers should follow again the excluded volume statistics and the ratio R^2/N (R-extension of the N -mers) should scale as $(P^2/N)^\alpha$ with $\alpha \approx 1 - 2\nu \approx -0.176$. Similar to experimental studies [Landry, Macromolecules 30, 7500 (1997)] we find an effective $\alpha \approx -0.09 \pm 0.01$. Possible reasons for the observed deviation to the theoretical prediction are discussed.

CPP 42.9 Fri 12:30 ZEU 160

Static and Dynamic Properties of Hyperbranched Polymers Modelled by Generalized Vicsek Fractals — ●TOBIAS PAROWITZ¹, MARTIN OLIVER STEINHAUSER², and ALEXANDER BLUMEN¹ — ¹University of Freiburg, Freiburg, Germany — ²Fraunhofer Ernst-Mach-Institut for High-Speed Dynamics, Freiburg, Germany

We study the properties of hyperbranched polymers modelled by generalised Vicsek fractals (GVF) in dilute solution. Due to their fractal (self similar) structure one expects the static as well as the dynamic properties to exhibit typical power law behaviour. Both equilibrium as well as non-equilibrium Brownian dynamics simulations of dilute GVF polymer solutions are performed. Of special interest in both cases is the influence of the excluded volume (EV).

We find the static scaling in good solvent to differ significantly from previous results obtained by a generalised Flory argument. Thus we put forward a different expression for fractal polymers which enables us to explain the simulation data as well as recent experimental observations.

Studying non-equilibrium situations such as micromanipulations and polymers under shear we obtain results in very good agreement with predictions made in the generalised Gaussian structure (GGs) framework. We are furthermore able to establish the influence of the EV on dynamical quantities, effects which are beyond the range of the GGS approach.

CPP 42.10 Fri 12:45 ZEU 160

Semi-flexible hydrogen-bonded and non-hydrogen bonded lattice polymers — ●KRAWCZYK JAROSLAW¹, PRELLBERG THOMAS², and ALEKSANDER L. OWCZAREK³ — ¹Technische Universität Dortmund — ²School of Mathematical Sciences, University of London, UK — ³The University of Melbourne, Australia

We investigate the addition of stiffness to the lattice model of hydrogen-bonded polymers in two and three dimensions. We find that, in contrast to polymers that interact via a homogeneous short-range interaction, the collapse transition is unchanged by any amount of stiffness: this supports the physical argument that hydrogen bonding already introduces an effective stiffness. Contrary to possible physical arguments, favouring bends in the polymer does not return the models behaviour to that comparable with the semi-flexible homogeneous interaction model, where the canonical θ -point occurs for a range of parameter values. In fact, for sufficiently large bending energies the crystal phase disappears altogether, and no phase transition of any type occurs. We also compare the order-disorder transition from the

globule phase to crystalline phase in the semi-flexible homogeneous interaction model to that for the fully-flexible hybrid model with both hydrogen and non-hydrogen like interactions. We show that these phase transitions are of the same type and are a novel polymer critical

phenomena in two dimensions. That is, it is confirmed that in two dimensions this transition is second-order, unlike in three dimensions where it is known to be first order.

CPP 43: New Materials

Time: Friday 10:30–12:15

Location: ZEU 114

CPP 43.1 Fri 10:30 ZEU 114

Electronic Properties of Conjugated Fullerenes using O-, NH-, or CH₂-Groups as Bridges — ●MARKUS REINMÖLLER^{1,2}, UWE RITTER¹, ERICH RUNGE², and WICHARD J. D. BEENKEN² — ¹Technische Universität Ilmenau, Institut für Physik, FG Chemie, Deutschland — ²Technische Universität Ilmenau, Institut für Physik, FG Theoretische Physik I, Deutschland

We performed quantum-chemical calculations by DFT methods on C₆₀ molecules connected by several conjugated bridges formed by –O–, –NH–, or –CH₂– groups. For the optimized structure, we obtain regularly an inter-fullerene-bond (C–C) near the bridging group. Both together form furane-, pyrrole-, or cyclopentane-rings. These molecules were compared with oligo-fullerenes directly connected by two C–C bonds, i.e., where the bridge is cyclobutadien-like. All fullerenes conjugated in the described way exhibit highest occupied molecular orbitals (HOMOs) that are anti-binding regarding the π -system on the bridge. The lowest unoccupied molecular orbital (LUMO) is non-binding in this respect; whereas some unoccupied MOs higher in energy are found to be binding over the bridges and consequently delocalized over the whole chain. These states are of some interest for effective band-like electron transport in conjugated fullerenes. Therefore, we determined the energetics of the localized and delocalized MOs in dependence of the number of conjugated C₆₀ molecules to examine the structure of an evolving conduction-band. Furthermore, we studied the optically excited states by time-dependent DFT in order to get some insights about possible photo-conduction.

CPP 43.2 Fri 10:45 ZEU 114

Resonant Raman Scattering on Chemically Functionalized Carbon Nanotubes — ●REINHARD MEINKE¹, MATTHIAS MÜLLER¹, JANINA MAULTZSCH¹, BENJAMIN GEBHARDT², CHRISTIAN THOMSEN¹, and ANDREAS HIRSCH² — ¹Institut für Festkörperphysik, TU Berlin, Germany — ²Zentralinstitut für Neue Materialien und Prozesstechnik, Universität Erlangen-Nürnberg, Germany

We present resonant Raman scattering on carbon nanotubes functionalized to various degrees of functionalization. From the resonance profiles of the radial breathing mode (RBM) we assign the chiral indices of the tubes [1] in order to study the reactivity as a function of tube species and diameter as has been observed for several reactants [2,3].

[1] J. Maultzsch et al., Phys. Rev. B 72, 205438 (2005). [2] M. Strano et al., Science 301, 1519 (2003). [3] M. Müller et al., phys. stat. sol. (b), 245, 1957 (2008).

CPP 43.3 Fri 11:00 ZEU 114

Towards understanding of C60-based nanowire growth with anomalous anisotropy — ●ILIA SOLOV'YOV¹, JUNFENG GENG², ANDREY SOLOV'YOV¹, and BRIAN JOHNSON² — ¹Frankfurt Institute for Advanced Studies, Goethe University, Frankfurt am Main, Germany — ²Department of Chemistry, University of Cambridge, Cambridge, United Kingdom

The growth of one-dimensional (1D) nanocrystals is an important research topic in crystal engineering for nanotechnology. In a recent study, we demonstrated that exceptionally long fullerene nanowires, with a length-to-width aspect ratio as large as ~ 3000 , can be grown from 1,2,4-trimethylbenzene solution of C₆₀.

We perform a thorough theoretical and experimental analysis, aimed to explain the exceptionally large aspect ratio of C₆₀-based nanowires. By accounting for different interactions in the system we have calculated the structure of the unit cell and determined the role of the fullerene and of the solvent molecules in the crystallization process of the nanowire. We have calculated the adhesion energy of C₆₀ molecules to the nanowire surface and demonstrated that it is related to the anisotropy of the crystal.

To get a more in-depth understanding of the nanowire growth mechanism we have also considered the influence of electron polarization on

the anisotropy of the C₆₀-based nanowires and studied the possible polymerization reactions in the system, which likely occur between the C₆₀ and the solvent molecules in the nanowire.

CPP 43.4 Fri 11:15 ZEU 114

Intercalated fullerene polymers and Raman spectroscopy - Vibrations and more? — ●MARKUS REINMÖLLER¹, THOMAS WÄGGERG², and BERTIL SUNDQVIST² — ¹Ilmenau University of Technology, Institute for Physics, Department of Chemistry, Ilmenau, Germany — ²Umeå University, Institute for Physics, Department of Nanophysics and Material Science, Umeå, Sweden

We have synthesised very homogeneous samples from two-dimensional intercalated fullerene polymers in the chemical compositions of Li₄C₆₀ and Na₄C₆₀. On both samples we performed Raman measurements with a He-Ne-laser from 300 K to 480 K.

In the temperature studies we analysed the temperature dependence of selected Raman active modes. The results can be compared to values from several other fullerene polymers [1]. A qualitative evaluation of the heat transport properties can be accomplished by a variation of the laser light intensity. From our analysis we deduced the temperature dependence of characteristic modes and explain differences between the materials by the unequal bonding types [2].

In our Raman studies of Li₄C₆₀ at elevated temperatures we find two different regimes. From the transition of these regions the initiation of depolymerisation can be estimated.

Raman spectroscopy is a powerful tool and we show that it can be used in an indirect and maybe uncommon way to learn more about materials.

[1] A. V. Talyzin et al., Sol. State Comm., 140 (2006) 178.

[2] S. Margadonna et al., J. Am. Chem. Soc., 126 (2004) 15032.

CPP 43.5 Fri 11:30 ZEU 114

Designed Polymer-Metal nanocomposites: On the use of colloidal polymer templates — ●STEPHAN V. ROTH¹, GERD HERZOG^{1,2}, ADELIN BUFFET¹, SEBASTIEN COUET¹, RAINER GEHRKE¹, RALF RÖHLSBERGER¹, ANDRE ROTHKIRCH¹, KAI SCHLAGE¹, WILFRIED WÜRTH², GUNAR KAUNE³, VOLKER KÖRSTGENS³, ROBERT MEIER³, EZZELDIN METWALLI³, and PETER MÜLLER-BUSCHBAUM³ — ¹HASYLAB at DESY, Notkestr. 85, D-22607 Hamburg, Germany — ²Inst. f. Exp.Phys., Univ. Hamburg, Luruper Chaussee 149, D-22761 Hamburg, Germany — ³TU München, Physik-Department Lehrstuhl E13, James-Frank-Str. 1, D-85747 Garching, Germany

Polymer-metal nanocomposites are important materials for data storage, optical and electronic technologies. In combination with the wide variety of nanostructures offered by polymer materials in thin film technology, new routes for tailoring such nanocomposite devices are possible. Especially the use of colloidal nanoparticles is very attractive for magnetic data storage by ordering the colloidal nanoparticles. In our route to produce new colloidal polymer-metal nanocomposites, we combine the advantages of ordering colloidal thin films, polymer material characteristics and sputter deposition, leading to order on multiple length scales, from metal nanoparticle to large-scale domains. To understand the build-up of these multiple length scales, we use microbeam grazing incidence small angle x-ray scattering. We investigate IN-SITU the growth kinetics of magnetic and non-magnetic metals on colloidal polystyrene thin films as a function of the template treatment and present the resulting different growth regimes.

CPP 43.6 Fri 11:45 ZEU 114

A Novel Lipid-Polyelectrolyte Composite Structure on Polyelectrolyte Multilayer Coated Colloidal Particles — ●EDWIN DONATH¹, IRINA ESTRELA-LOPIS¹, LUIS CUELLAR¹, MARTIN FISCHLECHNER², and SERGIO MOYA³ — ¹Institute of Medical Physics and Biophysics, 04107 Leipzig, Härtelstrasse 16/18, Germany — ²Nanoscience Centre, Cambridge, United Kingdom — ³CICBIOMAGUNE, San Sebastian, Spain

Polyelectrolyte multilayers from poly(diallyl dimethyl ammonium chloride) PDADMAC and poly(styrene sulfonate) were formed on silica particles. Then unilamellar lipid vesicles containing mixtures of acidic and zwitterionic lipids were added to the multilayer coated particles. While with other multilayer coatings not containing PDADMAC this resulted usually in the deposition of a lipid bilayer, we observed in the presence of PDADMAC a unique structural transition of the multilayer induced by the interaction with and the subsequent adsorption of lipids into the multilayer. The resulting structure showed a 3D-distribution of circular inhomogeneities on scales ranging from nanometers to microns. These inhomogeneities were identified by a different softness probed with AFM. Otherwise the surface was surprisingly smooth. FTIR investigations revealed the special properties of water near the quarternary ammonium groups which was subsequently replaced by lipids. We believe, this is beside electrostatic interaction one of the driving forces for the very strong interaction. The composite polyelectrolyte film on the particles shows unique transport properties and may find interesting applications as a novel material.

CPP 43.7 Fri 12:00 ZEU 114

Multi-responsive hybrid colloids based on gold nanorods and poly-(NIPAM-co-allyl-acetic acid) microgels: temperature- and pH-tunable plasmon resonance — MATTHIAS KARG¹, EN-

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This work describes the reversible changes of the optical properties of multiresponsive organic/inorganic hybrid particle colloids, which consist of a thermoresponsive poly-(NIPAM-co-allyl-acetic acid) microgel core and gold nanorods adsorbed to their surface. These composites combine the interesting optical properties of the rod-shaped gold particles – exhibiting two distinct pronounced plasmon modes – with the sensitivity of the microgel toward external stimuli, such as temperature or solution pH. We show here that the collapse of the microgel core, induced by changes in either temperature or pH, enhances the electronic interactions between gold nanorods on the gel surface, as a result of the subsequent increase of packing density derived from the reduced surface of the collapsed microgel [1]. These interactions lead to remarkable redshifts of the longitudinal plasmon resonance, which can be as large as 50 nm.

[1]. Karg, I. Pastoriza-Santos, J. Perez-Juste, T. Hellweg, L. M. Liz-Marzan, Nanorod-coated PNIPAM microgels: Thermoresponsive optical properties. *Small* 2007, 3, 1222.